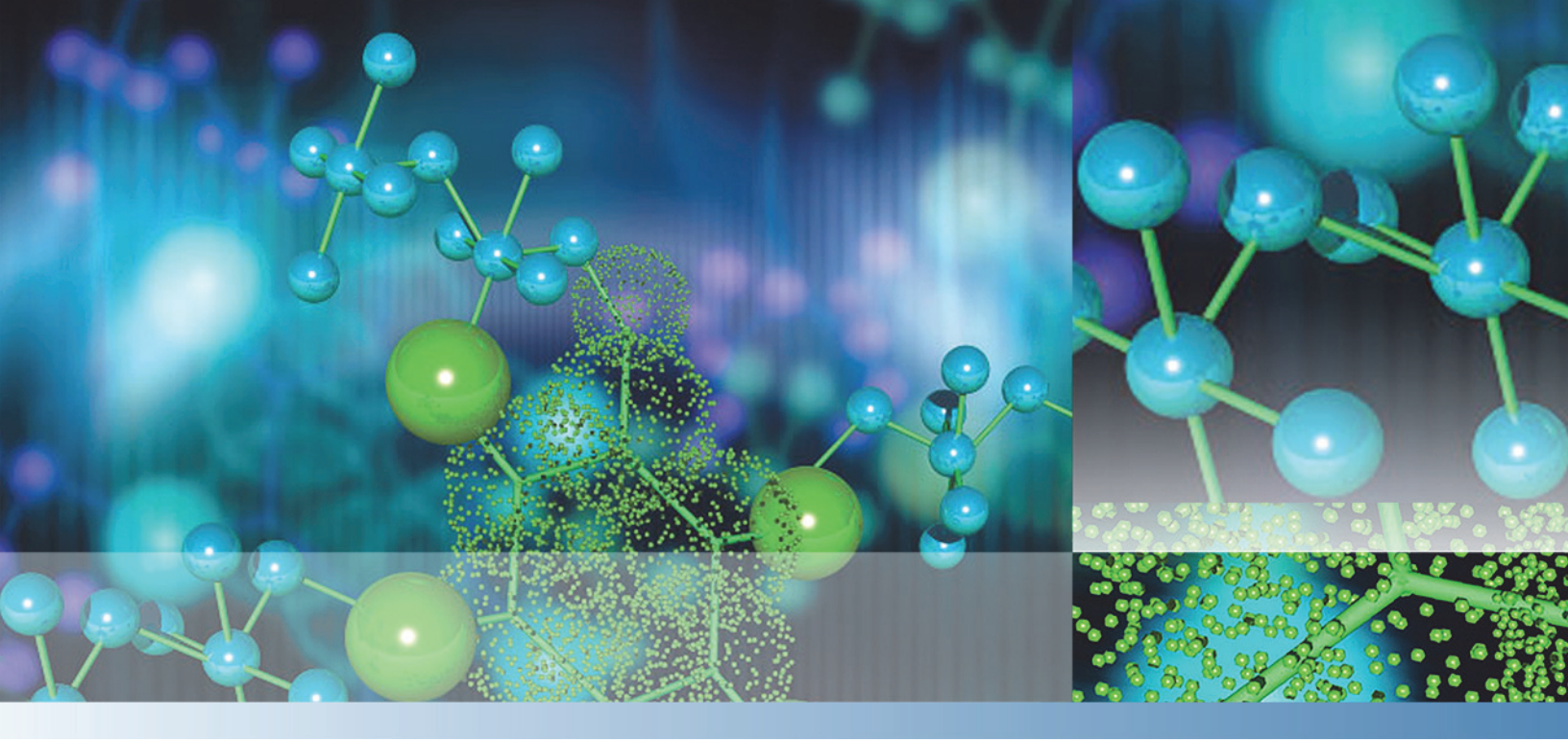

LCQ Fleet

Getting Connected Guide

97055-97224 Revision A September 2015

DOCUMENTATION SURVEY

Thermo SCIENTIFIC

Release history: Rev A, September 2015

Software version: Microsoft Windows 7 Professional (32-bit and 64-bit) SP1—Thermo Foundation 2.0 and later, and Thermo Xcalibur 2.2 and later; Windows XP Workstation SP3—Foundation 1.0.2 SP2 or earlier, and Xcalibur 2.1 SP1 or earlier; Thermo LTQ Tune Plus 2.7.0 and later

For Research Use Only. Not for use in diagnostic procedures.

Regulatory Compliance

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Changes that you make to your system may void compliance with one or more of these EMC and safety standards. Changes to your system include replacing a part or adding components, options, or peripherals not specifically authorized and qualified by Thermo Fisher Scientific. To ensure continued compliance with EMC and safety standards, replacement parts and additional components, options, and peripherals must be ordered from Thermo Fisher Scientific or one of its authorized representatives.

EMC Directive 2004/108/EC

EMC compliance has been evaluated by TUV Rheinland of North America.

- CFR 47, FCC Part 15, Subpart B, Class A: 2015
- CISPR 11: 2009 + A1
- ICES-003: 2014
- EN 55011: 2009 + A1
- EN 61326-1: 2013
- EN 61000-3- 2: 2006 + A1 + A2
- EN 61000-3-3: 2008
- EN 61000-4-2: 2009
- EN 61000-4-3: 2006 + A1 + A2
- EN 61000-4-4: 2004 + A1
- EN 61000-4-5: 2006
- EN 61000-4-6: 2009
- EN 61000-4-11: 2004

Low Voltage Safety Compliance

This device complies with Low Voltage Directive 2006/95/EC and harmonized standard IEC/EN/CSA/UL 61010-1, Third Edition.

FCC Compliance Statement

THIS DEVICE COMPLIES WITH PART 15 OF THE FCC RULES. OPERATION IS SUBJECT TO THE FOLLOWING TWO CONDITIONS: (1) THIS DEVICE MAY NOT CAUSE HARMFUL INTERFERENCE, AND (2) THIS DEVICE MUST ACCEPT ANY INTERFERENCE RECEIVED, INCLUDING INTERFERENCE THAT MAY CAUSE UNDESIRED OPERATION.

CAUTION Read and understand the various precautionary notes, signs, and symbols contained inside this manual pertaining to the safe use and operation of this product before using the device.

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2012/19/EU

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- Number of product pieces, and the estimated total weight and volume
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- Appropriate pick-up time
- Declaration of decontamination, stating that all hazardous fluids or material have been removed from the product

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Preface

The *LCQ Fleet Getting Connected Guide* describes how to connect the Thermo Scientific™ LCQ™ Fleet™ mass spectrometer (MS) to line power (ac mains power system), the data system computer, the external vacuum system, the waste exhaust system, and external peripheral devices. External devices include those that are controlled from or are independent of Thermo mass spectrometry applications, such as the Thermo Xcalibur™ data system.

Contents

❖ **To suggest changes to the documentation or to the Help**

Complete a brief survey about this document by clicking the button below. Thank you in advance for your help.

Related Documentation

The LCQ Fleet mass spectrometer includes complete documentation. In addition to this guide, you can also access the following documents as PDF files from the data system computer:

- *LCQ Fleet Preinstallation Requirements Guide*
- *LCQ Fleet Getting Started Guide*
- *LCQ Fleet Hardware Manual*

- *Ion Max and Ion Max-S API Source Hardware Manual*
- *Safety and Regulatory Guide*

  The LCQ Fleet also ships with a printed copy of the *Safety and Regulatory Guide*. This guide contains important safety information about Thermo Scientific liquid chromatography (LC) and mass spectrometry (MS) systems. Make sure that all lab personnel have read and have access to this document.

