

Agilent G1978B Multimode Source for 6100 Series Single Quad LC/MS

User Guide



Notices

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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 nanoelectospray ion source.

1 Basic Operation and Maintenance

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

2 Installation

This chapter tells you how to install the multimode ion source.

3 Reference

This chapter contains an overview of the multimode ion source, safety precautions, and technical specifications.

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This chapter describes the tasks that you need to operate and maintain the multimode source.





1 Basic Operation and Maintenance Setting up Methods

Setting up Methods

This section describes the tasks that you need to do to set up methods for your multimode source.

To setup a method to use the multimode source

To have your method use a multimode source, follow these steps:

- Open the MSD Spray Chamber dialog box by clicking Instrument > MSD Spray Chamber in the Method and Run Control view.
- 2 Set Method Spray Chamber to MM-ES+APCI.
- **3** Verify that **Installed Spray Chamber** is set to **MM-ES+APCI**.
- **4** Make any other changes that are necessary for your method.
- **5** Click the **OK** button.
- 6 Open The Set up MSD Signals dialog box by clicking Instrument > More > Set up MSD Signals in the Method and Run Control view.
- 7 Choose the desired ionization mode from the **Ionization** list. This list is only visible if the Method Spray Chamber was set to **MM-ES+APCI**. You may set the ionization mode to one of the following:
 - MM-ES
 - MM-APCI
 - MM-ES+APCI
- 8 Make any other changes that are necessary for your method.
- **9** Click the **OK** button.

WARNING

The 6100 Series Single Quad 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 and the system may catch fire.

To create a method for positive/negative mixed mode operation

- Open the MSD Spray Chamber dialog box by clicking the Instrument > Set Up MSD Signals in the Method and Run Control view.
- 2 Select MM-ES_APCI from the Method Spray Chamber drop-down list.
- 3 Check that Installed Spray Chamber is also set to MM-ES+APCI.
- 4 Make any other changes that are necessary for your method.
- **5** Click the **OK** button.
- 6 Open the Set up MSD Signals dialog box by clicking the Instrument > MSDSpray chamber in the Method and Run Control view.
- 7 Modify the settings so that Signal 1 has **Positive** polarity and Signal 2 has **Negative** polarity as shown in Figure 1.
- 8 Make any other changes that are necessary for your method.
- 9 Click the **OK** button.

Rapid polarity switching is a very useful technique but it requires time for the ion chemistry to be established and the optics path to refill with ions. The gas density plays a role in the speed of refilling the ion path. The gas density is affected by source temperature. For a method running positive/negative switching, it is advised to use a lower vaporizer temperature (150 to 200°C) and a lower Vcap (approximately 1000 V). These will greatly affect the quality of the results in positive/negative switching experiments.

1

1 Basic Operation and Maintenance

To create a method for positive/negative mixed mode operation





To create a method for alternating ESI and APCI operation

- Open The MSD Spray Chamber dialog box by clicking Instrument > MSD Spray Chamber in the Method and Run Control view.
- 2 Set Method Spray Chamber to MM-ES+APCI.

MSD Spray Chamber		X
Method Spray Chamber: MM-ES+APCI 💌	Lamp Sta	
Installed Spray Chamber: MM-ES+APCI	C ON	C OFF
Temperatures, Pressure, and Flow		
Actual <u>D</u> rying Gas Flow (I/min): 12.0	Setpoint 12.0	Maximum 13.0
Nebulizer Pressure (psig): 35	35	60
Drying Gas Temperature (*C): 250	250	350
Vaporizer Temperature (°C): 198	200	250
Parameters Positive	Negative	
Capillary Voltage (V): 4000	4000	
Corona Current (µA): 4.0	40	
Charging Voltage (V): 2000	2000	
Time (min) Parameter		alue
	- 1	- 1
Insert Append Cut	Сору	Paste
<u>D</u> K Cancel	<u>H</u> elp	1



- 3 Check that Installed Spray Chamber is also set to MM-ES+APCI.
- 4 Make any other changes that are necessary for your method.
- **5** Click the **OK** button.
- 6 Open the Set up MSD Signals dialog box by clicking Instrument > Set Up MSD Signals in the Method and Run Control view.
- 7 Modify the settings so that Signal 1 has **Ionization** value of **MM-ES** and Signal 2 has **Ionization** value of **MM-APCI** as shown in Figure 3.
- 8 Make any other changes that are necessary for your method.

1 Basic Operation and Maintenance

To create a method for alternating ESI and APCI operation

9 Click the **OK** button.

NOTE

In general, use the mixed mode operation (MM-ES+APCI setting with Signal 1) instead of alternating MM-ES (Signal 1) and MM-APCI (Signal 2) mode switching. Two times as many scans are obtained during elution of a chromatographic peak, and no delay is needed between scans, resulting in better data. It is rarely necessary to know whether a compound responds purely in ESI or APCI modes on a chromatographic time scale.





Maintenance

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 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.

- **2** Check that the vaporizer temperature sensor is straight and extends 15mm from back of chamber.
- **3** Check that the separator is aligned vertically.
- **4** Check that the APCI corona needle is in and extends approximately 3mm from the corona guide.
- **5** Check that the source is clean.
- **6** Close and latch the multimode source.

To open the multimode source

7 In the LC/MS ChemStation software **MSD Manual Tune** view, check that the system recognizes the source. The **Source** text box in the toolbar should read **MM-ES+APCI**.



