

Agilent 6460 Triple Quad Mass Spectrometer (Model K6460) System

Installation Guide

For in Vitro Diagnostic Use



Notices

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In This Guide...

This guide contains information to install the Agilent 6460 Triple Quad Mass Spectrometer (Model K6460) System.

1 Instrument Installation

This chapter describes the steps that are needed to install the K6460 Triple Quad MS.

2 Software Installation and Configuration

This chapter describes the steps that are needed to install the MassHunter software.

3 Installation Completion and System Verification

In this chapter, you finish the hardware setup.

4 Installation and Verification of the G1947B APCI Source

This chapter contains the steps needed to install and verify the operation of the APCI source.

5 Other Setup Tasks

This chapter contains tasks that are related to setting up your Triple Quad instrument.

6 Reference

This chapter contains parameters for verifying performance.

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Instrument Installation

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This chapter describes the steps that are needed to install the K6460 Triple Quad MS.



Figure 1 K6460 Triple Quad MS



Step 1. Unpack and set up the K6460 Triple Quad MS

Step 1. Unpack and set up the K6460 Triple Quad MS

NOTE

Do not open the shipping containers until an Agilent representative is present to verify the contents of each carton. Warranty claims for missing items are honored only if an Agilent representative is on site to verify the contents of each shipping container as it is unpacked.

Checkout and tuning samples are shipped separately to comply with shipping regulations and to ensure prompt delivery. Make sure that these samples have been stored correctly, as indicated in the instructions in the box.

1 Carefully examine all containers for external signs of damage. If damage is discovered, immediately contact the carrier and the Agilent Service Management.

Retain shipping containers and material until contents are checked for completeness and instrument performance is verified.

- **2** Check off each item on the packing list, and verify the serial numbers.
- **3** Record the serial numbers in the installation documentation.
- **4** Report any discrepancies to Agilent Technologies.
- **5** Check that site preparation is complete, which includes power and gas supplies and chemical supplies needed for installation and performance verification.
- **6** Check the line voltage in the lab.

Verify the proper line voltage and outlet ratings according to the instructions given in the *Site Preparation Guide*.

Step 2. Prepare to install the system

Before you begin, check that you have these parts:

- Utility knife and needle nose pliers
- 1 Unpack and set up the K6460 Triple Quad MS.
 - **a** Cut the tie wraps around the package. See Figure 2.



Figure 2 K6460 Triple Quad MS shipping container

b Lift the boxes off the top of the instrument. See Figure 3.

Step 2. Prepare to install the system



Figure 3 Instrument unpacked on shipping pallet (K6460 pictured)

c Remove the front, top, right, back-left, and lower front-left cosmetic covers so that you can remove the shipping brackets. You do not need to remove the upper front-left cover.

To remove the top cover, remove the two screws at the back side of the top cover that secure the back of the top cover to the instrument chassis (see Figure 4). These screws are only needed when shipping the instrument. You do not need to reinstall the screws when you reinstall the top cover.

Step 2. Prepare to install the system



Figure 4 Remove shipping screws from back of top panel. One of the screws to remove is circled in this picture.

d Remove the shipping brackets (a total of 7). You will need to use a 13-mm wrench.

Step 2. Prepare to install the system



Figure 5 Triple Quad on shipping pallet with covers removed (K6460 pictured)

- e Take an inventory of the contents of the packages.
- **f** Record serial numbers. The serial number label for the K6460 Triple Quad MS is located on the lower left corner to the left of the instrument power push button.
- **2** Use at least four people, one at each corner of the instrument, to lift the K6460 Triple Quad MS onto a stable bench or table. Be sure to comply with local standards on the limits that each individual is allowed to lift.

WARNING

Do not lift the Triple Quad without enough assistance to do so safely. The instrument weighs up to 115 kg (255 lbs). Be sure to use correct lifting procedures to avoid possible injury.

Step 2. Prepare to install the system

NOTE

Do *not* lift from under the power switch bracket on the front left corner of the instrument. The bracket will bend. See Figure 6.



Figure 6 Do *not* lift from under power switch bracket

1

Step 3. Set up the Agilent MS40+ pumps

Do these steps if your instrument include an Agilent MS40+ pump.

Before you begin, make sure that you have:

- Pump oil pan (p/n G1946-00034)
- Tygon 1/2-inch I.D. exhaust tubing (p/n G1946-80077)
- Agilent MS40+ foreline pump
- SW60 pump oil
- NW25 to 5/8-inch tube elbow (p/n G1960-20003)
- NW20/25 hinged clamp with wing nut (p/n 0100-1398)
- O-ring (p/n 0905-1592)
- pump power cord (p/n 8121-1753)

If the system is installed with G3215A Mass Spec Bench, follow the instructions in the Mass Spec Bench *User Guide* to install the pump or pumps inside of the Mass Spec Bench.



- 1 Unpack the Tygon 1/2-inch I.D. exhaust tubing (p/n G1946-80077) and Pump oil pan (p/n G1946-00034) from the shipping kit.
- 2 Remove the Agilent MS40+ foreline pump from its shipping container.

Step 3. Set up the Agilent MS40+ pumps

3 Set the Agilent MS40+ foreline pump into the Pump oil pan (p/n G1946-00034).

The pan is used to catch any small amounts of oil that can seep out of the pump. The pan can also hold all of the oil in the pump in case of a catastrophic seal failure.



- **4** Cut an appropriate length of the Tygon 1/2-inch I.D. exhaust tubing (p/n G1946-80077).
- 5 Find the NW25 to 5/8-inch tube elbow (p/n G1960-20003) and the O-ring (p/n 0905-1592). Put the O-ring on the exhaust adaptor.
- **6** Locate one NW20/25 hinged clamp with wing nut (p/n 0100-1398), open the swing clamp, and use it to clamp the exhaust adaptor onto the oil mist filter. Connect the Tygon 1/2-inch I.D. exhaust tubing (p/n G1946-80077) to the exhaust adaptor.
- **7** Add the entire 1-liter bottle of SW60 pump oil to the foreline pump.

CAUTION

Foreline pumps are shipped dry. Oil must be used for proper operation. Failure to add oil before a system is pumped down damages foreline pumps.

8 Plug the pump power cord (p/n 8121-1753) into the power inlet of the foreline pump. Secure the pump power cord in place using the retaining bale mechanism. Plug the other end into the Pump Expander assembly port labeled **Foreline**.

Step 3. Set up the Agilent MS40+ pumps



Figure 7 Pump expander box ports for K6460

Step 4. Connect the K6460 Triple Quad MS

- 1 Connect the rough hose (p/n G1969-20123) that is supplied in the ship kit to the KF-25 foreline pump hose connection on the back left of the instrument.
- **2** Connect the foreline pump hose to the KF-25 inlet adapter on the foreline pump.
- **3** Use the supplied hook/loop fastener tape to secure the drain bottle into a secondary containment tub.
- **4** Connect the spray chamber drain tube to the 1-inch fitting on the drain bottle. The drain tube can also be routed out the front of the Triple Quad if needed.
- **5** Attach the calibrant delivery system (CDS)/inlet module waste tubing from the solvent selection valve on the Triple Quad to the ¹/₄-inch fitting on the drain bottle.
- 6 Connect a length of the ½-inch Tygon tubing to the ½-inch fitting on the drain bottle, and then connect the other end of the tubing to a vent connection that is separate from the vent used for the foreline pump.

CAUTION

The drain bottle vent must be located away from the foreline pump vent to prevent the foreline pump exhaust from contaminating the Triple Quad spray chamber.