❖ To view the product manuals

From the Microsoft™ Windows™ taskbar, choose **Start > All Programs > Thermo Instruments > Manuals > LCQ Fleet**, and then open the PDF file to view it.

❖ To view the data system Help

- From the application window, choose **Help** from the menu bar.
- If information about setting parameters is available for a specific view, page, or dialog box, click **Help** or press the F1 key for information about setting parameters.

❖ To download user documentation from the Thermo Scientific website

1. Go to www.thermoscientific.com.
2. In the Search box, type the product name and press ENTER.
3. In the left pane, select **Documents & Videos**, and then under Refine By Category, click **Operations and Maintenance**.
4. (Optional) Narrow the search results or modify the display as applicable:
   - For all related user manuals and quick references, click **Operator Manuals**.
   - For installation and preinstallation requirements guides, click **Installation Instructions**.
   - For documents translated into a specific language, use the Refine By Language feature.
   - Use the Sort By options or the Refine Your Search box (above the search results display).
5. Download the document as follows:
   a. Click the document title or click **Download** to open the file.
   b. Save the file.

Cautions and Special Notices

Make sure you follow the cautions and special notices presented in this guide. Cautions and special notices appear in boxes; those concerning safety or possible system damage also have corresponding caution symbols.

This guide uses the following types of cautions and special notices.

CAUTION Highlights hazards to humans, property, or the environment. Each CAUTION notice is accompanied by an appropriate CAUTION symbol.

IMPORTANT Highlights information necessary to prevent damage to software, loss of data, or invalid test results; or might contain information that is critical for optimal performance of the system.

Note Highlights information of general interest.

Tip Highlights helpful information that can make a task easier.

The *LCQ Fleet Getting Connected Guide* contains the following caution-specific symbols (Table 1).

Table 1. Caution-specific symbols and their meaning (Sheet 1 of 2)

Symbol	Meaning
	**Chemical hazard:** Observe Good Laboratory Practices (GLP) when handling chemicals. Only work with volatile chemicals under a fume or exhaust hood.Wear gloves and other protective equipment, as appropriate, when handling toxic, carcinogenic, mutagenic, corrosive, or irritant chemicals. Use approved containers and proper procedures to dispose of waste oil and when handling wetted parts of the instrument.
	**Risk of eye injury:** Eye injury could occur from splattered chemicals or airborne particles. Wear safety glasses when handling chemicals or servicing the instrument.

Table 1. Caution-specific symbols and their meaning (Sheet 2 of 2)

Symbol	Meaning
	**Hot surface:** Allow heated components to cool before touching or servicing the instrument.
	**Sharp object:** Avoid handling the tip of the syringe needle.
	**Trip obstacle:** Be aware of cords, hoses, or other objects located on the floor.

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	us.customer-support.analyze@thermofisher.com	us.techsupport.analyze@thermofisher.com

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- Send an email message to Technical Publications (techpubs-lcms@thermofisher.com).
- Complete a survey at www.surveymonkey.com/s/PQM6P62.

1

Setting Up the Mass Spectrometer

This chapter describes how to connect the LCQ Fleet mass spectrometer to the gas supplies, vacuum system, data system computer, and line power (ac mains power system).

Note

- A Thermo Fisher Scientific field service engineer must install the mass spectrometer.
- The Glossary defines some of the terms used in this guide.
- For instructions about setting up the application parameters for tuning, calibrating, and testing, refer to the *LCQ Fleet Getting Started Guide*.

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Connecting the Gas Supplies

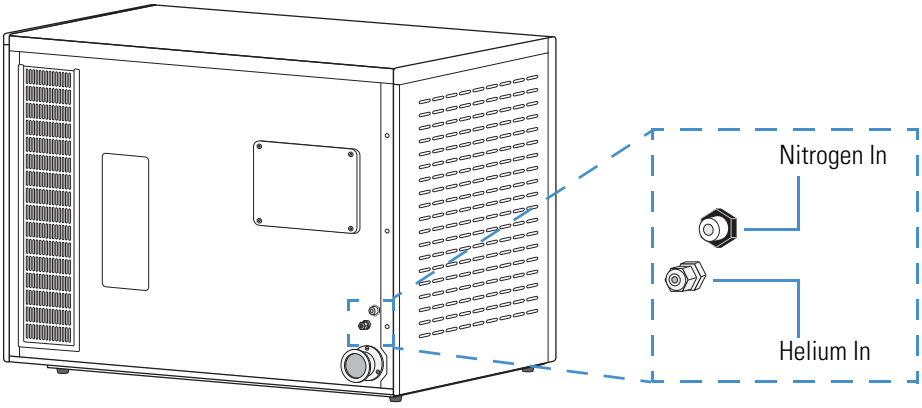
Table 2 lists the required gases and specifies their function.

Table 2. Summary of required gas types

Gas type	Gas function
Helium: • Ultra high purity (UHP), 99.999% • 275 ±70 kPa (40 ±10 psi)	collision gas and damping gas
Nitrogen: • High purity (HP), 99% • 690 ±140 kPa (100 ±20 psi)	auxiliary gas, collision gas, sheath gas, and sweep gas

Figure 1 shows the location of the gas inlets on the back of the instrument.

Figure 1. Gas connections on the back of the LCQ Fleet MS



Note

- Make sure that the lab already has the gas supply lines installed, properly terminated, and ready to connect to the MS. For information about the gas supply lines, refer to the *LCQ Fleet Preinstallation Requirements Guide*.
- If your system includes additional devices that require their own gas connections, refer to the connection instructions in the appropriate manuals for those devices.

Fittings, Parts, and Tools

Table 3 lists the parts required to connect the LCQ Fleet MS to the gas delivery system. Connections and gas delivery systems might vary. You are responsible for supplying any additional fittings or connections necessary during installation.

The following kits that shipped with the instrument contain the tubings and fittings listed in Table 3:

- MS Setup Kit (P/N 70111-62033)
- MS Accessory Kit (P/N 97055-62055)
- Special Accessory Kit for the LCQ Fleet (P/N 97055-62060)

Table 3. Shipped gas plumbing hardware

Gas type	Part description	Part number
Helium	Ferrule, two-piece set, brass, 1/8 in. ID	00101-02500 (back) 00101-08500 (front)
	Swagelok™-type nut, brass, 1/8 in. ID	00101-15500
	Tubing, copper, pre-cleaned, 1/8 in. OD, 3 m (10 ft) long You might need an additional length of tubing for the installation.	00301-22701
	Connection for the other end of the tubing to the helium gas source	–[a]
Nitrogen, HP	Ferrule, two-piece set, brass, 1/4 in. ID	00101-04000 (back) 00101-10000 (front)
	Swagelok-type nut, brass, 1/4 in. ID	00101-12500
	Tubing, Teflon™ PFA, 1/4 in. OD, 4.6 m (15 ft) long You might need an additional length of tubing for the installation.	00101-50100
	Connection for the other end of the tubing to the nitrogen gas source	–[a]

[a] Customer-supplied item

Connecting the Helium Gas Supply

The helium gas must be UHP (99.999%) with less than 1.0 ppm each of total hydrocarbons, oxygen, and water. The required gas pressure is 275 ±70 kPa (40 ±10 psi). Terminate the helium gas supply line with the parts listed in Table 3 on page 3.