Figure 4 List of Modes in Manual Tune View

The source listed is the source currently installed on the LC/MS instrument. If the G1978B multimode source is detected, it will indicate MM-ES+APCI.

The **Mode** is the ionization mode you have currently selected. The three Modes that a multimode source can use are MM-ES+APCI, MM-ES and MM-APCI.

MM-ES+APCI Mixed mode MM-ES Electrospray only

APCI only

MM-APCI

To turn off the instrument

Before you begin, check that:

• You have completed tuning and data acquisition and you have saved all data as needed.

Follow these steps to vent and completely power the instrument off.

1 Use the MSD Vent dialog box to vent the MSD instrument.

In the Diagnosis View, select Maintenance > MSD Vent

WARNING The quadrupole cools very slowly and will likely be near 100°C when the vent cycle is complete. The drying gas heater and APCI vaporizer heater will also still be hot. Wait for the instrument to cool off before continuing.

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.

- 2 When the vent cycle is completed, exit the ChemStation program.
- **3** Turn off the power switch on the front of the LC/MS.

1 Basic Operation and Maintenance

To clean the multimode source daily

To clean the multimode source daily

You should clean the multimode source daily or any time you suspect carryover (contamination) from one sample or analysis to another. The multimode source spray chamber is made of 316 stainless steal which is the same material the spray shield is made of.

Before you begin, check that you have:

- Abrasive paper, 8000 grit (p/n 8660-0852)
- Cloths, clean, lint-free (p/n 05980-60051)
- Cotton swabs (p/n 5080-5400)
- Gloves
- Mobile phase from the current method or clean isopropanol, reagent grade or better
- Wash bottle
- Water, reagent-grade or better
- **1** Turn off the spray chamber. Use the **Spray Chamber** menu item in Tune and set all gas flows and temperatures to minimum values of zero.

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

- **2** Remover the nebulizer and APCI corona needle.
- **3** Remove the cosmetic cover. The thermocouple probe will need to be removed if any wiping of the spray chamber will be done. Then, open the spray chamber.
- **4** Rinse the interior of the spray chamber using the wash bottle filled with the current mobile phase or with a mixture of isopropanol and water.

NOTE

Recent residue should be soluble in the mobile phase. If you are not sure what mobile phase was used recently, a mixture of 50% isopropanol and 50% water works well as a general cleaning solution.

WARNING

Some mobile phases are hazardous chemicals. Use caution that is appropriate for the current mobile phase.

5 Wipe the interior of the spray chamber with a clean, lint-free cloth.

WARNING There are sharp edges inside the spray chamber such as the separator. Pay close attention when wiping the interior of the spray chamber.

- **6** Rinse the area around the spray shield. Do not spray directly at the end of the capillary. This can cause pressure surges in the vacuum system.
- 7 Dampen a clean cloth with the mobile phase. Wipe the spray shield, field shaping electrodes and the area around the spray shield.
- 8 Replace the nebulizer and the APCI corona needle.
- **9** Install the thermocouple probe and adjust it so that it protrudes 15 mm from the inner spray chamber wall. See Figure 5.



Thermocouple probe

Figure 5 Installing the thermocouple probe and 15 mm adjustment

10 Replace the cosmetic cover.

1 Basic Operation and Maintenance

To clean the multimode source daily

11 Close the spray chamber.

NOTE

If symptoms of contamination persist, or if the spray shield or capillary cap show significant discoloration that cannot be removed by the regular, daily cleaning, use the weekly cleaning procedure.

To clean the multimode source weekly

The cleaning procedure for cleaning the multimode source weekly is similar to the procedure for cleaning the source daily. The main difference is that the multimode source is removed from the instrument.

Before you begin, check that you have:

- Abrasive paper, 8000 grit (p/n 8660-0852)
- Cloths, clean, lint-free (p/n 05980-60051)
- Cotton swabs (p/n 5080-5400)
- Gloves
- Mobile phase from the current method, or clean isopropanol, reagent grade or better
- Wash bottle
- Water, reagent-grade or better
- 1 Do the steps in "To remove the multimode source" on page 29.
- **2** Fill the spray chamber with clean mobile phase, or with a mixture of isopropanol and water.
- NOTE

Recent residue should be soluble in the mobile phase. If you are not sure what mobile phase was used recently, a mixture of 50% isopropanol and 50% water works well as a general cleaning solution.

WARNING

Some mobile phases are hazardous chemicals. Use caution that is appropriate for the current mobile phase.

- **3** Scrub the corona insulator and the interior of the spray chamber with a clean cotton swab.
- **4** Empty the spray chamber.
- **5** Wipe the interior of the spray chamber with a clean, lint-free cloth.

WARNING

The inside of the spray chamber has sharp edges, such as on the separator. Pay close attention when you wipe the interior of the spray chamber.

1 Basic Operation and Maintenance

To clean the multimode source weekly

- **6** Remove the spray shield. Use abrasive paper to gently clean the end of the capillary cap.
- 7 Dampen a clean cloth and wipe the end of the capillary cap.
- **8** Reinstall the spray shield.
- **9** Use abrasive paper to gently clean the spray shield. Dampen a clean cloth and wipe the spray shield.
- **10** Rinse the area around the spray shield. Then wipe the area around the spray shield.
- **11** Reinstall the spray chamber on the instrument.
- **12** Replace the nebulizer and APCI corona needle.
- **13** Install the thermocouple probe and adjust it so that it protrudes 15 mm from the inner spray chamber wall. See Figure 5 on page 17.
- **14** Replace the cosmetic cover.
- **15** Close the spray chamber.

