

**Agilent G1978B
Multimode Source for
6410 Triple Quad LC/MS**

Set-Up Guide



Agilent Technologies

Notices

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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.

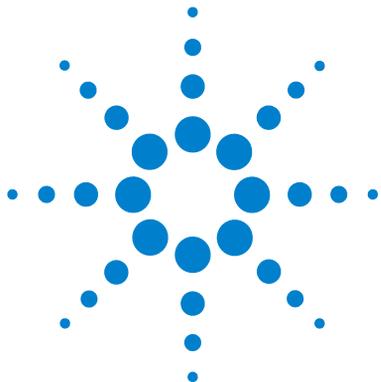
2 Performance Verification

This chapter describes how to set up methods and autotune the source.

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This chapter contains instructions to install the multimode source on a 6400 Series Triple Quad LC/MS system, and also to remove and replace the source.



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

Step 2. Install the HV control PCA and cables



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.

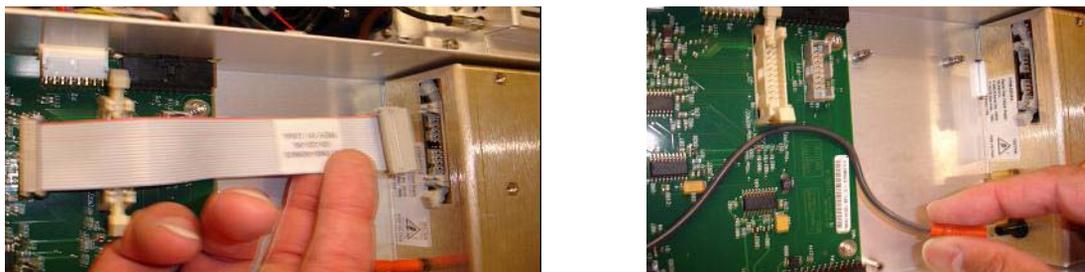


Figure 3 Disconnecting the Vcap/Vchamber power supply from the valve PCA (left) and the Vcap/Vchamber.

- 4 Place the MM 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.

1 Installation

Step 2. Install the HV control PCA and cables



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

- 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 Connecting the valve PCA to the Vcap/Vchamber power supply.

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

Step 2. Install the HV control PCA and cables



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.



Figure 7 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 (see [Figure 8](#)).



Figure 8 Connecting the APCI HV to the chassis.

1 Installation

Step 2. Install the HV control PCA and cables

- 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 9 Connecting the HV PCA to the chassis.

- 12** Close the AUX Module cover and reconnect all cables.

- 13** Install the multimode source onto the system and connect all connectors.

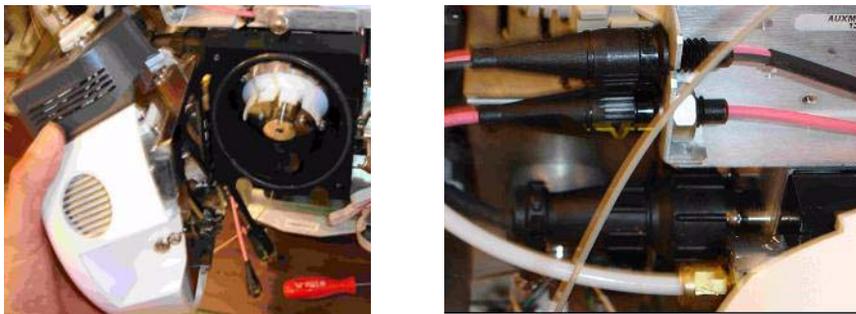


Figure 10 Installing the multimode source (left) and connecting all connectors.

- 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.

Changing Sources

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 QQQ** tab.
 - c Turn off all voltages and temperatures in the **Source** tab.

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.