❖ To connect the helium supply to the instrument

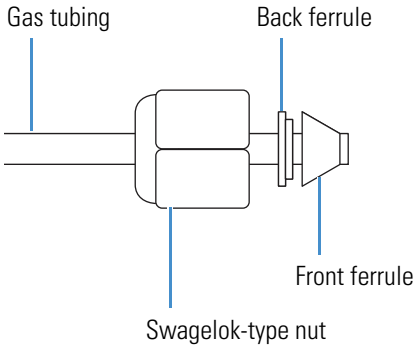
Note Use the appropriate 1/8 in. fittings and parts listed on page 3.

1. Cut an appropriate length of the precleaned, copper tubing.

   If you prefer, you can use stainless steel tubing.

2. Connect the Swagelok-type nut to one end of the tubing, followed by the two-piece ferrule set (Figure 2), and then connect this end of the tubing to the Helium In gas inlet on the back of the instrument (Figure 1 on page 2).

   Figure 2. Connector assembly for the helium tubing

3. On the other end of the tubing, connect an appropriate fitting for the gas supply.
4. Connect the tubing to the UHP helium gas supply.

IMPORTANT

- After you start using the LCQ Fleet MS, do not shut off the helium gas. Optimum performance requires a continuous flow of helium.
- If you intend to use helium for sparging your LC solvents, you must have a second tank and regulator.

Connecting the High-Purity Nitrogen Gas Supply

The nitrogen gas must be HP (99%). The required gas pressure is 690 ±140 kPa (100 ±20 psi).

❖ **To connect the HP nitrogen supply to the instrument**

Note Use the appropriate 1/4 in. fittings and parts listed on page 3.

1. Cut an appropriate length of the Teflon PFA tubing.
2. Connect the Swagelok-type nut to one end of the tubing, followed by the two-piece ferrule set (Figure 2 on page 4), and then connect this end of the tubing to the HP nitrogen gas supply.
3. Push the other end of the tubing into the Nitrogen In gas inlet on the back of the instrument (Figure 1 on page 2).

Connecting the Vacuum System

The LCQ Fleet MS requires one forepump (or roughing pump) to maintain the internal vacuum pressure.

CAUTION For forepump operation and maintenance, refer to the operating instructions provided with the pump. In particular, note the following:

- Prevent the forepump from over-heating by ensuring that there is sufficient air clearance around the pump.
- Maintain the exhaust pressure from atmospheric pressure minus 15 mbar to 1.15 bar absolute (0.15 bar relative).
- Follow the instructions for adding and changing the oil.

To connect the vacuum system, follow these procedures:

- Connecting the Mass Spectrometer to the Forepump
- Connecting the Forepump to the Lab Exhaust System
- Connecting Line Power to the Forepump

Connecting the Mass Spectrometer to the Forepump

The LCQ Fleet MS requires one forepump. Figure 3 shows the vacuum hose assembly that consists of the parts provided in the Vacuum Hose Accessory Kit (Table 4) and provided with the forepump (Table 5).

IMPORTANT To ensure the best pumping performance, limit the length of the vacuum hose to no more than 2.4 m (8 ft).

Figure 3. Vacuum hose assembly (P/N 97055-60135)

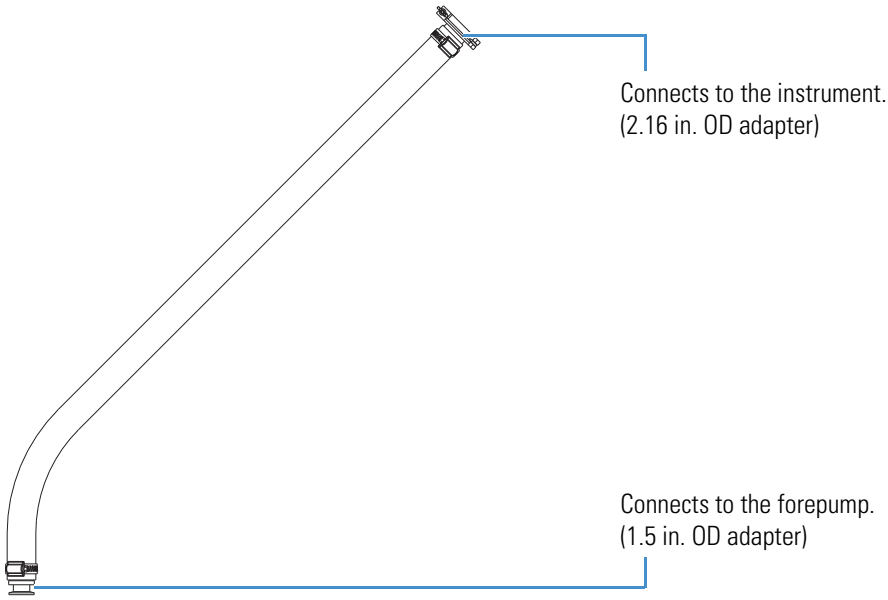


Table 4. Assembly parts in the Vacuum Hose Accessory Kit (Sheet 1 of 2)

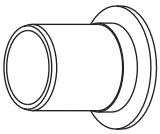
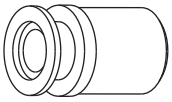
Image	Part description	Part number
—	Vacuum hose, reinforced PVC, 1.5 in. ID, 2.4 m (8 ft) long	00301-24163
	Centering ring with O-ring, nitrile and aluminum, NW40	00108-02-00005
	Hose adapter, aluminum, 1.5–2.2 in. OD (connects to the instrument)	97055-20714
	Hose adapter, aluminum, 1.5 in. OD (connects to the forepump)	70111-20210

Table 4. Assembly parts in the Vacuum Hose Accessory Kit (Sheet 2 of 2)

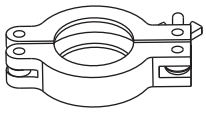
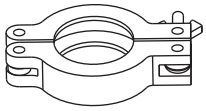
Image	Part description	Part number
	Hose clamp, high-torque, stainless steel, 1.25–2.125 in.	00201-99-00056
	Swing clamp, aluminum, NW40	00108-02-00004