To bake out the LC/MS

You will need to bake out the LC/MS the first time you turn the system on and any time that the system has been vented.

- 1 Connect the LC/MS inlet tubing (p/n 0890-1915).
- 2 Select the Tune view.
- **3** Select **Tune > Manual Tune**
- 4 Display the MS Tune Spray Chamber dialog box.
- **5** Set the drying gas flow to 7 L/min for MM-ES or 5 L/min for MM-ES+APCI or MM-APCI.
- 6 Set the nebulizer pressure to 40 psi.
- 7 Set the drying gas temperature to 300°C.
- 8 Set the vaporizer temperature to 250°C. (MM-ES+APCI or MM-APCI only)
- **9** Set the LC flow to 0.5 mL/min using the solvent mixture appropriate for your instrument model. Refer to the *6100 Series Installation Guide* for more information.
- **10** If you are doing performance verification on 6130 or 6140 only, install the 2.1 x 30mm x 3.5 micron B-C18 Rapid Resolution column.
- 11 Make sure the position of the MS selection valve is set so that the LC flow is diverted to the spray chamber (select Switch Stream > MSD)
- 12 Allow the system to bake out for at least 2 hours.

CAUTION

If the system has been exposed to humid conditions during shipping or storage, a minimum of 4 hours bake out is required to prevent arcing of the quadrupole.

1 Basic Operation and Maintenance To do an autotune

To do an autotune

Tuning the multimode source is done in MM-APCI mode only. Autotune is performed from the same menu as with all sources.

• From the **MSD Tune view**, select **Instrument > Autotune** menu item.

The tune report will have a header with either the title **MM-APCI Positive Mode - Standard Scan** or **MM-APCI Negative Mode - Standard Scan**. You can run the check tune after autotuning to validate that the instrument is passing check tune criteria. Do the autotuning after the system has had at least 8 hours to equilibrate vacuum and temperatures.







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Installation

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This chapter contains instructions to install the multimode source on a 6100 Series Single Quad LC/MS system, and also to remove and replace the source.



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







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, p/nG1960-60802
- Valve BD-APCI Needle Interlock, p/n G1960-60856







Figure 8 From left to right: G1946-80058, G1960-60802 and G1960-60856

2

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 CE works on the electronics. The switch box is for CE 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 MM HV power supply PCA in the slot between the valve PCA and the Vcap/Vchamber. Secure the board by pressing it down into its slot and then attach it with two screws.
- **5** Connect the short gray cable from valve PCA to the multimode HV power supply.



Figure 10 Connecting the valve PCA to the multimode HV power supply.

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 valve PCA and Vcap/Vchamber power supply.



Figure 11 Connecting the valve PCA to the Vcap/Vchamber power supply.

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



Figure 12 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



Figure 13 Connecting the APCI HV power supply to the valve PCA.

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.





Figure 14 Connecting the APCI HV to the chassis.

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.





Figure 15 Connecting the HV PCA to the chassis.

12 Close the AUX Module cover and reconnect all cables.13 Install the MM source to the system and connect all connectors.

Step 2. Install the HV control PCA and cables



Figure 16 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 ChemStation program.
- **17** Click **Method and Run Control View > MSD > Spray Chamber** and verify that the source is an MM Source.
- 18 Go to MSD Tune window and start the Auto tune with MM source.
- **19** Verify that the multimode source is working correctly.

2

To remove the multimode source

Do the following steps to remove the multimode source.

1 Set the source temperatures for vaporizer heater and drying gas heater to minimum values to cool the source.

Use the **Tune > Instrument > Edit Spray Chamber** menu item to display the Edit Spray Chamber dialog box. The drying gas flow, nebulizer gas flow, drying gas temperature and the vaporizer temperature should be set to minimum values.

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, APCI or APPI

To convert from multimode to ESI, APCI or APPI

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 If the source to be installed is an APPI source, disconnect the multimode high voltage PCA RS-232 serial cable from the serial port B connector of Smart Card.
- **2** Unscrew and remove the multimode spray shield with the field shaping electrodes.
- **3** 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.
- **4** For APCI and APPI ion source, connect the vaporizer heater cable and the APCI high voltage cable. For the APPI source, connect the RS-232 cable to the serial port B connector of Smart Card.
- **5** For all sources, reconnect the nebulizer gas line tubing and the LC/MS sample tubing.

To convert from ESI, APCI or APPI 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 23.

- 1 Switch to the MSD Tune view.
- **2** Select **Instrument/Set Spray Chamber** and set all gas flows and temperatures to 0.
 - Drying Gas (L/min)
 - Nebulizer Pressure (psig)
 - Drying Gas Temperature (°C)
 - Vaporizer Temperature (APCI source only)
 - Lamp Off (APPI source only)
- **3** Wait for the source to cool (until temperatures are at least below 100°C).
- **4** Disconnect the nebulizer gas tubing from the currently installed ion source.
- 5 Disconnect the LC/MS sample inlet tubing.
- **6** If the APCI or APPI source is installed, remove the APCI vaporizer heater cable and APCI high voltage cable.
- 7 If the APPI source is installed, remove the serial port B RS-232 cable.
- 8 Remove the currently installed ion source.
- **9** Unscrew and remove the spray shield. See Figure 17.

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.