Step 4. Connect the K6460 Triple Quad MS



Figure 8 Drain bottle

7 Install the gas filter(s):

For K6460 Triple Quad MSs without AJS ESI source:

- **a** Cut an appropriate length of the 1/4-inch PTFE gas tubing (G1946-80078) and connect to the nitrogen gas supply regulator or nitrogen generator.
- b Use the supplied nut and ferrule kit (5183-0392) to attach the other length of tubing to the RMSN-4 gas filter. This configures the filter in series with the supply tubing. See Figure 9 as an example for assembling the gas trap in the correct configuration.



Step 4. Connect the K6460 Triple Quad MS

For K6460 with AJS ESI source:

- **a** Cut an appropriate length of the 1/4-inch PTFE gas tubing (p/n G1946-80078) and connect to the nitrogen gas supply regulator or nitrogen generator.
- **b** Locate the 2 1/4-inch brass T-unions (0100-0088) and loosen the brass nuts on the T-unions.
- **c** Connect the other end of the supply tubing to the T-union.
- **d** Cut four 4-inch lengths of PTFE tubing from the supplied 10 meter length (G1946-80078).
- e Connect two of the 4 inch lengths to each side of the T-unions. Use the supplied nut and ferrule kit



source

Figure 10 Gas filter connected in parallel

(5183-0392) to attach the other side 4 inch the tubing to the two RMSN-4 gas filters. This configures the filters in parallel. See Figure 10 as an example for assembling the gas traps in the correct configuration.

Step 4. Connect the K6460 Triple Quad MS



Figure 11 Power and gas connections on back left of the K6460

- 8 Set the pressure on the nitrogen supply regulator at 80 to 100 psi (550 to 690 kPa). Turn on the nitrogen gas for a few minutes to purge the tubing and gas conditioner before you connect the nitrogen gas supply to the Triple Quad. Regulator pressures above 110 psi (760 kPa) cause nitrogen waste due to release from the bleed valve on the flow-control module.
- **9** Use the tubing cutters (p/n 8710-1709) supplied in the ship kit to cut an appropriate length of the 1/8-inch copper supply tubing (p/n 5180-4196) to connect from the outlet fitting on the collision cell nitrogen tank regulator to the nitrogen gas conditioner (p/n RMSN-2) for the collision cell gas, and then cut a second length of the 1/8 -inch copper supply tubing to connect from the nitrogen gas conditioner to the collision cell gas inlet fitting on the left side of the Triple Quad (see Figure 11). Secure the gas filters in a vertical position with tie wraps.

Step 4. Connect the K6460 Triple Quad MS



Foreline pump power cord connection/ Pump Expander Assembly control connection

AC line power connection

Figure 12 Power and electrical connection at back left side of Triple Quad (K6460). If two LAN connections exist, make sure to use the upper connection.

10 Set the pressure on the Collision Cell supply regulator at 10 to 30 psi (70 to 210 kPa).

CAUTION

Do not attach the Collision Cell gas fitting to the nitrogen supply regulator at 80 to 100 psi (550 to 690 kPa). Pressure to the Collision Cell Gas Flow Module greater than 30 psi (210 kPa) can cause fewer collisions to be available for secondary collision induced dissociation (CID) and poor peak shapes, as well as poor high vacuum. The Collision Cell can use the same nitrogen supply as the regular supply (i.e. for drying gas, nebulizer, CDS pressure) if it is the required purity (99.999%) but it must be down-regulated to 30 psi (210 kPa).

- **11** Connect the remote start cable to its connector on the back left side of the Triple Quad. See Figure 12.
- **12** Connect the foreline pump power cord into the foreline pump connector on the back left side of the Triple Quad. See Figure 12.
- **13** Verify the front power switch is in the OFF position.

Step 4. Connect the K6460 Triple Quad MS

- **14** Plug the Triple Quad power cord into the Triple Quad power connector on the Triple Quad and the other end of the Triple Quad power cord into the wall outlet. See Figure 12.
- **15** Plug the Pump Expander Assembly power cord into the wall outlet.



Figure 13 Pump Expander Assembly box for K6460.

Step 5. Install the spray chamber

Agilent Jet Stream ESI Source

Before you begin, check that you have these parts:

- Agilent Jet Stream (AJS) ESI source
- ESI-L Low Concentration Tuning Mix (p/n G1969-85000)
- **1** Remove the top cover by loosening the T10 lock screw and lifting off the instrument chassis.
- **2** Remove the AJS ESI source from the packaging inside the instrument chassis next to the e-Module. See Figure 14.



Figure 14 Packaging for AJS ESI source for K6460

- **3** Remove the foil that covers the spray chamber mount, and remove the shipping cover from the Electrospray spray chamber.
- **4** Put the nebulizer in the nebulizer adjustment fixture supplied in the shipping kit and check that the nebulizer needle is properly adjusted. The nebulizer needle should be even with the end of the nebulizer nozzle.
- **5** Install the nebulizer in the spray chamber.

Step 5. Install the spray chamber

- **6** Install the spray chamber on the spray chamber mount, close the spray chamber, and fasten the latch. You may need to adjust the latch to ensure that the O-ring seals completely. Use a $\frac{1}{4}$ -inch x $\frac{5}{16}$ -inch wrench to loosen the lock nut, and then adjust the latch to the proper fit, and then tighten the lock nut so that the latch maintains its adjustment.
- 7 Connect the high voltage and vaporizer cables to the connectors on the left side panel of the instrument.
- 8 Connect the 1/8-inch nebulizing gas tubing from the Triple Quad mainframe to the nebulizer gas fitting.
- **9** Connect the 1/8-inch sheath gas tubing from the Triple Quad mainframe to the sheath gas fitting on the AJS ESI source.
- **10** Connect the PEEK tubing from the selection valve (inside the front cover) to the top of the nebulizer.



Figure 15 Connections for AJS ESI source

- **11** Rinse the calibrant bottle three times with hot (60°C) water and then three times with methanol. Then rinse it once with acetonitrile.
- **12** Add the ESI-L Low Concentration Tuning Mix to the calibrant bottle.

CAUTION

Never use aliphatic, aromatic or halogenated hydrocarbons in the CDS. These solvents are not compatible with the O-ring in the CDS.

13 Turn on the Triple Quad front power switch to start the pump-down of the Triple Quad.

The foreline pump(s) will become quieter within a few seconds.

Agilent G1948B Electrospray Source

Before you begin, check that you have these parts:

- Agilent G1948B Electrospray interface (the G1948A Electrospray interface is not supported)
- Nebulizer spacer kit (p/n G1946-60254)
- ESI-L Low Concentration Tuning Mix (p/n G1969-85000)
- **1** Remove the foil that covers the spray chamber mount, and remove the shipping cover from the Electrospray spray chamber.
- **2** Install the nebulizer spacer as follows:
 - **a** Use a flat-bladed screwdriver to remove the two nebulizer shoulder screws from the top of the spray chamber.
 - **b** Use the two m3×8 Torx T10 screws to install the nebulizer spacer onto the top of the spray chamber.
 - **c** Install the two nebulizer shoulder screws into the top of the nebulizer spacer.
- **3** Put the nebulizer in the nebulizer adjustment fixture supplied in the shipping kit and check that the nebulizer needle is properly adjusted. The nebulizer needle should be even with the end of the nebulizer nozzle.
- **4** Install the nebulizer in the spray chamber.
- **5** Install the spray chamber on the spray chamber mount, close the spray chamber, and fasten the latch. You may need to adjust the latch to ensure that the O-ring seals completely. Use a ¹/₄-inch x 5/16-inch wrench to loosen

Step 5. Install the spray chamber

the lock nut, adjust the latch to the proper fit, and then tighten the lock nut so that the latch maintains its adjustment.