1 Installation

To convert from multimode to ESI or APCI

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 QQQ** tab.
 - c Turn off all voltages and temperatures in the **Source** tab.
- 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

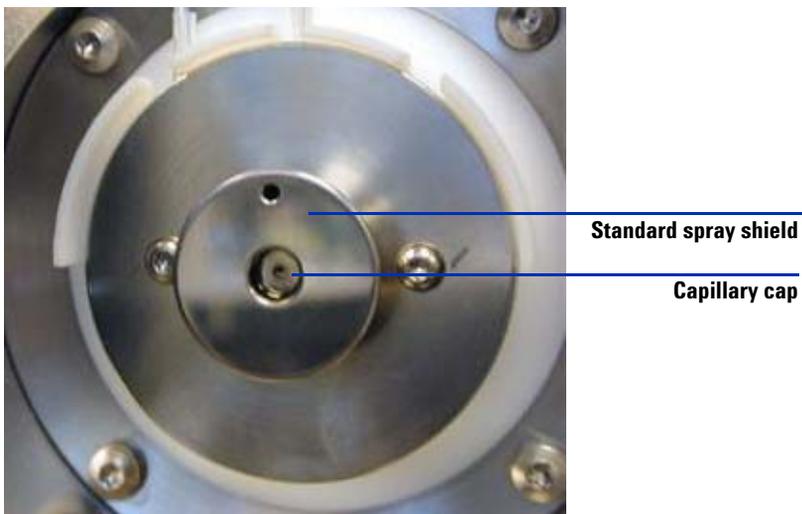


Figure 11 Standard spray shield and capillary cap for ESI or APCI

- 8 Remove the capillary cap. If needed, moisten a clean cloth with isopropyl alcohol and wipe the capillary cap. See [Figure 12](#).

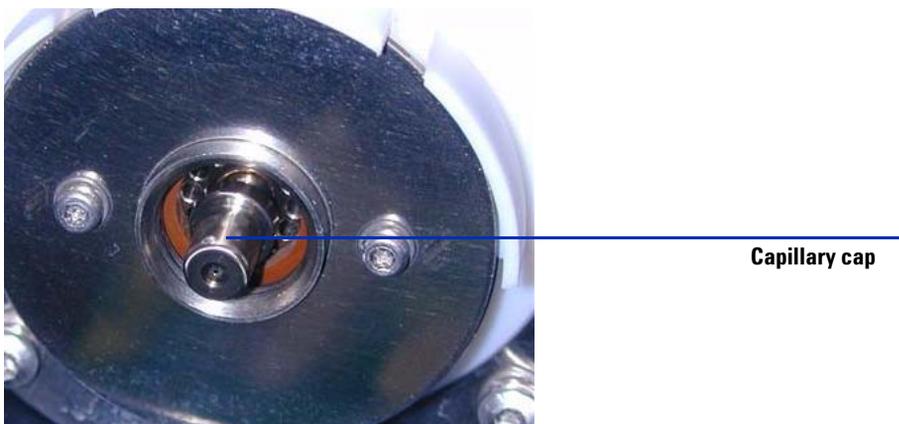


Figure 12 Spray shield removed.

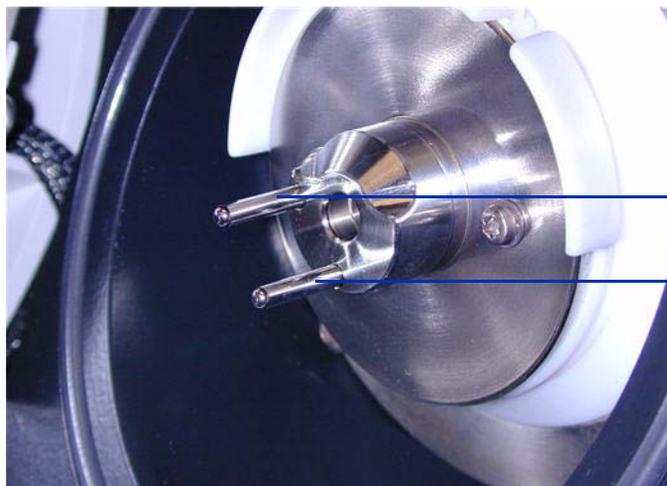
- 9 Place the capillary cap back on the capillary.
- 10 Install the new spray shield with field shaping electrodes. See [Figure 13](#).