Table 5. Assembly parts supplied with the forepump

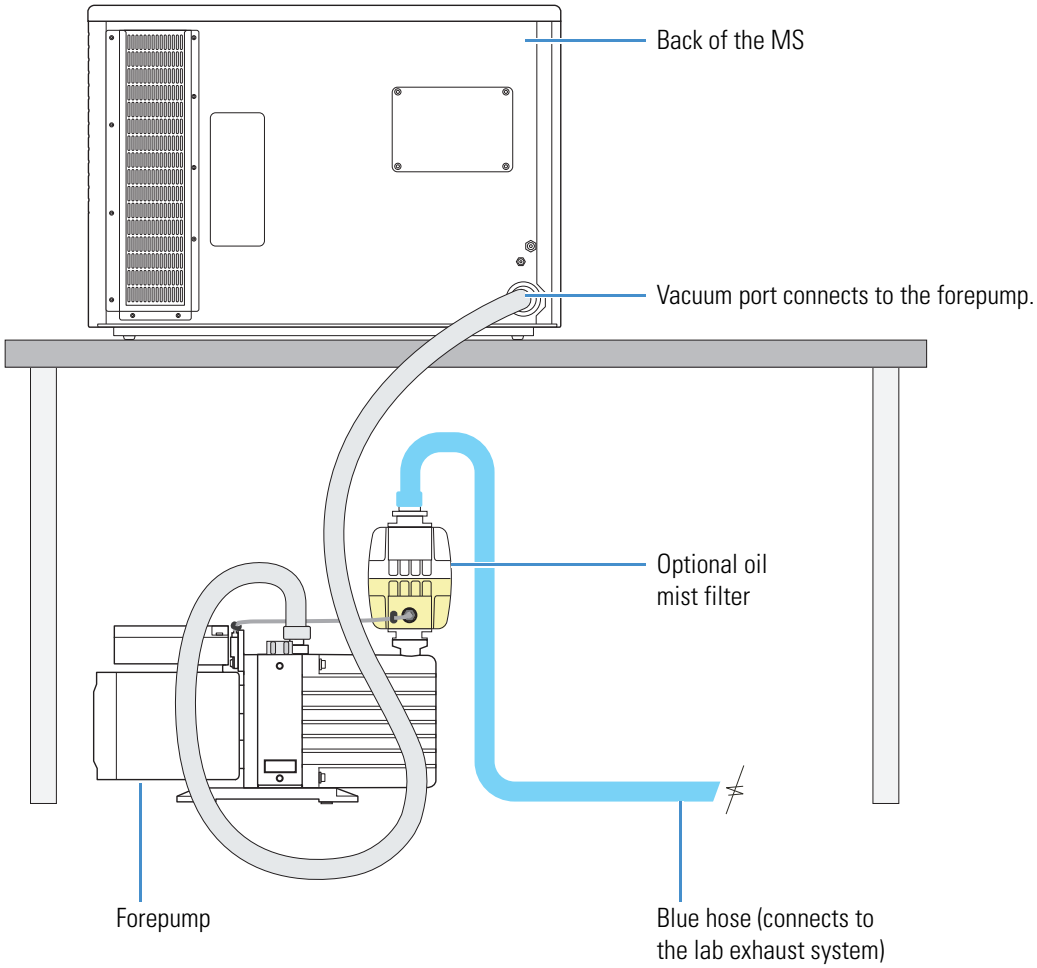
Image	Part description	Part number
	Centering ring with O-ring, Viton™ and aluminum, NW25	00108-02011
	Swing clamp, aluminum, NW25	00102-10020

❖ To connect the forepump to the instrument

1. Connect the vacuum hose to the instrument as follows:
   a. Place the NW40 centering ring on the flange of the vacuum port located on the back of the instrument.
   b. Using the NW40 swing clamp, secure the end of the vacuum hose that has the instrument adapter to the vacuum port.
2. Connect the other end of the vacuum hose to the forepump as follows:
   a. Place a NW25 centering ring on the flange of the forepump inlet port.
   b. Using a NW25 swing clamp, secure the vacuum hose to the forepump.

   Figure 4 show the connections for the LCQ Fleet vacuum system.

Figure 4. Connections between the MS vacuum port, forepump, and lab exhaust system



Connecting the Forepump to the Lab Exhaust System

To operate the forepump properly requires an efficient fume exhaust system. Most atmospheric pressure ionization (API) applications contribute to solvents accumulating in the forepump. While Thermo Fisher Scientific recommends that you periodically open the gas ballast valve (on the top of the pump) to purge the accumulated solvents, opening the valve might allow a large volume of volatile solvent waste to enter the fume exhaust system. Because the optional oil mist filter connects to the ballast port, be aware that opening the valve also drains the oil mist filter. Choose an exhaust system that can accommodate the periodic purging of these solvents. The frequency of the purging depends on the throughput of the system—never operate a pump continuously with the gas ballast valve open.

CAUTION Because the forepump exhaust is a health hazard, make sure that it vents to an appropriate external exhaust system.

Table 6 lists the parts required to connect the forepump to the lab exhaust system. These parts are in the MS Setup Kit (P/N 70111-62033) and the Mechanical Pump Accessory Kit (P/N 70111-62048).

Table 6. Shipped forepump exhaust system hardware

Image	Part description	Quantity	Part number
	Exhaust hose, blue, 1 in. ID, 6.1 m (20 ft) long	1	00301-08301
	Hose clamp, high-torque, stainless steel, 1.25–2.125 in.	2	00201-99-00056

❖ To connect the forepump to the lab exhaust system

1. Using a hose clamp, secure the blue exhaust hose to the forepump exhaust port.
2. Using a hose clamp, secure the other end of the hose to the lab exhaust system.

Figure 4 on page 8 shows the blue exhaust hose connection.

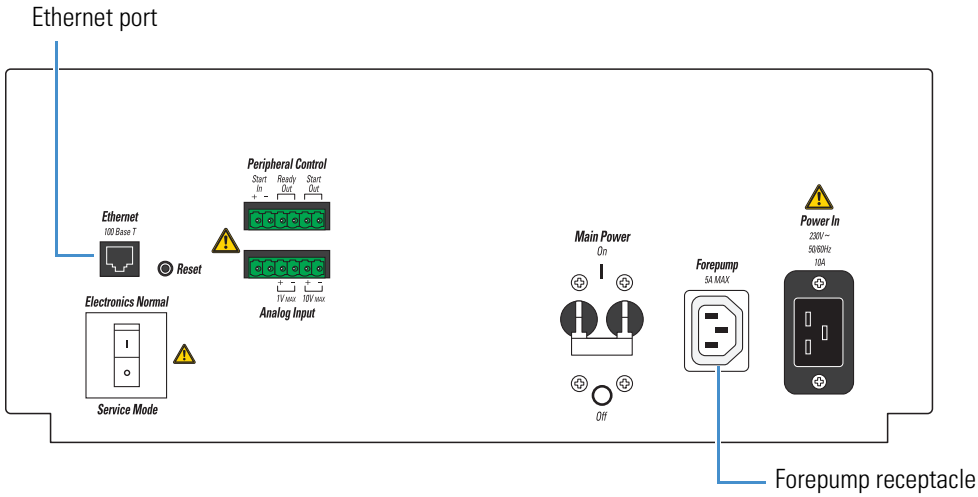
CAUTION Run the exhaust hose at floor level for at least 2 m (6.6 ft). This hose acts as a trap for exhaust fumes that would otherwise recondense in the forepump oil.

Connecting Line Power to the Forepump

This section describes how to connect the forepump to line power (ac mains power system). The forepump receives 230 Vac power through its connection to the Forepump receptacle on the right side of the instrument (Figure 5).

IMPORTANT Do not connect the forepump to a wall outlet.

Figure 5. Power panel for the LCQ Fleet MS



❖ To connect line power to the forepump

1. Turn off (0) the power switches on both the instrument and the forepump.
2. Connect the forepump's nondetachable power supply cord to the Forepump receptacle.

IMPORTANT Do not turn on the forepump until after you complete all of the system connections and connect the instrument to line power.

CAUTION Trip hazard. After completing the forepump connections, move the pump to the floor, either under or to the side of the workbench. Do not place it on the workbench. Route the hose so that it is not a trip hazard.

Connecting the Data System Computer

The data system for the LCQ Fleet MS includes a computer, a monitor, and an Ethernet switch. You can also add a printer. The instrument communicates with the data system computer through an Ethernet network.

Table 7 lists the parts required to connect the data system computer to the instrument. These parts are in the MS Setup Kit (P/N 70111-62033).

Table 7. Shipped data system connection hardware

Description	Quantity	Part number
Ethernet cable, Category 5, 2.1 m (7 ft) long	2	00302-01838
Fast Ethernet switch, 10T/100Base-TX, 5-port	1	00825-01-00024

CAUTION Safety and EMC regulations require the use of Category 5 shielded Ethernet communication cables, maximum 3 m (10 ft) long.