2

To convert from ESI, APCI or APPI to the multimode source



Figure 17 Standard spray shield and capillary cap for ESI or APCI

10 Remove the capillary cap. If needed, moisten a clean cloth with isopropyl alcohol and wipe the capillary cap. See Figure 18.



Figure 18 Spray shield removed.

11 Place the capillary cap back on the capillary.

12 Install the new spray shield with field shaping electrodes. See Figure 19.

To convert from ESI, APCI or APPI to the multimode source



Figure 19 Multimode spray shield

13 Screw the multimode spray shield into the holder for the spray shield. See Figure 20.



Figure 20Multimode spray shield installed

NOTE

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.

14 Remove the shipping cover from the multimode source spray chamber.

To convert from ESI, APCI or APPI to the multimode source



Figure 21 Multimode Spray Chamber

15 Install the spray chamber on the spray chamber mount.



Figure 22 Multimode source with I-Button

16 Install the nebulizer on the multimode source spray chamber.

To convert from ESI, APCI or APPI to the multimode source



Figure 23 No nebulizer on top of the multimode source

17 Connect the 1/8-inch nebulizer gas tubing from the LC/MS mainframe to the nebulizer gas fitting. See Figure 24.



Figure 24 Nebulizer with gas tubing connected

To convert from ESI, APCI or APPI to the multimode source

18 Connect the LC/MS sample tubing to the LC/MS diverter valve inlet filter. See Figure 25 on page 36.

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.



Figure 25 LC/MS sample tubing connected to LC/MS inlet filter

19 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 25.


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This chapter contains reference information to help you run your 6100 Series Single Quad LC/MS with a multimode source.



Safety and Specifications

Safety and Specifications

This section describes safety, safety symbols, and technical specifications.

Safety

Some of the procedures in this chapter require access to parts of the instrument and multimode source while it is in Shutdown state or shortly after it is turned off. If you do not perform these procedures correctly, you are exposed to dangerous temperatures, voltages, and chemical hazards. This topic describes the potential dangers.

Nebulizer Needle Hazard

- The nebulizer needle tip is very fragile. Do not touch the tip to any objects, such as the capillary cap or spray chamber. If you accidentally touch the nebulizer needle tip, replace the needle.
- The vaporizer temperature sensor is very sharp and can pierce your skin. Do not touch the tip, especially when you analyze toxic substances or when you use toxic solvents.
- Use care when you adjust the nebulizer needle. Do not damage the end of the needle.

High temperatures

Most parts in the multimode source operate at or reach temperatures high enough to cause serious burns. These parts include, but are not limited to the capillary, capillary cap, spray shield, vaporizer temperature sensor, APCI corona needle, counter electrode, source hinge and spray chamber.

Do not touch these parts.

• Certain parts remain hot for many minutes after the instrument is shut down or turned off. In particular the spray shield and the capillary cap could be very hot after working with APCI, ESI or MM-ES+APCI. Use extreme care when you work on an instrument that has recently been turned off.

- The Infrared medium-wave twin tube emitters are made of quartz glass. The IR radiation is not hazardous and is radiated as heat.
- Do not touch any surfaces in the source spray chamber. The spray chamber in most cases will be very hot

Hazardous voltages

Whenever the instrument is not in Standby, hazardous voltages are present on one or more interior parts. Parts that use hazardous voltages include, but are not limited to, the capillary cap and counter electrode.

These parts are usually covered or shielded. As long as the covers and shields are in place, you will not make contact with hazardous voltages.

- Never open the multimode spray chamber while the instrument is in the operation or the HV voltages are turned on.
- Do not insert fingers or tools through the openings on the multimode spray chamber. During operation the capillary and capillary cap are at high voltage up to 4 kV.
- If you connect the instrument to an ungrounded or improperly grounded power source, you create a shock hazard for the operator and can damage the instrument. Intentional interruption of instrument grounding is strictly prohibited.

Biohazardous residue

The multimode interface does not ionize all of the sample and solvent. The vacuum pumps of the instrument removes the sample that is not ionized and solvent. The exhaust from these pumps can contain traces of sample and solvents. Vent all pump exhaust outside the building or into a fume hood. Comply with your local air quality regulations

• The exhaust fumes from the vacuum system and spray chamber contains trace amounts of the chemicals you analyze. Health hazards include chemical toxicity of solvents, samples, buffers, and pump fluid vapor, as well as potentially biohazardous aerosols of biological samples. Vent all exhausts out of the building where they cannot be recirculated by environmental control systems. Do not vent exhausts into your laboratory. Comply with your local air quality regulations.

3 Reference Safety

- Fluid drained from the multimode chamber is made of solvent and sample from your analyses. The fluid in the mechanical pump collects traces of samples and solvents. In addition, unnebulized solvent and sample collects at the bottom of the spray chamber. Connect the drain on the bottom of the spray chamber to a closed container.
- Handle and dispose of all fluids using precautions appropriate for their biohazardous and biological content. Comply with local environmental regulations.
- Handle all used pump fluid as hazardous waste. Dispose of used pump fluid as specified by your local regulations.

Environmental Conditions

This equipment must be installed in an environment of Category II installation as defined in IEC 664. Check that the supply voltage does not fluctuate more than +10% or -10% of rated voltage.

Equipment Class Class 1 Laboratory Equipment
Pollution Degree 2
Installation Category II
Environment Indoor Use
Altitude Not to exceed 2300 m
Electrical supply 100 - 240 V AC, 50/60 Hz, 1.2 A
Mains supply voltage Fluctuations not to exceed 10% of nominal supply voltage
Operating Temperature $15 \text{ to } 35^{\circ}\text{C} (59 \text{ to } 95^{\circ}\text{F})$
Humidity < 90% RH at 35°C
Anarational Conditions

Operational Conditions

If the G1978B is used in a manner not specified by Agilent Technologies, the protections provided by the G1978B may be impaired.