- **6** Connect the 1/8-inch nebulizing gas tubing from the Triple Quad mainframe to the nebulizer gas fitting.
- 7 Connect the PEEK tubing from the selection valve (inside the front cover) to the top of the nebulizer.
- 8 Rinse the calibrant bottle three times with hot (60°C) water and then three times with methanol. Then rinse it once with acetonitrile.
- **9** Add the Electrospray calibrant to the calibrant bottle.

CAUTION Never use aliphatic, aromatic or halogenated hydrocarbons in the CDS. These solvents are not compatible with the O-ring in the CDS.

10 Turn on the Triple Quad front power switch to start the pump-down of the Triple Quad.

The foreline pump(s) will become quieter within a few seconds.

Step 6. Install the Agilent LC system

Before you begin, check that you have these parts:

- HPLC grade methanol, or better
- HPLC grade water, or better
- **1** Install the Agilent LC system. Follow its installation documents. Other LCs are not supported.
- **2** Connect the remote start cable from the Triple Quad to a Remote Start connector on the LC sampler, pump or other detector module only.
- **3** Install an Agilent G1369 LAN Interface card into the LC detector module if required. If a detector module is not present, install the Agilent G1369 LAN Interface card into the pump module. Before you install the LAN Interface card, set switches 5 and 6 to the ON position. This will force the Agilent LAN Interface Card to use its default IP address and subnet mask.

The default IP address is 192.168.254.11 and the default subnet mask is 255.255.255.0.

CAUTION

Do not use any other LAN interface card besides the G1369 (e.g. the older Jet Direct card J4100A).

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If you purchased a bundled K6460 Triple Quad MS system, the MassHunter Workstation software has been installed for you. In this case, start at "Step 4. Install the Data Acquisition program".

If you are upgrading MassHunter software that is already installed, refer to the *Upgrade Guide* that came with your system.



Step 1. Set up the computer system

- **1** Set up the PC:
 - **a** Unpack the PC and put it on a suitable bench top or table.
 - **b** Connect the keyboard, mouse, monitor and printer to the computer.
- **2** Install the network hub:
 - **a** Put the hub on the table next to the PC.
 - **b** Plug the power supply into the hub.
 - c Connect the power supply to a power outlet.
- **3** Connect one end of a Category 5, shielded twisted pair (STP) cable to any port (1 to 7) on the network hub. Connect the other end of the cable to the 10/100 Base-T network card in slot 1 of the PC. The card should be labeled **LC/MS**.

Do not connect to port 8 on the hub/switch.

- **4** Connect a second Category 5 STP LAN cable from one of the open ports 1 to 7 on the hub to the Agilent LAN Card in the pump or detector.
- **5** Connect a third Category 5 STP LAN cable from one of the open ports 1 to 8 on the hub to the LAN interface connection on the LAN/MS control card in the Triple Quad instrument.
- **6** Install the printer if included with your system. See the installation documentation supplied with the printer.
- 7 Turn on the printer, hub, monitor, and PC, in that order.

The computer comes installed with software and the appropriate drivers for the installed accessories.

8 When the computer starts, create a user account. This account will be used to acquire data. Do not use the Windows Admin account for this purpose.

Step 2. Check PC network card configuration

1 Click Start > Control Panel, and then under Network and Internet, click View network status and tasks.

If Control Panel displays in Small icons view, click **Network and Sharing Centers**.

- 2 Click Change adapter settings.
- **3** From the list of network connections, double-click the network connection that corresponds to the instrument LAN connection.
- **4** Scroll down the list to **Internet IP Protocol 4 (TCP/IPv4)** (or **Internet IP Protocol**), select it, and then click **Properties**.

Connect using:		
Broadcom Net	Xtreme Gigabit Ethernet	
This connection uses	s the following items:	Configure
Client for Mi	icrosoft Networks t Scheduler	od slove - 274 -
File and Prin	nter Sharing for Microsoft	Networks
Broadcom A	Advanced Server Progra	m Driver
Internet Pro	tocol Version 6 (TCP/IP)	(6)
✓ → Link-Laver	Topology Discovery Map	per I/O Driver
🗹 🔺 Link-Layer	Topology Discovery Res	ponder
Install	Uninstall	Properties
Description		
Description Transmission Cont wide area network across diverse inte	trol Protocol/Internet Pro c protocol that provides c erconnected networks.	tocol. The default communication

Figure 16 LCMS Connection Properties dialog box - Networking tab

Step 3. Prepare for installation

5 Make sure the Network Adapter is set to these settings: IP address: 192.168.254.1 Subnet mask: 255.255.255.0

You can get IP settings assigne this capability. Otherwise, you r for the appropriate IP settings.	ed automatically if your network supports need to ask your network administrator
🔘 Obtain an IP address auto	omatically
Use the following IP addre	ess:
IP address:	192 . 168 . 254 . 1
Subnet mask:	255 . 255 . 255 . 0
Default gateway:	2 2 2
Obtain DNS server addres	ss automatically
Use the following DNS served	ver addresses:
Preferred DNS server:	· · · · · ·
Alternate DNS server:	
Walidate settings upon evi	it Advanced

Figure 17 Internet Protocol Version 4 (TCP/IP) Properties dialog box

Step 3. Prepare for installation

• Run Windows Update to make sure you have the latest critical updates and security fixes.

Make sure Windows Update is completed before you continue.

CAUTION

If you do not run Windows Update, your system can be vulnerable to security problems. Confirm that the LAN power management has not been activated by a Windows Update program.

Step 4. Install the Data Acquisition program

The installation of the Data Acquisition program includes installation of Optimizer and Study Manager. Do not separately install these programs.

- 1 Check that no other program is running on your system, including Windows Update.
- **2** Put the Data Acquisition installation disc into the disc drive.

The welcome page appears.

- **3** Click **Install Microsoft .NET 4.5**. Follow the instructions to install Microsoft .NET 4.5.
- **4** Click **Install MassHunter Data Acquisition Software**, and then follow the instructions to install the software.
 - In the License Agreement page, click I accept the terms in the License Agreement, and then click Next.
 - In the **Choose destination location** page, click **Next** to accept the default destination location.

The default is C:\Program Files (×86)\Agilent\MassHunter\Workstation\Acq.

- If prompted, in the **Choose location for customer data files** screen, check that the default of D: \MassHunter is displayed in the text box, and then click **Next**.
- In the **Ready to install** page, click **Install**.

The Setup Status page now appears.

- If you are asked to allow Agilent Technologies to install software on the computer, click **Yes**.
- If you get a message that indicates that the screen resolution is *not* set to the required resolution, click **OK**.
- If you see a Notepad window that prompts you to install other options, close the Notepad window.
- When the installation completion message is displayed, click **Finish**.
- **5** Make sure that the most current firmware for the K6460 is installed.

2 Software Installation and Configuration

Step 5. Install the Qualitative Analysis program

- 6 Click Install MassHunter Data Acquisition Manuals, and then:
 - **a** Make sure all check boxes are marked.
 - **b** Click Start Copy.

Manuals for Help must be marked so that user guides can be opened from online Help after installation. **Manuals** can be marked to copy the user guides to a second location of your choice.

Video Maintenance Guide must be marked so that the animated maintenance instructions can be opened from online Help after installation.

7 Click **Install Software Verification Tool** if you need to qualify the installation.

Step 5. Install the Qualitative Analysis program

• Refer to the *Offline Qualitative and Quantitative Analysis Installation Guide* for the K6460 Mass Spectrometer to install the Qualitative Analysis program.

CAUTION You must use the **Run as administrator** option to install the program. Failure to do so can result in an incomplete installation, which can cause the system to run unreliably.

Do not install any other MassHunter program until instructed to do so.

Step 6. Install the Quantitative Analysis program

• Refer to the *Offline Qualitative and Quantitative Analysis Installation Guide* for the K6460 Mass Spectrometer to install the Quantitative Analysis program.