❖ To connect the instrument to the data system computer

1. Connect one Ethernet cable from a port on the Ethernet switch to the Ethernet port on the right side of the instrument (see page 10).
2. Connect the second Ethernet cable from a port on the Ethernet switch to the Ethernet network card (labeled LC/MS) in the data system computer.
3. Connect a power supply cord from the Ethernet switch to a wall outlet, and then turn on the Ethernet switch.
4. If the Ethernet switch has an ECO button (for power conservation), make sure that it is in the Off position to maintain the communication link between the instrument and data system computer.
5. Connect another power supply cord from the computer to a wall outlet, and then turn on the computer.

Tip For troubleshooting purposes, you might want to record which devices connect to which Ethernet ports.

Connecting the Mass Spectrometer to Line Power

Note For information about the line power requirements, refer to the *LCQ Fleet Preinstallation Requirements Guide*.

❖ To connect the instrument to line power

1. Turn off (0) the main power switch.
2. Place the electronics service switch to Service Mode (down position).
3. Connect the power supply cord to the Power In receptacle on the right side of the instrument, and then plug the cord into a 230 Vac wall outlet.

2

Ion Max and Ion Max-S Ion Sources

This chapter briefly describes the Ion Max™ and Ion Max-S™ ion source assemblies and the source drain connection to the LCQ Fleet MS.

Note For information about available ionization modes, and how to install or remove the API source housing, refer to the *Ion Max and Ion Max-S API Source Hardware Manual*.

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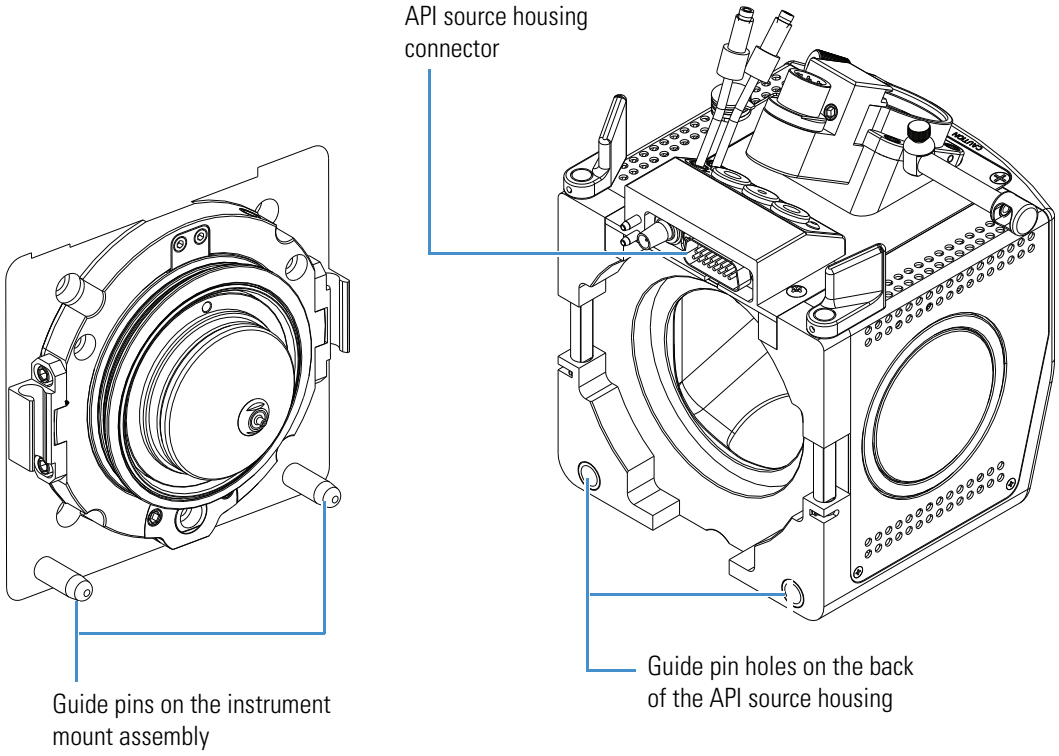
API Source Housing

The Ion Max or Ion Max-S API source housing holds the ESI, HESI-II, or APCI probe. The Ion Max has two features that the Ion Max-S does not have: an adjustable probe port and a front door with a window. Aside from these two features, these two source housings have the same functionality and mount to the LCQ Fleet MS in the same way. No tools are needed to remove or install the API source housing or source drain. For information about installing or removing the API source housing, refer to the *LCQ Fleet Getting Started Guide* and the *Ion Max and Ion Max-S API Source Hardware Manual*.

Figure 6 shows the API source mounting assembly located on the front of the instrument (left drawing) and the back view of the API source housing (right drawing). The API source housing receives power for the heater, high-voltage safety interlock, and readback through the housing connector.

CAUTION Hot surface. While the mass spectrometer is in operation, the external surface of the API source housing can become extremely hot. Let the API probe and housing cool to room temperature (approximately 20 minutes) before you touch them.

Figure 6. API source housing connection



API Source Housing Drain

When installing the API source, connect the drain at the bottom of the API source housing to the solvent waste container (Figure 7). For instructions, refer to the *Ion Max and Ion Max-S API Source Hardware Manual*.