To convert from ESI or APCI to the multimode source



Figure 13 Multimode spray shield

11 Screw the multimode spray shield into the holder for the spray shield. See [Figure 14](#).



Field shaping electrode
9 o'clock position

Field shaping electrode
6 o'clock position

Figure 14 Multimode spray shield installed

NOTE

The field shaping electrodes should be in the nine o'clock and the six o'clock positions. Failure to place the field shaping electrodes in the correct positions will result in greatly reduced response by the multimode source. Loosen the end plate screws on each side to adjust the field shaping electrodes position.

1 Installation

To convert from ESI or APCI to the multimode source

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



Figure 15 Multimode Spray Chamber

13 Install the spray chamber on the spray chamber mount.

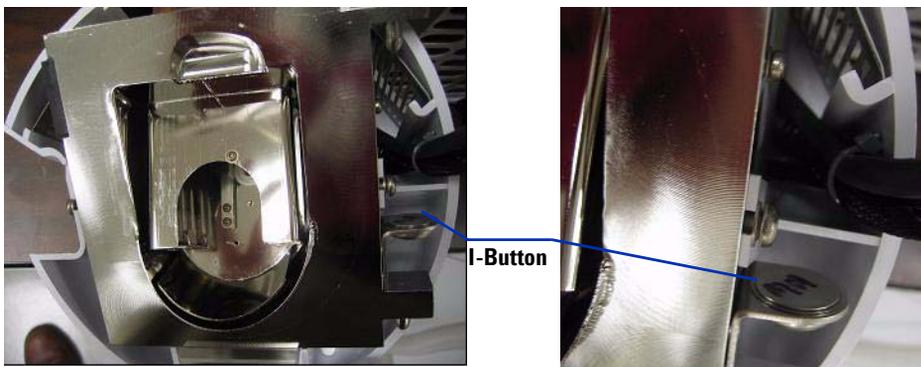


Figure 16 Multimode source with I-Button

14 Install the nebulizer on the multimode source spray chamber.

To convert from ESI or APCI to the multimode source



Figure 17 No nebulizer on top of 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](#).

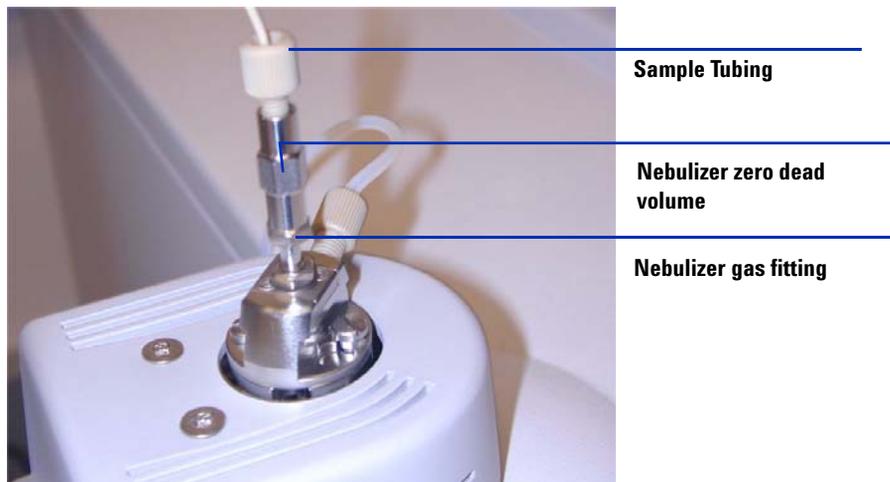


Figure 18 Nebulizer with gas tubing connected

1 Installation

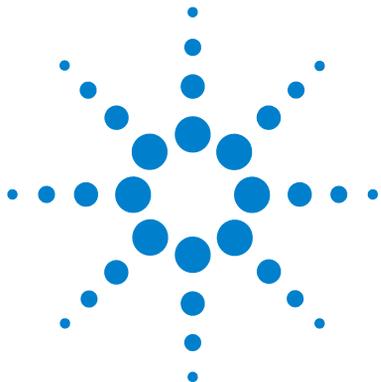
To convert from ESI or APCI to the multimode source

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.