CAUTION

You must use the **Run as administrator** option to install the program. Failure to do so can result in an incomplete installation, which can cause the system to run unreliably.

Do not install any other MassHunter program until instructed to do so.

Step 7. Install Microsoft Excel (optional)

The MassHunter Qualitative Analysis and Quantitative Analysis programs include PDF-based report templates. You need to install Excel only if you want to use custom Excel report templates.

• Refer to the *Offline Qualitative and Quantitative Analysis Installation Guide* for the K6460 Mass Spectrometer to install Excel.

Do not install any other MassHunter program until instructed to do so.

Step 8. Install Service Packs for Data Acquisition

Make sure that you install Service Packs specifically for K6460, if available.

1 Put the Data Acquisition installation disc into the disc drive.

If you received a separate Service Pack installation disc, insert that disc instead.

- 2 If the folder **Service Packs** exists on the installation disc, then:
 - a Open the **Service Packs** folder. If the folder contains another folder, such as **SP1**, open that folder.
 - **b** Locate the installation file, which ends with **SP** *x*.exe.
 - c Right-click the installation file and select Run as administrator.
 - d Follow the instructions to install the service pack.

2 Software Installation and Configuration

Step 9. Install Quantitative Analysis Reporting

Step 9. Install Quantitative Analysis Reporting

• Refer to the *Offline Qualitative and Quantitative Analysis Installation Guide* for the K6460 Mass Spectrometer to install the Quantitative Analysis Reporting program.

CAUTION You must use the **Run as administrator** option to install the program. Failure to do so can result in an incomplete installation, which can cause the system to run unreliably.

Do not install any other MassHunter program until instructed to do so.

Step 10. Configure Excel for MassHunter (optional)

• Refer to the *Offline Qualitative and Quantitative Analysis Installation Guide* for the K6460 Mass Spectrometer to verify the installation of Excel Add-Ins for MassHunter.
Step 11. Configure the instrument

If available, configure the device from the Device Configuration tool in the Data Acquisition program. Go to **Tools > Device Config**.

Some HPLC instrument setups can be configured only through the Device Configuration tool from the Data Acquisition program. The Capillary Pump and the Nano pump with the Chip Cube are examples.

In this step, you configure the K6460 Triple Quad MS and the HPLC instrument.

- **1** Open the **Agilent MassHunter Workstation** folder on the desktop, and then double-click **Acq Tools**.
- **2** Double-click the **Instrument Configuration** tool.
- **3** If you are prompted to log in to OpenLAB, provide the user name and password for an OpenLAB administrator account.

You are prompted if OpenLAB Shared Services is installed on this computer.

- **4** In the Instrument Configuration dialog box:
 - **a** If you want to change the name of the instrument, type a new name for **Instrument name**.
 - **b** Mark the **Mass Spectrometer** check box.
 - c Click the option for your LC/MS instrument.
 - d Mark the Agilent LC (1100/1120/1200/1220/1260/1290)/CE check box.
 - e Click Agilent LC System Access.
 - f Click Device Config and configure the LC system.
 - g Click OK.

2 Software Installation and Configuration

Step 11. Configure the instrument

istrument name:	Instrument 1	
Mass Spectrometer		
Agilent 6400 Series Tri	ple Quadrupole	192.168.254.12
🔿 Agilent 6500 Series Qu	adrupole Time of Flight	
🔿 Agilent 6200 Series Tir	ne of Flight	
Agilent LC (1100/1120/	(1200/1220/1260/1290) / CE	
	100 100 051 11	
Agilent LC System Acc	ess 192.168.254.11	Device Config
 Agilent LC System Acc Agilent CE System Acc 	Sess 192.168.254.11 Sess 192.168.254.11	Device Config
Agilent LC System Acc Agilent CE System Acc Agilent 35900E A/D Co	isess 192.168.254.11 inverter 192.168.254.13	Device Config
Agilent LC System Acc Agilent CE System Acc Agilent 35900E A/D Co HTC/HTS Autosampler	192.168.254.11 press 192.168.254.11 inverter 192.168.254.13 r 1	Device Config

Figure 18 Instrument Configuration Dialog Box

5 When configuration is completed, click **OK**.

Step 12. Copy the support folder to the computer

In this step, you copy the **\Support** folder from the Data Acquisition installation disk to the **D**:**\MassHunter**\ folder.

- 1 In a Windows Explorer window, open the installation disk drive.
- 2 Right-click the **Support** folder and click **Copy**.
- **3** Right-click the **D**:**MassHunter** folder and click **Paste**.
- 4 In Windows Explorer, right-click the D:\MassHunter\Support folder and click Properties.

s	upport Proper	ties	<u>? X</u>		
	General Shari	ing Security Customize			
		Support			
	Туре:	File Folder			
	Location:	D:\MassHunter			
	Size:	58.1 MB (60,992,589 bytes)			
	Size on disk:	58.4 MB (61,329,408 bytes)			
	Contains:	159 Files, 17 Folders			
	Created:	Today, August 29, 2008, 8:11	1:39 PM		
	Attributes:	Eead-only	A <u>d</u> vanced		
		☐ <u>H</u> idden			

Figure 19 Support Properties dialog box

5 Clear the Read-only check box, and then click Apply.The Confirm Attribute Changes dialog box is displayed.

2 Software Installation and Configuration

Step 12. Copy the support folder to the computer

Confirm Attribute Changes				
You have chosen to make the following attribute changes:				
unset read-only				
Do you want to apply this change to this folder only, or do you want to apply it to all subfolders and files as well? O Apply changes to this folder only O Apply changes to this folder, subfolders and files				
OK Cancel				

Figure 20 Confirm Attribute Changes dialog box

6 Click Apply changes to this folder, subfolders and files, and then click OK.

Step 13. Confirm the LC firmware revision

- **1** Start the Data Acquisition program.
- 2 Click File > Print > Instrument Configuration Report.
- 3 Click Screen.
- 4 Click OK.
- 5 Go to

http://www.chem.agilent.com/_layouts/agilent/downloadFirmware.aspx?w hid=69761 and check that you have the most recent firmware for the K1260 LC instrument.

- **6** If you need to update your LC firmware, follow the instructions on the web site. Make sure you use the latest firmware update tool, as instructed on the web site.
- **7** Check that the firmware for the G1369A Agilent LAN Interface card is the latest version available:
 - **a** Start a Command Prompt in Windows.
 - **b** Type telnet 192.168.254.11 in the Command Prompt window and press **Enter**.
 - c Type / in the Telnet window.

The LAN Interface card displays its current configuration information.

The LAN Interface card requires 1.10 firmware or higher. If an upgrade is needed, please contact your Agilent representative.

Step 14. Finish the installation

1 Create a system recovery disc of your installed system.

Check with your IT department for the appropriate backup procedure.

- **2** Install or enable any other program that you will use with your MassHunter workstation. Refer to the installation guide or quick start guide for these programs.
- **3** Make sure that the trust settings in Excel are set for all MassHunter users, including the guest account that is set up for compliance. See the *Offline Qualitative and Quantitative Analysis Installation Guide* for the K6460 Mass Spectrometer for more information.
- **4** Run the installation program for the K6460 Resource Disc to install the K6460 manuals to your MassHunter Workstation.