Cleanliness

Cleanliness and the prevention of accidental contamination during maintenance are very important. Contamination of the interior of the vacuum system or the sample path can affect the results of your analyses.

- Always wear clean gloves when handling parts that come in contact with the sample path. Oil from your fingers is difficult to remove.
- When you set parts down, place them on clean, lint free cloths or clean aluminum foil, not directly on the laboratory bench.
- Keep parts covered so they do not get dirty.
- If possible, maintain a separate set of tools that have been thoroughly cleaned. Use these tools only when working on clean assemblies.
- With open ion sources, such as API, avoid dusty and fibrous environments. Dust particles can enter MS ion source and deposit on ion optics, causing sensitivity loss.

3 Reference Safety Symbols

Safety Symbols



NOTE

This symbol is placed on the product where it is necessary for you to refer to the **manual** in order to understand a **hazar**d.



WARNING CAUTION

This symbol is placed on the product within the area where **hazardous voltage** is present or shock hazard can occur. Only trained service persons should perform work in this area.



WARNING

This symbol is placed on the product within the area where **hot parts and surfaces** are present. Allow the product to cool before performing work in this area.



WARNING

This symbol is placed on the product within the area where **biohazards** are present. Handle these areas with the respective care.

Size			
	Height	Length	Width
	17 cm	18 cm	9.5 cm
	6.8 in	7.1 in	3.7 in
Weight	2.27 kg / 5 lbs.		
Power source	Power 60 VA		
	Primary		
	Voltage		100 V to 240 V
	Current		0.85 A to 0.40 A
	Frequency		50 Hz / 60 Hz
	Secondary		
	Voltage		12 V
	Current		3.3 A
Operating Temperature		F to 95°F) (Analytics ge of 21°C ± 3°C (70	al specifications will be met only within °F ± 6°F).
Operating Humidity	15% to 95% (non co	ondensing at 35°C)	
Operating Altitude	< 2300 meters / < '	7500 feet	

Technical Creations

Multimode Source for 6100 Series Single Quad LC/MS User Guide



Overview

Benefits of a multimode source



Figure 26 Multimode source.

The multimode source is an ion source for LC/MS that can operate as an APCI, ESI or simultaneous APCI/ESI source. See Figure 26. The source is intended to operate at normal chromatographic flow rates 50 to 2000 μ L /min. It is capable of fast reversing pos/neg switching. The multimode source can be run in three different modes of operation (MM-ES, MM-APCI or MM-ES+APCI).

Why use the multimode source?

- A single ion source with a single nebulizer performing MM-ES, MM-APCI, or MM-ES+APCI
- MM-ES to MM-APCI without source exchange
- Operates in MM-ES only, MM-APCI only, or MM-ES+APCI mixed mode
- Operates at typical HPLC flow rates up to 2 mL/min, even in MM-ES mode
- Multimode source provides higher throughput for data requiring validation in both MM-ES and MM-APCI
- More universal response

3

- Permits analysis of fast-eluting peaks
- Operation at flow rates used for high-throughput analysis without splitting
- Operation at lower flow rates for higher-sensitivity analysis

The design uses a single nebulizer through which the LC effluent flows. You do not need to switch back and forth between APCI and ESI modes. While this option will be available, the great value of the source is its ability to produce APCI and ESI generated ions simultaneously. This ability increases the effective duty cycle of the mass spectrometer. Another key feature is the much greater operational flow rate that is available in this design.

Ionization Mode	Polarity
APCI	positive
APCI	negative
APCI	fast switching
ESI	positive
ESI	negative
ESI	fast switching
Multi-Mode	positive
Multi-Mode	negative
Multi-Mode	fast switching

Mixed mode operation is generally a balance between optimal ESI and APCI conditions. Changing the vaporizer temperature, the nebulizer pressure, and the corona current alters the balance between the ionization modes.

Parameter adjustment	APCI response in mixed mode generally	ESI response in mixed mode generally
Higher vaporizer temperature	Increases	Stays the same
Higher nebulizer pressure	Decreases	Increases
Higher corona current	Increases	Decreases

Benefits of a multimode source



Multimode source operational description

Figure 27 Graphical representation of multimode source

- **1** Liquid enters the grounded nebulizer
- 2 A charged aerosol is made in the ESI Zone
- **3** The aerosol is dried by IR lamps
- 4 Neutral analytes and ESI charged analytes pass through the APCI Zone
- **5** ESI and APCI ions enter the capillary

Benefits of a multimode source



Figure 28 Graphical representation of MM-ES zone

- **1** Liquid enters the grounded nebulizer.
- **2** The charging electrode charges the liquid
- **3** Nebulizing gas pushes the charged aerosol past the charging and reversing electrodes
- **4** The reversing electrode separates the ESI formation from the APCI formation

Multimode Source for 6100 Series Single Quad LC/MS User Guide

Benefits of a multimode source



Infrared Drying



- **1** The charged aerosol passes the reversing electrode and enters the thermal container.
- **2** The thermal container confines the heat and aerosol
- **3** Infrared lamps dry the charged aerosol on the way to the APCI Zone

Reference Benefits of a multimode source

3



Figure 30 Graphical representation of MM-APCI zone

- 1 Neutral analytes and MM-ES charged analytes pass through the MM-APCI Zone.
- **2** A corona is formed between the APCI corona needle and the pin.
- **3** Neutral analytes in or very near this gap are ionized.
- **4** MM-ES and MM-APCI ions are merged and follow the electric field into the mass spectrometer.