2 Performance Verification

To review methods and run worklist [22](#)

To do sensitivity verification [24](#)

To autotune with the multimode source [27](#)

To set up a method to use the multimode source [28](#)

This chapter contains the steps necessary to complete the hardware setup and verify the performance specifications of the installed system.



2 Performance Verification

To review methods and run worklist

To review methods and run worklist

You use the multimode source in Positive MRM Mode.

- 1 Verify that the Collision Cell gas flow rate produces a high vacuum gauge reading in the range of 2.7 to 3.3 x 10e-5 torr.

To view the high vacuum gauge reading, click the **Cell** tab in the Tune Context and check that the high vacuum gauge reading is within range. If not, see “[To reset the Collision Cell gas flow rate](#)” in the Triple Quad *Installation Guide*.

- 2 Start the Data Acquisition program, change the **Context** to **Tune**, and start an **Autotune**.

After the autotune has completed, you may need to wait up to 30 minutes to allow for the calibrant solution to be pumped out of the Triple Quad. This minimizes any background signal attributable to the calibrant. In addition, you can sonicate the nebulizer in a small graduated cylinder filled with acetonitrile for 10 minutes.

- 3 Change the Context to **Acquisition**, click **File > Load** and then load the method **MMI-ES Pos MRM Reserpine Checkout.m**. The checkout method includes the following acquisition parameters:
 - 2 µL injection
 - isocratic from channel A at 0.4 mL/min.
 - 2.5 minutes run time
 - 250°C drying gas temperature
 - 5 L/minute drying gas flow (can be optimized, typical 10 to 13 L/min)
 - 60 psi nebulizer pressure (can be optimized, typical 35 to 40 psi)
 - 2000 V capillary voltage
 - 250°C Vaporizer temperature
 - 2000 V charge voltage
 - 37 V collision cell energy (can be optimized, typical between 37 to 41 V)
 - 240 V fragmentor voltage (can be optimized, typical between 140 to 250 V)
 - 700 V Delta EMV (can be optimized, typical between 400 to 800 V)
 - MS1 Resolution set to Wide and MS2 Resolution set to Unit

- 4 In the method, select channel A, the 75:25 methanol/water solution with 5 mM ammonium formate, as the LC solvent.
- 5 Click **File > Load** and then load the method **MMI-ES Pos MS2 Scan.m**.
- 6 In the method, select channel A, 75:25 methanol/water solution with 5mM ammonium formate, as the LC solvent.
- 7 Place the vials into the LC autosampler.
 - Position #1: An empty, uncapped vial
 - Position #2: A vial containing the solvent used for dilution (this is the solvent blank)
 - Position #3: A vial containing the reserpine sample (500 fg/μl)
- 8 From the **File** menu click **Load** and then load the worklist: **MMI-ES Pos Reserpine Checkout.wkl**.

The worklist is set up to do one injection of the solvent blank using the **ESI Pos MS2 Scan.m** method in order to collect background ion data, then using the **ESI Pos MRM Reserpine Checkout.m** method for the remaining runs, one injection of the empty vial, five injections of the solvent blank, and five injections of the reserpine sample.