6460 Triple Quad Mass Spectrometer (Model K6460) System Installation Guide

3 Installation Completion and System Verification

Step 1. Condition the Agilent LC instrument 44
Step 2. Reset the collision cell gas flow rate 47
Step 3. Prepare the performance evaluation samples 49
Step 4. Set up methods and worklists 50
Step 5. Verify the Triple Quad sensitivity 52

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



Step 1. Condition the Agilent LC instrument

Before you begin, check that you have:

- 18 MΩ, HPLC grade deionized water (p/n 8500-2236)
- high-purity HPLC grade isopropanol
- premixed LC flushing solvent (50:25:15:10 isopropanol/acetonitrile/cyclohexane/dichloromethane) (p/n G1969-85026)
- high-purity HPLC grade acetonitrile (p/n G2453-85050)
- high-purity HPLC grade methanol (p/n 8500-1867)
- high purity formic acid (p/n G2453-85060)
- for 6470/6495: RRHD Zorbax Eclipse Plus C18 trapping column (p/n 959757-302)
- **1** Flush the LC system.

This flushing procedure is very effective at reducing background contaminants from the LC systems when they are interfaced with a mass spectrometer. The flushing procedure must be done for each solvent channel to ensure contaminants are removed from separate degasser and pumping channels.

- 2 Remove any column(s), install a restriction capillary, and bypass the flow cell for the UV detector, unless it is rated for high-pressure (400 bar) operation. Route the outlet capillary to a waste container.
- **3** If required by your degasser model, connect A1/A2 degasser channels in series and B1/B2 degasser channels in series. Use the c-tubes included with the degasser.

Don't try to re-use solvents used for the flushing procedure.

- **4** Use a hand-held controller or the Data Acquisition program to set up the pump module to deliver deionized water for 15 minutes at 3 mL/minute to remove any salt buffers. Do 5 injections with deionized water to clean the injector path and sample loop.
- **5** Set up the pump module to deliver HPLC grade isopropanol for 5 minutes at 3 mL/minute. Do 5 injections with isopropanol to clean the injector path and sample loop.
- **6** Set up the pump module to deliver the premixed LC flushing solvent (50:25:15:10 isopropanol/acetonitrile/cyclohexane/dichloromethane) for 15

minutes at 3 mL/minute. Do 5 injections with the flushing solvent to clean the injector path and sample loop.

Alternatively, while the K6460 Triple Quad MS pumps down, the flushing solvent can be pumped at a low flow rate (e.g. 0.1 mL/minute) overnight.

CAUTION

Make sure that the flushing solvent does not stay in the LC for an extended period of time (for example, several days) because the cyclohexane may be harmful to the pump seals.

- 7 Set up the pump module again to deliver HPLC grade isopropanol for 5 minutes at 3 mL/minute. Do 5 injections with isopropanol to clean the injector path and sample loop.
- 8 If applicable, remove the c-tubes from the degasser channels plumbed in series and reconnect the degasser tubing to the original configuration.
- ${\bf 9}$ Install the column used for installation verification (p/n 959757-902) and wet the column with 100% methanol.

All columns shipped with the K6460 Triple Quad MS are shipped dry. Upon installation, these columns must be primed or wetted with Methanol to properly condition the column.

10 Set up the pump module again to deliver HPLC grade methanol for at least 30 minutes at 0.5 mL/minute. Make sure that the solvent stream selector valve on the K6460 Triple Quad MS is set to waste position or the outlet tubing from the column is *not* connected to the instrument.

If the HPLC Stack has a Thermostatted Column Compartment (TCC), set the temperature of the column compartment to 60°C to reduce the back pressure and to help remove any contaminants on the column.

- **11** For positive mode checkout:
 - **a** For Channel A, install 1 liter of water with 0.1% formic acid.
 - **b** For Channel B, install 1 liter of 100% acetonitrile.

3 Installation Completion and System Verification

Step 1. Condition the Agilent LC instrument

c Do 5 injections with the blank premixed mobile phase (70:30 water: methanol) to clean the injector path and sample loop.

NOTE Up to 0.1 percent formic acid can be added to the solvent that you just prepared to help ionize the reserpine checkout sample. Do not add the formic acid until after you prepare the Reserpine checkout sample.

NOTE

Use solvents that are at a minimum HPLC grade. Solvents that are acceptable for most LC applications may contain high levels of background that are detectable by the more sensitive LC/MS instrument. LC solvents used with the LC/MS instrument should be rated for both HPLC and pesticide, environmental, or GC/MS analyses. Use the highest purity solvents you can obtain. Acceptability of solvents must be empirically determined.

12 Autotune the LC/MS in both Positive and Negative Ion Polarities after the system has reached equilibration (approximately 11 hours after initial pumpdown) and the Quadrupole Frequencies have been adjusted.

The factory provided instrument disc contains an Autotune file that can be copied to the MassHunter tune folder for the configured model: D:\MassHunter\Tune\QQQ\model

Step 2. Reset the collision cell gas flow rate

Most parameters such as the collision cell gas flow rate work with values set at the factory. In case the default flow rate does not give a high vacuum reading in the acceptable range, follow the steps in this topic to:

- Determine the optimal flow rate (DAC steps) to achieve the correct high vacuum gauge reading.
- Enter this value into the SmartCard using the "back door" command.

High Vacuum measurements with Collision Cell gas turned off can vary depending upon how long ago the LC/MS instrument was pumped down.

For best results, allow the instrument to pump overnight at Autotune settings, but with Collision Cell gas turned OFF, before taking the High Vacuum measurement.

Acceptable ranges are listed in Table 1.

Model	Rough Vacuum	High Vacuum (CC Gas OFF)	High Vacuum (CC Gas ON)
K6460	1.8 to 2.2 Torr	2.0 to 5.0 × 10 ⁻⁶ Torr	$2.0 \text{ to } 3.0 \times 10^{-5} \text{ Torr}$

Table 1Acceptable vacuum ranges

- **1** Determine the optimal Flow Rate:
 - a Open a Command Prompt window (click **Start > Run**, type cmd and click **OK**).
 - **b** Type telnet 192.168.254.12 5123 to open a "back door" into the Triple Quad's MS Interface Card firmware.
 - c Press Enter.

NOTE

- **d** Find the high vacuum gauge reading in the **Cell** tab of the Manual Tune program.
- **e** Type getccgasflow and press **Enter** to get the current value of the collision cell gas flow DAC.

3 Installation Completion and System Verification

Step 2. Reset the collision cell gas flow rate

f Use the setccgasflow command to adjust the Collision Cell DAC value in iterative steps until the **High Vaccum** reading on the instrument is within the acceptable range.

Typical values are between 550 to 650. As a guideline, adjust collision cell gas flow by 5 or 10 units at a time.

The target High Vaccuum Pressure with CC Gas on is 2.0 x 10-5 Torr.

Wait 20 to 30 seconds for the collision cell pressure and gas flow to stabilize after each adjustment.

g Close the Command Prompt window:

>bye

NOTE

Step 3. Prepare the performance evaluation samples

In this step, you dilute the supplied performance evaluation sample (reserpine) to the concentrations needed for the Triple Quad system checkout.

Use the diluted samples within a day of dilution. Refrigerate the intermediate (first) dilution in the supplied bottle.

- Always rinse the graduated pipettes and volumetric flasks thoroughly with deionized water before and between each use.
- Use polypropylene labware for preparing performance evaluation samples, since glass vessels introduce unacceptable levels of sodium.
- Always rinse the autosampler vials and caps with the solvent mix used for sample dilution before filling them with the performance verification samples. This minimizes any background that can be contributed by the vials and caps. The vials may be run uncapped if the septa are found to be a source of background contamination.