Figure 7. API source drain assembly and waste container

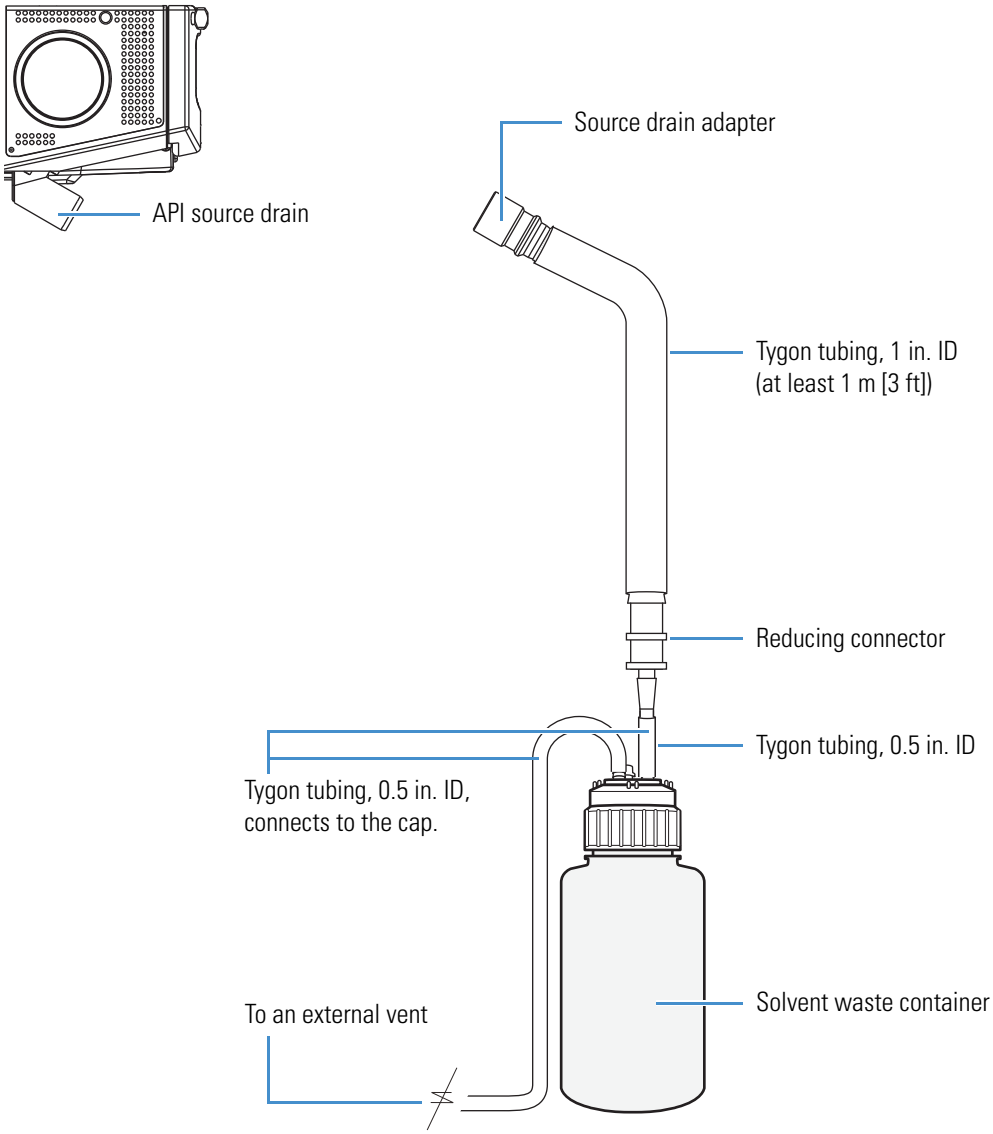


Table 8 lists the components of the solvent waste system. During the initial installation of the instrument, a Thermo Fisher Scientific field service engineer installs the solvent waste system.

Table 8. Solvent waste system parts

Description	Part number	Kit
Cap, filling/venting	00301-57022	MS Setup Kit
Container, Nalgene™, heavy-duty, 4 L	00301-57020	MS Setup Kit
Reducing connector, single barbed fitting, 1 to 0.5 in. ID	00101-03-00001	MS Setup Kit
Source drain adapter, Teflon	70111-20971	MS Accessory Kit
Tubing, Tygon™, 0.5 in. ID, 3/4 in. OD	00301-22920	MS Setup Kit
Tubing, Tygon PVC, 1 in. ID, 1-3/8 in. OD	00301-22922	MS Setup Kit

Use these guidelines for the API source drain:

- Use the PVC tubing provided with the solvent waste container to connect the solvent waste container to a fume exhaust system. Do not connect silicone tubing to the API source drain. If silicone tubing connects to the outlet drain, you might observe background ions at *m/z* 536, 610, and 684.

CAUTION Do not vent the PVC drain tube (or any vent tubing connected to the waste container) to the same fume exhaust system that connects to the forepump. Vent the waste container to a dedicated fume exhaust system. The exhaust system for the API source must accommodate a flow rate of up to 30 L/min (64 ft^3/h).

- Use the Teflon source drain adapter (see Table 8). Do not connect Tygon tubing directly to the API source drain. At high temperatures, Tygon releases volatile contaminates.

CAUTION When you reconnect the API source drain tubing to the bottom of the API source housing, make sure that you first connect the Teflon source drain adapter. This adapter can withstand the high temperatures produced by the H-ESI or APCI source.

- To prevent solvent waste from backing up into the mass spectrometer, make sure that all tubing is above the level of liquid in the waste container as follows:
  - Tygon tubing from the mass spectrometer to the solvent waste container
  - PVC tubing from the waste container to the exhaust system

3

External Peripheral Devices

This chapter provides information on how to control an external device that connects to the LCQ Fleet MS through a contact closure cable. Control of external devices might or might not be through one of the Thermo Scientific mass spectrometry applications, such as the Xcalibur data system.

Note For information about connecting LC devices that are controlled by a layered application, refer to the appropriate manual provided on the LC Devices software DVD.

Contents

Interface Kits

Table 9 lists the kits that connect the instrument to various external devices.

Table 9. Data system interface kits

Description	Part Number
Xcalibur Ethernet Communication Kit (Agilent 1200 Series LC): • Contact closure cable with 15-pin connector • Contact closure PCB • Ethernet Category 5 shielded cables (2) • Ethernet switch, 10T/100Base-TX, 5-port • Agilent G1369A LAN card	OPTON-30012
Xcalibur JetDirect™ Ethernet Control Kit (Agilent™ 1100 Series LC): • Contact closure cable with 15-pin connector • Contact closure PCB • Ethernet Category 5 shielded cables (2) • Ethernet switch, 10T/100Base-TX, 5-port • HP™ JetDirect 400N print server PCB	OPTON-30018
Mass Spectrometer Contact Closure Cable (for devices not controlled by the Xcalibur data system): • 2-wire trigger cable • 8-position screw connector	OPTON-21705

External Devices Controlled by a Mass Spectrometry Application

Thermo mass spectrometry applications, such as the Xcalibur data system, control external devices (for example, autosamplers, pumps, and detectors) from several manufacturers including Thermo Fisher Scientific, Agilent Technologies, and Waters™ Corporation.

The LCQ Fleet MS can start data acquisition upon receiving a contact closure (start) signal from an external device, which is typically an autosampler. This external device connects to the contact closure pins (Start In ±) by using the contact closure cable provided with the LC device. For instructions, refer to the instrument manual.

CAUTION The external device providing the start signal must have proper earth grounding. Ground loops can cause problems and create a safety hazard. The complementary metal-oxide-semiconductor (CMOS) integrated circuits that are mounted on the internal input/output (I/O) printed circuit board (PCB) fail if they receive more than 5 V or 5 mA.

To connect and set up the external device, follow these procedures:

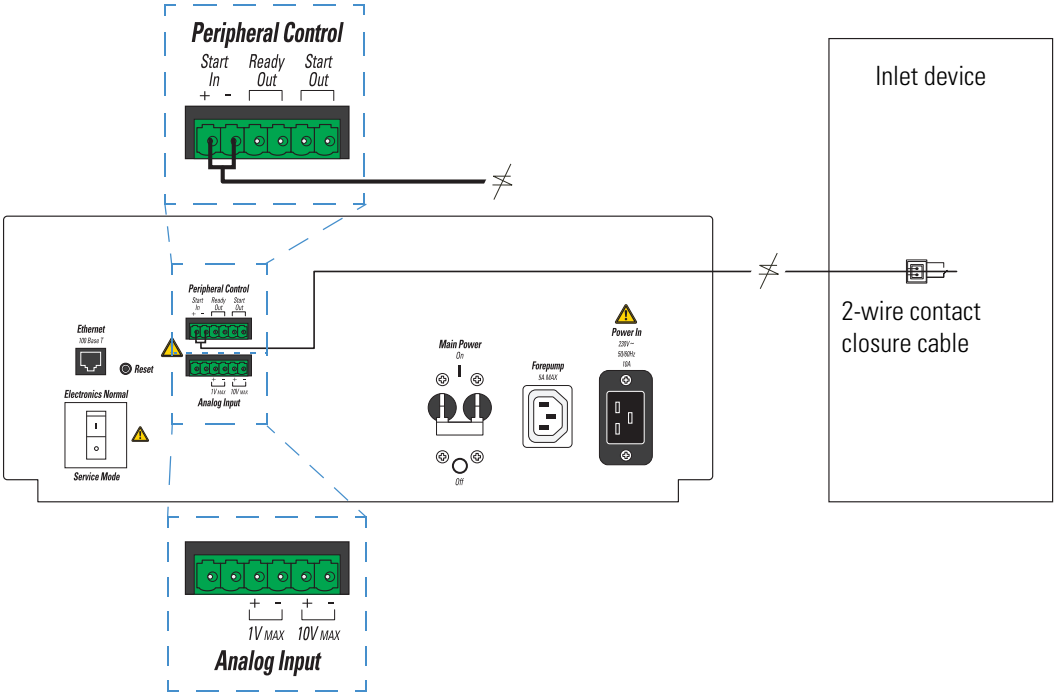
1. Connecting the Contact Closure Cable
2. Selecting the Start Instrument

Connecting the Contact Closure Cable

Thermo Fisher Scientific provides instructions for connecting supported LC systems to a Thermo Scientific mass spectrometer. You can access the appropriate manual from the data system computer by choosing **Start > All Programs > Thermo Instruments > Manuals > LC Devices** and so on to find the applicable manual for your specific device.