Benefits of a multimode source

Multimode source side view



Figure 31 Graphical representation of a side view of the multimode source

Benefits of a multimode source

Multimode source top down view



Figure 32 Graphical representation of a top view of the multimode source

Mobile phase considerations when using the multimode source

Mobile phase considerations when using the multimode source

Flow rate

In general, once the analyte response is optimized, the flow rate or mobile phase composition may be changed without having to re-optimize the vaporizer temperature or drying gas temperature. The IR emitters have a feedback control that is provided by the vapor temperature sensor. Power to the IR emitters is dynamically changed to maintain the vapor temperature at the desired setpoint regardless of mobile phase changes.

ESI mode (or for compounds that have an ESI response in mixed mode)

Improved response will be obtained when lower amounts of electrolyte are used in the mobile phase. The recommended electrolyte concentration is lower, approximately one fifth that of prior recommendations. The need for lower electrolyte concentrations is due to the physics of ESI ion formation and charge separation in the multimode source. The following are example recommended electrolyte concentrations:

- 1 mM ammonium acetate instead of 5 mM
- 0.02% formic acid instead of 0.1%

NOTE

The electrolyte-response effect is not present in the dedicated ESI source; continue to use higher electrolyte concentrations with the dedicated ESI source.

NOTE

Do not use pure solvents (i.e., no electrolyte) as mobile phases for ESI work as this practice results in unpredictable analyte response.

APCI mode (or for compounds that have an APCI response in mixed mode)

- In positive APCI mode, higher response is obtained using protic or neutral solvents as the organic mobile phase component instead of acetonitrile.
- Acetronitrile is a strong enough gas-phase base to deprotonate some analyte ions, leading to reduced response (30-fold reduction has been seen).
- Methanol, isopropyl alcohol, and acetone are preferred for positive mode APCI.

• In negative APCI mode, the use of acetonitrile has also been linked with a reduction in response of the analytes.

For electrolytes added to the mobile phase used for mixed mode operation, use care in selecting the anion as it may affect the response in negative APCI mode. For example, acetate is preferred over formate as it is more likely to accept a proton from the neutral analyte to produce a negatively-charged analyte ion under APCI conditions.

Positive/negative mode switching

- In general, you need an intermediate pH (compromise) so protonated and deprotonated analyte ions may co-exist in significant concentrations.
- Sensitivity and/or chromatographic peak shape are generally not as good as when the analysis conditions are optimized using a single polarity.
- 0.2% acetic acid or 1 mM ammonium acetate (not ammonium formate) are suggested as mobile phase modifiers.

3

Flowchart summarizing parameter choices for different modes

Flowchart summarizing parameter choices for different modes



3

Source comparison in positive ion mode

Using the multimode source in MM-ES+APCI mode with positive polarity, you can acquire a single data file containing the two compounds, indol and crystal violet.



Source comparison in negative ion mode

Source comparison in negative ion mode

Using the multimode source in MM-ES+APCI mode with negative polarity, you can acquire both hexanesulfonic acid and dinitrobenzotrifluride in the same file. Neither ESI nor APCI can acquire both of these compounds.



Single analysis in MM-ES+APCI mode with fast switching

Single analysis in MM-ES+APCI mode with fast switching

Using the multimode source in MM-ES+APCI mode, you can use fast switching to acquire all four peaks during the same run.



Guidelines

Guidelines for multimode source settings in MM-ES mode

NOTE

Click **Instrument > MSD Spray Chamber** to set the Method Spray Chamber to MM-ES+APCI before you edit the Set Up MSD Signals dialog box.

Nebulizer pressure Always set to 60 psi.

Drying gas flow Always set to 5 L/min (IR does the drying).

Drying gas temperature Depends on the vaporizer temperature. A good starting temperature is 250°C. If running a cold vaporizer temperature, then set the drying gas temperature to vapor temperature or lower. If running the vaporizer hot (>175°C), then set the drying gas temperature to 350°C. Remember you want the vaporizer to control the drying and to be able to maintain the set point.

Vaporizer Start at 150°C. ESI works across a broad vaporizer range. If you are getting excessive sodium adducts, lower the temperature. You can run as low as 60°C. It is recommend to run 100°C or greater. Negative ion TFA adducts work best at lower temperature (<150°C).

Vcap Set to 2000 V. A lower voltage works better for fast switching. High mass ions (>1000) prefer a higher Vcap.

Charging Voltage Set to 200 V.

Guidelines for multimode source settings in MM-APCI mode

NOTE

Click **Instrument > MSD Spray Chamber** to set the Method Spray Chamber to MM-ES+APCI before you edit the Set Up MSD Signals dialog box.

Nebulizer pressure Start at 20 psi. The signal decreases with higher nebulizer pressure.

Drying gas flow Always set to 5 L/min (IR does the drying)

Drying gas temperature Just set to 350°C. Remember you want the vaporizer to control the drying and to be able to maintain set point.

Vaporizer Start at 250°C. APCI is gas phase chemistry. A higher temperature usually works better. The vaporizer will compensate for flow rate or solvent composition.

Corona current Set to 5 μ A positive or negative. The corona voltage will be ~4000 V at 6 μ A.