Required Parts • 1 mL graduated pipette (p/n 9301-1423)

- 2 × 100 mL volumetric flasks (p/n 9301-1344)
- ES/APCI Positive Ion Performance Standard (p/n G2423A)
- Plastic bottle for storing first dilution (p/n 9301-1433)
- 1 Prepare 2 liters of a 60:40 mixture of acetonitrile:water w/ 0.1% formic acid.
- **2** Prepare the first dilution (50 pg/ μ L) reserpine:
 - **a** Use a clean graduated pipette to transfer 1.0 mL of the 5 ng/μL reserpine (p/n G2423A) standard to a pre-rinsed 100 mL volumetric flask.
 - **b** Dilute to the 100 mL mark with the 60:40 mixture of acetonitrile:water w/0.1% formic acid solution that was prepared in step 1. Invert the flask at least 10 times to ensure proper mixing of the checkout sample.
 - **c** Use 5 to 10 mL of this solution to rinse one of the plastic storage bottles and fill it with the remaining solution.
 - d Label this bottle "50 pg/µL reserpine" along with the preparation date.
- **3** Prepare the second dilution (500 fg/ μ L) reserpine:
 - **a** a Use a clean graduated pipette to transfer 2 mL of the 100 pg/ μ L reserpine dilution to a pre-rinsed 100 mL volumetric flask.
 - ${\bm b}~$ Dilute to the 100 mL mark with the 60:40 mixture of acetonitrile:water w/~0.1% formic acid solution.

Step 4. Set up methods and worklists

- **c** Use 5 to 10 mL of this solution to rinse one of the plastic storage bottles and fill it with the remaining solution.
- **d** Label this bottle "1 pg/ μ L reserpine" along with the preparation date.
- 4 Refrigerate this solution and use on the day it is prepared

This provides 1 pg reserpine amount that is needed for performance verification.

Step 4. Set up methods and worklists

Before you begin, copy the methods and worklists according to your instrument model.

The methods are the same for each performance verification, regardless of whether a standard installation checkout or Marketing Bid Specification checkout is done.

For the appropriate method and worklist for your instrument, see Table 2, "Checkout methods and worklists," on page 51.

Positive ion mode checkout conditions are found in "Positive Ion Mode Checkout Conditions" on page 72.

- 1 Click **Method > Open** and then load the appropriate MRM method. Change the method as needed to match the values found in "Positive Ion Mode Checkout Conditions" on page 72, and then save the method.
- 2 Click **Method** > **Open** and then load the appropriate scan method. Change the method as needed to match the values found in "Positive Ion Mode Checkout Conditions" on page 72, and then save the method.
- **3** Put the vials into the LC autosampler:
 - Position #1: An empty, uncapped vial
 - Position #2: A vial that contains the solvent used for dilution (solvent blank)
 - Position #3: A vial that contains the checkout sample $(500 \text{ fg}/\mu\text{L})$
- 4 Click Worklist > Open, and then open the appropriate worklist.

The worklist is set up to:

- Do one injection of the solvent blank with the scan method to collect background ion data.
- Use the MRM method for the remaining runs to do:
 - one injection of the empty vial
 - five injections of the solvent blank
 - five injections of the checkout sample

Table 2 Checkout methods and worklists

Source	Mode	Positive Ion Mode Installation Checkout
AJS	Scan Method	6460 ESI_AJT Pos MS2 Scan Grad.m
	MRM Method	6460 ESI_AJT Pos MRM Checkout Grad.m
	Worklist	6460 ESI_AJT Pos MRM Checkout Grad.wkl
ESI	Scan Method	6460 ESI Pos MS2 Scan Grad.m
	MRM Method	6460 ESI Pos MRM Checkout Grad.m
	Worklist	6460 ESI Pos MRM Checkout Grad.wkl

Step 5. Verify the Triple Quad sensitivity

The Performance Specification Services (G6061A and G6067A) can be purchased only at the time of original Agilent 6460 Triple Quad Mass Spectrometer (Model K6460) System bundle purchase.

• For standard Marketing Bid Specification Services (G6061A for Positive Ion Mode), the same checkout conditions as the installation checkout methods are used.

	Sample Name	Sample Position	Data File	Sample Type	Level Name	lnj Vol (μl)	Comment
1	Background Scan	Vial 2	D:\MassHunter\Data\Checkout\6460\BackgroundScan001.d	Blank		1	
2	Air Blank	Vial 1	D:\MassHunter\Data\Checkout\6460\AirBlank001.d	Blank		1	
3	Solvent Blank	Vial 2	D:\MassHunter\Data\Checkout\6460\SolventBlank001.d	Blank		1	
4	Solvent Blank	Vial 2	D:\MassHunter\Data\Checkout\6460\SolventBlank002.d	Blank		1	
5	Solvent Blank	Vial 2	D:\MassHunter\Data\Checkout\6460\SolventBlank003.d	Blank		1	
6	Solvent Blank	Vial 2	D:\MassHunter\Data\Checkout\6460\SolventBlank004.d	Blank		1	
7	Solvent Blank	Vial 2	D:\MassHunter\Data\Checkout\6460\SolventBlank005.d	Blank		1	
8	Reserpine 500 fg	Vial 3	D:\MassHunter\Data\Checkout\6460\ReserpineCheckout001	Sample		1	
9	Reserpine 500 fg	Vial 3	D:\MassHunter\Data\Checkout\6460\ReserpineCheckout002	Sample		1	
10>	Reservine 500 fg	Vial 3	D\MassHunter\Data\Checkout\6460\ReserpineCheckout003	Sample		1	
11	Reservine 500 fg	Vial 3	D:\MassHunter\Data\Checkout\6460\ReserpineCheckout004	Sample		1	
12		Vial 3	D:\MassHunter\Data\Checkout\6460\ReserpineCheckout005	Sample		1	
			Worklist				
			T OKIIN				

Figure 21 Reserpine checkout worklist

- 1 Review the worklist to be sure that the method and data paths are correct. Check that the data file names given in the worklist are unique and have not already been acquired.
- 2 Run the Positive Ion Mode checkout worklist.
 - a Run the appropriate Positive Ion Mode checkout worklist.
 - **b** Load each solvent blank and reserpine peak into the Qualitative Analysis program.
 - **c** Generate Extracted Ion Chromatograms of the ion product (195.10 m/z for Positive Ion Mode).

Installation Completion and System Verification 3

Step 5. Verify the Triple Quad sensitivity

Extract Chromatograms	
Extract Chromatograms List of opened data files 6495 Pos MRM Checkout_016	Type: MRM Integrate when extracted MS Chromatogram Advanced Excluded Masses MS level: MS/MS Polarity: Positivi Scans: Multiple reaction monitor Transition: 509 3000>195 1000
< <u> </u>	OK Cancel

Figure 22 Extract Chromatogram dialog box for Reserpine (Positive mode)

d Smooth the extracted chromatogram by setting **Smoothing Function** to **Quadratic/Cubic Savitzky-Golay**, and **Function width** to **9** points.

noothing function:	Quadratic/Cub	ic Savitzky-Go
unction width:	9	points
Gaussian width:	5.000	points

e Integrate each reserpine peak, and click **Calculate Signal to Noise**. Use the **General** integrator.

3 Installation Completion and System Verification

Step 5. Verify the Triple Quad sensitivity

nitegrator Su	itability Peak Filt	ers Results		
Seneral				_ ▼ <u>A</u>
otions				
Detector Point samplin	g: 1	Start thres	nold: 0	.200
Smoothin	Ig	Stop thresh	nold:	0.0
Filtering:	5 point 👻	Peak locat	ion: Top	-
Baseline alloc	ation			
Baseline rese	et >	5		
lf either edge	<	100 %		
then:	Orop else ta	ngent skim		
	Tangent skir	m else drop		

f Calculate the signal-to-noise using **Height**.

g For standard sensitivity verification, or performed under standard Marketing Bid Specification Service:

Under Noise Measurement, for **Noise definition**, select **Auto-RMS** (available in MassHunter Qualitative Analysis B.05.00 and higher).

Set the **Noise region boundary** to **Start time 0 minute** and **End time 1 minute**. Make sure that the noise region does not include the chloramphenicol peak (or reserpine peak for Positive Ion Mode).