2 Performance Verification

To do sensitivity verification

To do sensitivity verification

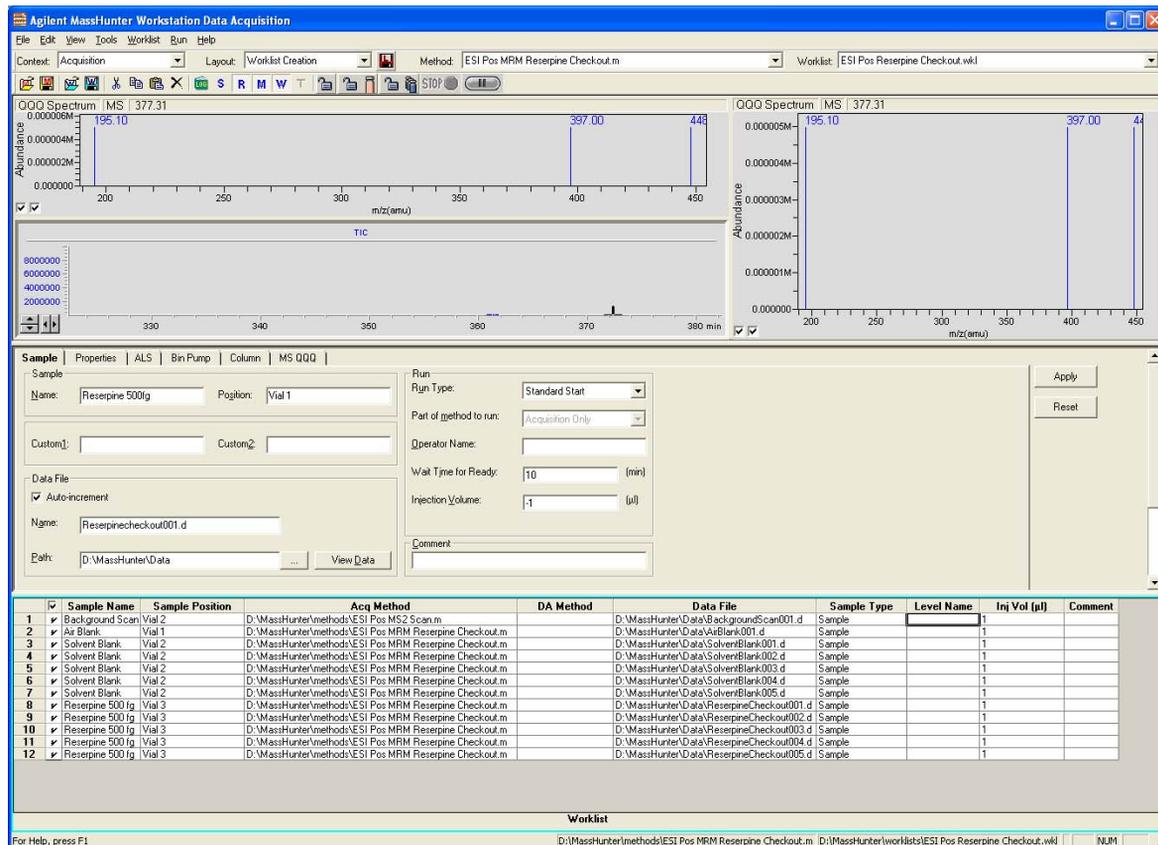


Figure 19 Reserpine checkout worklist

- 1 Review the worklist to be sure that the method and data paths are correct, and that the data file names given in the worklist are unique and have not already been acquired.
- 2 Run the worklist.
- 3 When the worklist is finished, calculate signal-to-noise for each injection:
 - a Load each solvent blank and reserpine sample data file into the Qualitative Analysis program.
 - b Generate Extracted Ion Chromatograms of the 195.1 ion.