Vcap Set to 2000 V. The lower voltage works better for fast switching. The APCI response is usually better at the higher end of the Vcap range.

Charging Voltage Set to 2000.

NOTE

The above set of parameters is provided as a starting point and should yield good response for many analytes. To obtain a specific response, i.e., high sensitivity detection of a compound or class of compounds, or a balanced response to a wide variety of compound classes, these parameters and the LC mobile phase composition should be examined further using traditional techniques for optimizing a method. The four most important parameters and the suggested optimization order are: vaporizer temperature, then capillary voltage, then nebulizer pressure, and then corona current.

3

Guidelines for multimode source settings in MM-ES+APCI mode

Guidelines for multimode source settings in MM-ES+APCI mode

NOTE

Click **Instrument > MSD Spray Chamber** to set the Method Spray Chamber to MM-ES+APCI before you edit the Set Up MSD Signals dialog box.

Drying gas flow Always set to 5 L/min (IR does the drying)

Nebulizer pressure Start at 40 psi. You will use the nebulizer pressure and the corona current to balance ESI and APCI. A higher nebulizer pressure results in more ESI. A lower nebulizer pressure results in more APCI.

Drying gas temperature Set to 300°C. Remember you want the vaporizer to control the drying and to be able to maintain the set point.

Vaporizer Start at 200°C. A higher temperature usually works better for MM-APCI. MM-ESI is usually unaffected except for sodium adduction. The vaporizer will compensate for flow rate or solvent composition.

Capillary Voltage Set to 2000 V. A lower voltage works better for fast switching. You are balancing ESI and APCI response. A setting of 2000 is a good compromise.

Corona current Set to $1 \ \mu A$ for positive or negative polarity. More corona current will reduce the ESI signal and increase the APCI signal.

Charging Voltage Set the charging voltage to 2000 V.

NOTE

The above set of parameters is provided as a starting point and should yield good response for many analytes. To obtain a specific response, i.e., high sensitivity detection of a compound or class of compounds, or a balanced response to a wide variety of compound classes, these parameters and the LC mobile phase composition should be examined further using traditional techniques for optimizing a method.

Guidelines for positive/negative polarity switching in mixed mode

NOTE

Click **Instrument > MSD Spray Chamber** to set the Method Spray Chamber to MM-ES+APCI before you edit the Set Up MSD Signals dialog box.

The following settings are a good starting point when you are doing positive/negative polarity switching in MM-ES+APCI mode.

Drying gas flow Always set to 5 L/min (IR does the drying).

Nebulizer pressure Start at 40 psi. You will use the nebulizer pressure and the corona current to balance ESI and APCI. A higher nebulizer pressure results in more ESI. A lower nebulizer pressure results in more APCI.

Drying gas temperature Set to 250°C. Remember you want the vaporizer to control the drying and to be able to maintain the set point.

Vaporizer Start at 150°C. A higher temperature usually works better for MM-APCI. MM-ESI is usually unaffected except for sodium adduction. The vaporizer will compensate for flow rate or solvent composition.

Capillary Voltage Set to 1000 V. The lower voltage works better for fast switching. You are balancing ESI and APCI response.

Corona current Set to $1 \mu A$ for positive or negative polarity. The corona voltage will be approximately 3500 at $2 \mu A$. More corona current will reduce the ESI signal and increase the APCI signal.

Charging Voltage Set the charging voltage to 2000 V.

NOTE

Refer to "To create a method for positive/negative mixed mode operation" on page 9 for additional information.

3

Guidelines for positive/negative polarity switching in mixed mode

NOTE

The above set of parameters is provided as a starting point and should yield good response for many analytes. To obtain a specific response, i.e., high sensitivity detection of a compound or class of compounds, or a balanced response to a wide variety of compound classes, these parameters and the LC mobile phase composition should be examined further using traditional techniques for optimizing a method.