The contact closure connector (Start In pins) for the instrument is on the right side (Figure 8).

Figure 8. Peripheral Control and Analog Input terminals



Selecting the Start Instrument

You can now turn on the data system computer, Ethernet switch, forepump, mass spectrometer, and LC system. By default, the Xcalibur data system, for example, selects the configured autosampler as the start instrument for a sequence run. The following procedure shows you how to verify this setting and, if necessary, change the selection.

❖ To select the external start instrument

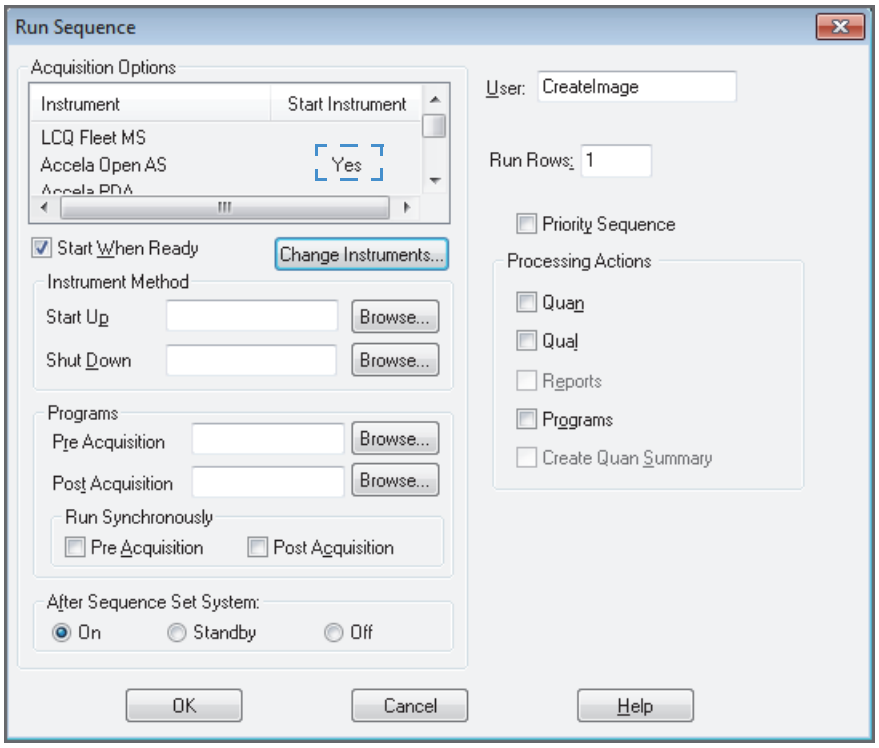
1. Open the Xcalibur data system, and then choose **View > Sequence Setup View** to open the Sequence Setup window.
2. Open the sequence that you want to run as follows:

   a. Click the **Open** button and browse to the appropriate folder.
   b. Select the sequence (SLD) file and click **Open**.

3. Choose **Actions > Run Sequence** or **Actions > Run This Sample** to open the Run Sequence dialog box (Figure 9).

   The Yes in the Start Instrument column indicates that the default start instrument for the sequence run is the Thermo Scientific Accela Open Autosampler.

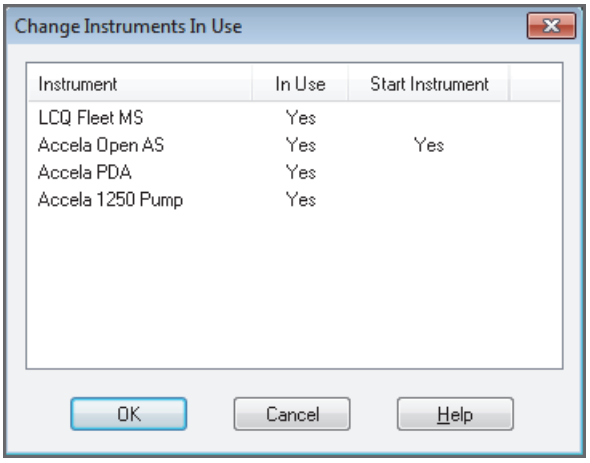
   Figure 9. Run Sequence dialog box showing the default start instrument



4. If you must change the start instrument, do the following:

   a. Click **Change Instruments** to open the Change Instruments In Use dialog box (Figure 10).

      Figure 10. Change Instruments In Use dialog box showing the default start instrument



b. In the Start Instrument column, click the blank field to the right of the appropriate triggering device (typically an autosampler) to move the word *Yes* to this field.

c. Click **OK**.

5. In the Run Sequence dialog box, complete the remaining selections.

6. Click **OK**.

External Devices Not Controlled by a Mass Spectrometry Application

When an external device is not controlled by a Thermo mass spectrometry application, such as the Xcalibur data system, you must properly connect it to send its contact closure (start) signal. In addition, the Xcalibur Run Sequence dialog box must indicate the appropriate instrument as the start instrument.

The LCQ Fleet MS can start data acquisition upon receiving a contact closure (start) signal from an external device, typically an autosampler. This external device connects to the contact closure pins (Start In ±) by using a contact closure cable.

To connect and set up the external device, follow these procedures, as applicable:

1. Connecting the Contact Closure Cable

2. Starting a Sequence Run from the Xcalibur Data System on page 22

Connecting the Contact Closure Cable

Before proceeding, verify that the external device is suitable for use with the instrument.

Note To start data acquisition, the output (start) signal from the external device must be *Normally Hi* (5 V) and momentarily go to *Low* (less than 2.5 V). If you cannot configure the external device to go from *Normally Hi* to *Low* momentarily, you cannot use it with the instrument.

If the Xcalibur data system does not control your external device, use the supplied contact closure mating connector to assemble a two-wire contact closure cable. This cable connects the Start In pins on the instrument (Figure 8 on page 19) to your device. However, you are responsible for providing the cable for the Ready Out and Start Out pin connections, which are described in Table 10.

The Analog Input terminal (Figure 8) converts the signal from an analog external input device to a digital signal for the LCQ Fleet MS. Analog devices are typically those that are not controlled by a mass spectrometry application.

The 1 V Max and 10 V Max inputs are 12-bit analog-to-digital converters (ADCs) that acquire a 1 V or 10 V input signal from the connected external device. The output signals from the ADCs are low resolution and suitable for qualitative data acquisition. The 1 V Max input accepts a 0–1 V signal and the 10 V max input accepts a 0–10 V signal. For a high resolution ADC output signal suitable for quantitative data acquisition, use an external high resolution analog converter.

Table 10. Pin-out descriptions for an external device contact closure connection

Peripheral control pin	Description
Start In +	A digital latch circuit (TTL) that sends a 5 V signal to the connected external device, which must be able to pull the signal to less than 2.5 V.
Start In –	Earth ground.
Ready Out (2 pins)	Provides ready status. The relay switch circuit sends a programmable output signal to the external receiving device. Rated maximum 3 A, switching 60 W.
Start Out (2 pins)	Provides a connection for an external device that requires a programmable start signal, such as a fraction collector. The relay switch circuit sends a programmable output signal to the external receiving device. Rated maximum 3 A, switching 60 W.