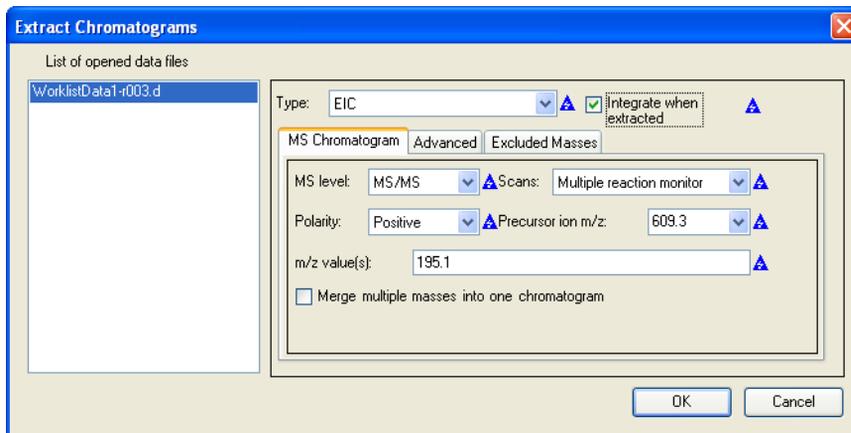


Figure 20 Extract Chromatogram dialog box

- c** Integrate each reserpine peak, and click **Calculate Signal to Noise**.
- d** Calculate the signal-to-noise using **Height**.
- e** Under Noise Measurement, for **Noise definition**, click **RMS** and select **X 3**. For **Noise regions**, type 1.00 - 1.45. (Make sure that the noise region does not include the reserpine peak. If the reserpine peak elutes within the default noise region, shift the noise region such that it is 0.45 to 0.90 minutes after the retention time of the reserpine peak.)

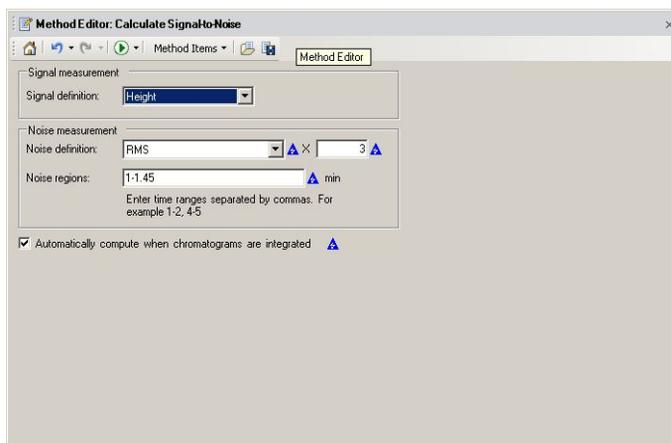


Figure 21 Calculate Signal to Noise dialog box

To autotune with the multimode source

- 1 Remove the G1948B Electrospray source and install the G1978B multimode source.
- 2 Pour the Electrospray or APCI calibrant back into its original bottle or another suitable container, rinse the calibrant bottle with acetonitrile, pour the MMI-L Low Concentration Tuning Mix (G1969-85020) calibrant into the calibrant bottle, and attach the calibrant bottle back onto the CDS.
- 3 Set the **Context** view to **Tune** in the MassHunter Workstation program.
- 4 Load an autotune file that was generated with the G1948B Electrospray source.
- 5 Run an Autotune using the G1978B multimode source.

2 Performance Verification

To set up a method to use the multimode source

To set up a method to use the multimode source

- 1 In the MassHunter software, change the **Context** to **Acquisition**.
- 2 In the MS QQQ tab, set **Ion source** to **MMI** (see [Figure 22](#) on page 29).
- 3 In the **Time Segments** table, chose an ionization mode from the **Ion Mode** list. You may set the ionization mode to one of the following:
 - ESI
 - APCI
 - ESI+APCI

The Ion Mode selection ESI + APCI will specify a method for Simultaneous ESI and APCI operation.

Note that the Ion Mode selection is only visible if **Ion source** is set to **MMI**.

- 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

Sample | Properties | WPS | Bin Pump | Column | VWD | **MS QQQ**

Ion source: MMI

Tune file: Autotune_092806_175408\atun...

Time segments:

#	Time	Scan Type	Ion Mode	Ion Polarity	Diverter Valve	Delta EMV
1	0	MRM	ESI+APCI	Negative	To MS	400

Stop time: 1 min

Time filtering: Peak width 0.07 min

Source parameters:

Gas Temp: 325 301.5 °C

Vaporizer: 200 °C

Gas Flow: 5 2.99159 l/min

Nebulizer: 40 14.9962 psi

Capillary: 2000 V 3.90720 nA

Corona Current: 1 µA

Charging: 2000 V

Chamber Current: 9.00219 µA

4.91 cycles/s 203.5 ms/cycle

Buttons: Copy, Paste, Paste to All Seg

Figure 22 Multimode acquisition settings

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.

2 Performance Verification

To set up a method to use the multimode source

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In This Book

This book contains installation, operation, maintenance and troubleshooting instruction for the Multimode Source for 6410 Triple Quad LC/MS.

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