3

Empirical Formulas for high resolution MS

G2421A MM-ES Calibration Ions

	Positive Ion (m/z)	Empirical Formula
Betaine+H	118.086809	C5.H12.O2.N
HP-0321+H	322.048699	C6.H19.O6.N3.P3
HP-0622+H	622.029499	C12.H19.O6.N3.P3.F12
HP-0922+H	922.010300	C18.H19.O6.N3.P3.F24
	1307.969049	C25.H17.O6.N3.P3.F40
HP-1521+H	1521.971900	C30.H19.O6.N3.P3.F48
fragment	1807.937049	C35.H17.O6.N3.P3.F60
HP-2121+H	2121.933500	C42.H19.O6.N3.P3.F72
fragment	2307.905049	C45.H17.O6.N3.P3.F80
HP-2721+H	2721.895100	C54.H19.O6.N3.P3.F96
	Negative Ion (m/z)	Empirical Formula
TFA-H	Negative lon (m/z) 112.985039	Empirical Formula C2.O2.F3
TFA-H fragment		-
	112.985039	C2.02.F3
fragment	112.985039 431.981740	C2.O2.F3 C9.O.N3.F14
fragment adduct	112.985039 431.981740 601.978370	C2.O2.F3 C9.O.N3.F14 C12.H.O.N3.F21
fragment adduct adduct	112.985039 431.981740 601.978370 w 734.006709	C2.O2.F3 C9.O.N3.F14 C12.H.O.N3.F21 C14.H18.O8.N3.P3.F15
fragment adduct adduct adduct	112.985039 431.981740 601.978370 w 734.006709 1033.987509	C2.02.F3 C9.0.N3.F14 C12.H.0.N3.F21 C14.H18.08.N3.P3.F15 C20.H18.08.N3.P3.F27
fragment adduct adduct adduct fragment	112.985039 431.981740 601.978370 w 734.006709 1033.987509 1305.953400	C2.02.F3 C9.0.N3.F14 C12.H.0.N3.F21 C14.H18.08.N3.P3.F15 C20.H18.08.N3.P3.F27 C25.H15.06.N3.P3.F40
fragment adduct adduct adduct fragment adduct	112.985039 431.981740 601.978370 w 734.006709 1033.987509 1305.953400 1633.949110	C2.02.F3 C9.0.N3.F14 C12.H.0.N3.F21 C14.H18.08.N3.P3.F15 C20.H18.08.N3.P3.F27 C25.H15.06.N3.P3.F40 C32.H18.08.N3.P3.F51
fragment adduct adduct adduct fragment adduct fragment	112.985039 431.981740 601.978370 w 734.006709 1033.987509 1305.953400 1633.949110 1805.921399	C2.02.F3 C9.0.N3.F14 C12.H.0.N3.F21 C14.H18.08.N3.P3.F15 C20.H18.08.N3.P3.F27 C25.H15.06.N3.P3.F40 C32.H18.08.N3.P3.F51 C35.H15.06.N3.P3.F60
fragment adduct adduct adduct fragment adduct fragment adduct	112.985039 431.981740 601.978370 w 734.006709 1033.987509 1305.953400 1633.949110 1805.921399 2233.910709	C2.02.F3 C9.0.N3.F14 C12.H.0.N3.F21 C14.H18.08.N3.P3.F15 C20.H18.08.N3.P3.F27 C25.H15.06.N3.P3.F40 C32.H18.08.N3.P3.F51 C35.H15.06.N3.P3.F60 C44.H18.08.N3.P3.F75

w indicates a weak adduct signal.

G2422A MM-APCI Calibration Ions

NOTE

Fragment ion signals are progressively stronger at higher m/z by increasing CID energy.

G2422A MM-APCI Calibration Ions

	Positive Ion (m/z)	Empirical Formula
Purine+H	121.051421	C5.H5.N4
HP-0321+H	322.048699	C6.H19.O6.N3.P3
HP-0622+H	622.029499	C12.H19.O6.N3.P3.F12
HP-0921+H	922.010300	C18.H19.O6.N3.P3.F24
fragment	1307.969049	C25.H17.O6.N3.P3.F40
HP-1521+H	1521.971900	C30.H19.O6.N3.P3.F48
fragment	1807.937049	C35.H17.O6.N3.P3.F60
HP-2121+H	2121.933500	C42.H19.O6.N3.P3.F72
	Negative Ion (m/z)	Empirical Formula
Purine-H	119.035771	C5.H3.N4
fragment	556.001426	C10.H15.O6.N3.P3.F10
fragment	805.985476	C15.H15.O6.N3.P3.F20
fragment	1305.953400	C25.H15.O6.N3.P3.F40
fragment	1805.921399	C35.H15.O6.N3.P3.F60

NOTE

Fragment ion signals are progressively stronger at higher m/z by increasing CID energy.

3

Tuning Mix and Test Mix

G2421A ES Tuning Mix (100mL)

Item-Description	Quantity	
es tune mix label	1 each	
plastic bottle	1 each	
acetonitrile	74.67 g	
hp-0321	<1 mg	
hp-0621	<1 mg	
hp-0921	<5 mg	
hp-1521	<5 mg	
hp-2121	<5 mg	
hp-2721	<10 mg	
hp-0585	<5 mg	
betaine	<1 mg	
tfa ammonium salt	26.2 mg	

Trade Name	Chemical Description
HP-0321	Non-fluorinated triazatriphosphorine
HP-0621	Fluorinated triazatriphosphorine
HP-0921	Fluorinated triazatriphosphorine
HP-1521	Fluorinated triazatriphosphorine
HP-2121	Fluorinated triazatriphosphorine
HP-2721	Fluorinated triazatriphosphorine
HP-0585	Tris(heptafluoropropyl)-triazine

G2422A APCI Tuning Mix (100mL)

G2422A APCI Tuning Mix (100mL)

Item-Description	Quantity
apci tune mix label	1 each
plastic bottle	1 each
acetonitrile	62.88 g
methanol	11.87 g
hp-0321	<1 mg
hp-0621	<1 mg
hp-0921	<5 mg
hp-1521	<5 mg
hp-2121	<5 mg
purine	<1 mg
chloroform	1.476 g

Trade Name	Chemical Description
HP-0321	Non-fluorinated triazatriphosphorine
HP-0621	Fluorinated triazatriphosphorine
HP-0921	Fluorinated triazatriphosphorine
HP-1521	Fluorinated triazatriphosphorine
HP-2121	Fluorinated triazatriphosphorine
HP-2721	Fluorinated triazatriphosphorine
HP-0585	Tris(heptafluoropropyl)-triazine

Chemical structures in the multimode test mix

Chemical structures in the multimode test mix

The following diagram shows the chemical structure of the four components in the multimode test mix.



Chemical structures in the multimode test mix

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Multimode Source for 6100 Series Single Quad LC/MS User Guide

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In This Book

This book contains installation, operation, maintenance and troubleshooting instruction for the Multimode Source for 6100 Series Single Quad LC/MS.

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