Set the Noise region width to 0.075.

oise measurement			
loise definition: Au	to-RMS	-	X 1
loise region boundary			
Start time	0.000	min	
End time	1.000	min	
Noise region width	0.075	🔺 min	
	to when chrometo	areme ero	integrated

- Figure 23 Calculate Signal-to-Noise dialog box (for an installation checkout or standard marketing Bid Specification Service checkout), shown with Noise region width of 0.075.
- **3** Generate a printout of each signal-to-noise calculation report for each solvent blank and sample injection. Include the chromatogram in the printout.
- 4 Open the Excel spreadsheet D:\MassHunter\Support\Checkout\Sensitivity Checkout Report.xlsx. Fill in the values to calculate the average signal to noise and save the spreadsheet.

The average signal-to-noise must be greater than that listed in these tables, depending on the checkout type. See Table 3 on page 57.

3 Installation Completion and System Verification

Step 5. Verify the Triple Quad sensitivity

- **5** Generate a printout of the Excel signal-to-noise report.
- **6** Change solvents (to A = water w/0.1% formic acid and B = acetonitrile for Positive Ion Polarity).
- 7 Clean the injectors. See step 11 on page 45.
- 8 Equilibrate the column for 1 hour at 30:70 A:B.

		6400 Series Q	QQ LC/M	S Sensitivity Check	out Report
Seri	al Number:	SG14497326		Paramet	ers
	Model:	G6460C			
lo	on Polarity:	Positive		Compound	Reserpine
Chec	kout Type:	Installation		Amount Injected, pg	1
	Test Date:	05/07/2015		Sensitivity Specification	5000
				(1 pg on-column, Auto-RMS,	0.1 min noise)
			Signal-to- Noise		
-	Injection #	Compound	(Height)		
_	1	Blank	0.03		
-	2	Blank	0.05		
_	3	Blank	0.06		
-	4	Blank	0.06		
•	5	Blank	0.02		
A	verage	Dialik	0.044		
			Signal-to- Noise		
	Injection #	Compound	(Height)	Peak Area	Peak Height
	1	Reserpine	20305.1	2147	1235
	2	Reserpine	23691.6	2181	1245
	3	Reserpine	27316.6	2222	1258
	4	Reserpine	22582.4	2217	1265
	5	Reserpine	24384.3	2314	1318
A	verage	Reserpine	23656	2216.2	1264.2
				62.5035999	32.22886905
				2.82%	2.55%
	Avera	ge Signal-to-Noise:	23656:1	(blank subtracted)	
		Result:	PASS		
					Revision: B.07.00

Figure 24 Example of a Positive mode signal-to-noise report.

Mode	G1948B Electrospray	Agilent Jet Stream
Sensitivity Performance	5,000:1 (Auto-RMS,1 pg)	15,000:1 (Auto-RMS,1 pg)
G6061A Marketing Bid Sensitivity Performance	10,000:1 (Auto-RMS, 1 pg)	30,000:1 (Auto-RMS,1 pg)

 Table 3
 K6460 Positive Mode Specifications

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4

6460 Triple Quad Mass Spectrometer (Model K6460) System Installation Guide

Installation and Verification of the G1947B APCI Source

To install the G1947B APCI source 60 To verify the operation of the G1947B APCI source 61

This chapter contains the steps needed to install and verify the operation of the APCI source.

If the APCI source was purchased with the K6460 Triple Quad MS, you will need to install the source and verify its operation.

You can complete only a check tune with the different source types: G1948B and G1978B. Make sure you use the correct tune calibrant.



To install the G1947B APCI source

- **1** Install these parts from the APCI enablement kits that ship with the G1947B APCI source into the Aux module on the K6460 Triple Quad MS:
 - APCI High Voltage Power Supply (p/n G1946-80058)
- **2** Pour the Electrospray calibrant back into its original bottle or another suitable container, rinse the calibrant bottle with acetonitrile, pour the APCI calibrant into the calibrant bottle, and attach the calibrant bottle back onto the CDS.
- **3** Remove the electrospray source and install the APCI source:
 - **a** Put the nebulizer into the nebulizer adjustment fixture that is supplied in the shipping kit. Check that the nebulizer needle is properly adjusted. Make sure that the nebulizer needle is even with the end of the nebulizer nozzle.
 - **b** Install the nebulizer in the spray chamber.

WARNING Surfaces can be extremely hot. Let the instrument surfaces cool before you touch them.

- **c** Remove the previously installed spray chamber. Install the standard spray shield if not already installed.
- **d** Orient the standard spray shield so the off-axis hole is at the 12 o'clock position by loosening the two T10 screws that secure the end plate, orienting the spray shield, and re-tightening the two T10 screws (do not over-tighten).
- **e** Install the APCI spray chamber on the spray chamber mount, close the spray chamber, and fasten the latch. If needed, adjust the latch to ensure that the O-ring seals completely. Use a $\frac{1}{4}$ -inch × $\frac{5}{16}$ -inch wrench to loosen the lock nut, adjust the latch to the proper fit, and then tighten the lock nut so that the latch maintains its adjustment.
- **f** Connect the APCI corona and vaporizer heater cables to the connector on the left side panel of the instrument.
- **g** Connect the 1/8-inch nebulizing gas tubing from the LC/MS mainframe to the nebulizer gas fitting.
- **h** Connect the PEEK tubing from the selection valve (inside the front cover) to the top of the nebulizer.

To verify the operation of the G1947B APCI source

There is no sensitivity checkout with the G1947B APCI source on the K6460 Triple Quad MS. To verify its proper operation, run a manual tune with the G2432A APCI/APPI Calibration Solution.

Note that Auto Tune is not supported with this source.

- 1 Install the G2432A APCI/APPI Calibration Solution.
- **2** Check the tuning of the APCI source:
 - a In Data Acquisition program, set Context to Tune.
 - **b** Open the auto tune file that was generated with the electrospray source.
 - **c** In the **Manual Tune** tab, mark the **Calibrant on** check box, and then acquire the data.
 - **d** Verify that the masses in the **MS1** and **MS2** tabs are correct for the loaded source before you manually tune the peaks.
 - **e** Verify that you have sufficient abundance for the tune peaks, that the tune peaks have peak widths of 0.7 ± 0.05 amu, and that mass assignments are within ± 0.15 amu of the target mass assignments.

If needed, click **Adjust Gain & Offset** to establish the Mass Axis and Peak Width values. Repeat these for both MS1 and MS2 tabs.

3 Save the tune file.

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6460 Triple Quad Mass Spectrometer (Model K6460) System Installation Guide

Other Setup Tasks

5

To start the Data Acquisition program 64 To stop MassHunter Engines 64 To stop MassHunter processes in case of unrecoverable errors 65 To view the log book 65 To configure the network interface card 66 To remove the MassHunter Workstation software 67 To reconfigure the instrument 68

This chapter contains tasks that are related to setting up your K6460 Triple Quad MS.

For complete information on using the your K6460 Triple Quad MS, refer to the list of resources found in the *Quick Start Guide*.



To start the Data Acquisition program

To start the Data Acquisition program

You can start the Data Acquisition program in one of two ways:

- Double-click the **Data Acquisition** icon in the Agilent MassHunter program group, or
- Click Start > Programs > Agilent > MassHunter Workstation > Data Acquisition.

CAUTION

Do not start Data Acquisition as administrator. (*Do not* right-click **Data Acquisition** and select **Run as administrator**.)

To stop MassHunter Engines

- **1** Close the **Data Acquisition** program.
- 2 Right-click the **Engine Launcher** icon in the system tray.
- **3** Click **Shutdown Engines** to stop the engines.

To start the MassHunter Engines, restart the Data Acquisition program. Alternatively, to start the MassHunter Engines without starting the Data Acquisition program, click **Start Engines**.

To stop MassHunter processes in case of unrecoverable errors

When you stop MassHunter processes, loss of data can occur.

- 1 Click Programs > Agilent > MassHunter Workstation > Acq Tools > Remove MassHunter Processes.
- **2** Click **Yes** when you are asked whether you want to remove all MassHunter processes.

Only the Data Acquisition processes are stopped.

To view the log book

 Double-click the Acq System Logbook icon in the Agilent MassHunter program group, or click Start > Programs > Agilent > MassHunter Workstation> Acq System Logbook.

You can also start the Logbook Viewer program within the MassHunter Data Acquisition program.

To configure the network interface card

To configure the network interface card

The computer that is shipped with the K6460 Triple Quad MS is equipped with two network cards (LAN-cards). The first LAN-card is for connection to the "house network" (via 10/100/1000 Base-T network card). The IP address for this card can either be "static" or dynamically assigned (e.g. obtained by a DHCP server). By default, TCP/IP is configured as the network protocol for this card, which is built-in to the PC.

The second LAN-card (in slot #1) is dedicated for instrument communication with the K6460 Triple Quad MS and the Agilent 1100/1200 Series LC system. *This network card should NOT be connected to the site LAN.*

To verify is the Instrument LAN network card settings are correct, follow these steps.

- 1 Click Start > Settings > Control Panel.
- 2 Double-click Network Connections.
- **3** Right-click the icon for the network card for the house LAN, click **Properties**, and then configure the network card as needed.

Because this network card is independent from the card used for instrument control, it may be configured using a static IP address or using a DHCP server.

- **4** Right-click the icon for the network card for the K6460 Triple Quad MS, click **Properties**, and then check that these parameters are set:
 - Subnet Mask 255.255.255.0
 - Gateway leave blank

NOTE

Because network configurations vary widely from site to site, get assistance from an IT representative when you connect to the site network. Configuration by an Agilent Customer Engineer is on a best-effort basis only.

To remove the MassHunter Workstation software

- 1 If you have any data, methods, libraries, or other files or directories that you want to save, and then move or copy them to a folder outside of those to be deleted.
- **2** Close all MassHunter Workstation programs, including the Data Acquisition, Qualitative Analysis and Quantitative Analysis programs.
- 3 Click Start > Control Panel > Programs and Features.
- **4** Remove these programs:
 - Agilent MassHunter Workstation Data Acquisition
 - Agilent MassHunter Workstation Qualitative Analysis
 - Agilent MassHunter Workstation Quantitative Analysis
 - Agilent MassHunter Workstation Quantitative Analysis Reporting
- **5** Close *all* applications.
- 6 Reboot the computer. You are now ready to install new software.

To reconfigure the instrument

If you have more than one stack of HPLC modules from which to choose, or a new supported LC module is installed, the Instrument Configuration registry must be cleared for MassHunter Workstation.

- 1 Put the K6460 Triple Quad MS into standby mode.
- 2 Close the MassHunter Acquisition program.
- **3** Stop MassHunter processes.

See "To stop MassHunter processes in case of unrecoverable errors" on page 65.

- 4 Start the Instrument Configuration program (**Programs > Agilent >** MassHunter Workstation > Acq Tools > Instrument Configuration).
- **5** Mark the **Mass Spectrometer** check box, and then click the K6460 Triple Quad MS. Leave all other check boxes cleared.

Instrument Configuration		
Instrument name:	Instrument 1	
Mass Spectrometer		
Agilent 6400 Series Triple Quadrupole		192.168.254.12
O Agilent 6500 Series Quadrupole Time of Flight		
Agilent 6200 Series Time of	f Flight	
Agilent LC (1100/1200/1260)/1290) / CE	
Agilent LC System Access	192.168.254.11	Device Config
O Agilent CE System Access	192.168.254.11	
Agilent 35900E A/D Conver	ter	192.168.254.13
HTC/HTS Autosampler		1
		OK Cancel

Figure 25 Instrument Configuration

6 Click OK.

- **7** Start the MassHunter Workstation Acquisition program and confirm that only the MS instrument is available.
- 8 Close the Data Acquisition program.
- **9** Stop MassHunter processes.
- **10** Open Instrument Configuration again.
- 11 Click the K6460 Triple Quad MS and mark the Agilent LC (1100, 1120, 1200, 1220, 1260, 1290)/CE check box.

Agilent LC System Access	192.168.294.11	Device Config
) Agilent CE System Access	192.168.254.11	
		_
Agilent 35900E A/D Converter	192.168.254.13	
HTC/HTS Autosampler	1	Device Config
SFC	1	Device Config
	·	

Figure 26 Instrument Configuration dialog box

12 Click OK.

The registry has now been cleared and configured for any new LC module(s).

Additional configuration steps may be required to set up LC devices.

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This chapter contains acquisition parameters for the checkout methods.

For a list of the checkout methods for each instrument, see Table 2, "Checkout methods and worklists," on page 51.



6 Reference

Positive Ion Mode Checkout Conditions

Positive Ion Mode Checkout Conditions

These conditions are used in a Positive Ion Mode checkout.

Time	%A (water w/0.1% formic acid)	%B (acetonitrile w/0.1% formic acid)	Flow
Initial	90	10	0.4 mL/min
0.1	90	10	0.4 mL/min
1	2	98	0.4 mL/min
4	2	98	0.4 mL/min
4.1	90	10	0.4 mL/min
5	Stop		

Table 4HPLC Pump

Post time of 3 minutes.

Table 5 HPLC Autosampler

Injection volume	1 μL
Autosampler temperature	4°C
Needle wash flushport	70:30 methanol:water
Needle wash location	Flushport, 3 seconds
6

Positive Ion Mode Checkout Conditions

	ESI	AJS
Gas Temp	350°C	325°C
Gas Flow	10 L/min	10 L/min
Nebulizer	60 psi	20 psi
Sheath Gas Temp		400°C
Sheath Gas Flow		12 L/min
Nozzle Voltage		0 V

Table 6Source parameters

Table 7MS parameters

	ESI	AJS	
Capillary	4000 V	4000 V	
Collision Energy	41 V	41 V	
Fragmentor	150 V	150 V	
Accelerator voltage	7 V	7 V	
Delta EMV	200 V	200 V	
Time Filtering	0.03 min	0.03 min	
Compound	Reserpine	Reserpine	
Scan	MRM	MRM	
MS1 Res	Unit	Unit	
MS2 Res	Unit	Unit	
Precursor Ion	609.3 m/z	609.3 m/z	
Product Ion	195.1 m/z	195.1 m/z	
Dwell	200 ms	200 ms	
Low Pressure Funnel RF			
High Pressure Funnel RF			

6 Reference

Positive Ion Mode Checkout Conditions

	ESI	AJS
Sample (stock)	Reserpine, 5 ng/µL	Reserpine, 5 ng/µL
Concentration after dilution	1 pg/µL	1 pg/µL
Dilution solvent	60:40 aceonitrile w/ 0.1% formic acid: water w/ 0.1% formic acid	60:40 aceonitrile w/ 0.1% formic acid: water w/ 0.1% formic acid
Total sample amount injected on column	1 pg	1 pg
Sample order number (p/n)	G2423A	G2423A

Table 7 MS parameters (continued)

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In This Book

This book contains installation, configuration, verification, and start-up tasks to operate your Agilent 6460 Triple Quad Mass Spectrometer (Model K6460) System.

For In Vitro Diagnostic Use

The K6460 mass spectrometer is intended to be used to identify inorganic or organic compounds in human specimens by ionizing the compounds and separating the resulting ions by means of electrical field according to their mass.

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