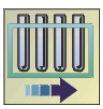
❖ To connect the contact closure cable

1. Connect the contact closure cable to the Start In pins on the right side of the instrument (Figure 8 on page 19).
2. Connect the other end of the cable to the external device according to its manual.

Starting a Sequence Run from the Xcalibur Data System

You can now turn on the data system computer, Ethernet switch, forepump, mass spectrometer, and LC system. When the Xcalibur data system, for example, does not control the autosampler, it selects the mass spectrometer as the start instrument for a sequence run. Therefore, you must change the start instrument as part of the sequence run setting.

❖ To start the sequence run



1. Open the Xcalibur data system, and click the **Sequence Setup** icon to open the Sequence Setup window.
2. Open the sequence that you want to run as follows:

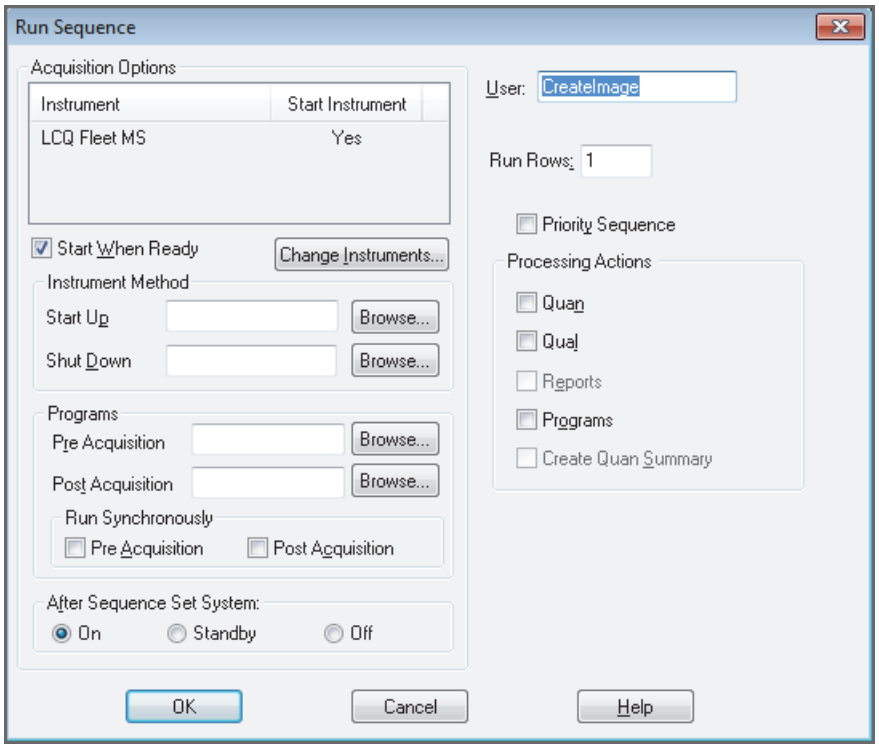
   a. Click the **Open** button and browse to the appropriate folder.

b. Select the sequence (.sld) file and click **Open**.

3. Choose **Actions > Run Sequence** or **Actions > Run This Sample** to open the Run Sequence dialog box (Figure 11).

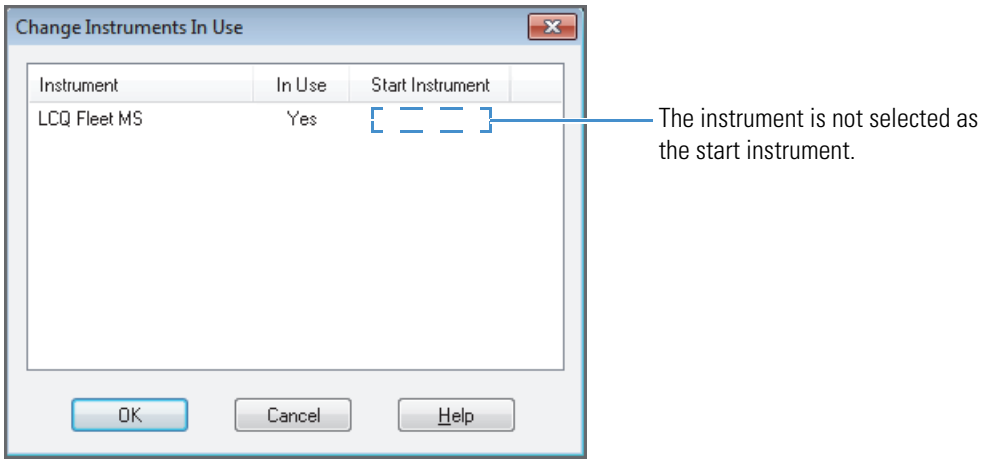
   The Yes in the Start Instrument column indicates that the default start instrument for the sequence run is the mass spectrometer.

Figure 11. Run Sequence dialog box with the mass spectrometer as the start instrument



4. Click **Change Instruments** to open the Change Instruments In Use dialog box (Figure 12).

Figure 12. Change Instruments In Use dialog box without a specified start instrument



5. Do one of the following:
   - If Yes appears in the Start Instrument column for the mass spectrometer, click **Yes** to clear this device as the start instrument.
   - If Yes does not appear in the Start Instrument column for the mass spectrometer, click **OK**.
6. Under Acquisition Options, select the **Start When Ready** check box, and then click **OK**.

   The instrument method downloads to the instrument, and the Status page displays the following message:

   Waiting - Contact Closure

7. If the Xcalibur Roadmap page does not display the Info View pane, click the **Information View** button, and then click the **Status** tab.
8. Start the external device.

   Acquisition from the instrument begins after the external device sends the contact closure (start) signal.

   In situations where the Xcalibur data system does not control external devices such as autosamplers, control might be through a third-party system or a built-in control system. For example, you can control the Thermo Scientific SpectraSYSTEM™ AS3000 autosampler from its front-panel command center.

Note The SpectraSYSTEM LC modules are external devices because Thermo Fisher Scientific does not provide Xcalibur-compatible device drivers for them. You can control the SpectraSYSTEM LC modules from their front-panel control modules.

Triggering External Devices

You can use Thermo Scientific mass spectrometry applications, such as the Xcalibur data system, to trigger (activate or deactivate) an external device, such as a fraction collector, when the LCQ Fleet MS detects a specified target.

A contact closure signal that triggers an external device can occur when one or more external trigger activation masses are present in the mass spectrum, or the base peak intensity exceeds a preset threshold.

To select the first option, specify the external trigger activation masses for each sample in the Sequence Setup view in the columns for predefined user labels: ETMW (external trigger molecular weight) or MWFC (molecular weight for fraction collection). The data system automatically tests for the presence of external trigger activation masses and the presence of these masses with common solvent adducts. When the external trigger activation mass is no longer present in the scan or when the base peak intensity is less than the preset threshold, the contact closure is deactivated.

Note For additional information about triggering an external device, refer to the Tune Plus Help.

Glossary

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

A

API source The sample interface between the liquid chromatograph (LC) and the mass spectrometer (MS).

atmospheric pressure chemical ionization (APCI) A soft ionization technique done in an ion source operating at atmospheric pressure. Electrons from a corona discharge initiate the process by ionizing the mobile phase vapor molecules, forming a reagent gas.

atmospheric pressure ionization (API) Ionization performed at atmospheric pressure by using atmospheric pressure chemical ionization (APCI), heated-electrospray ionization (H-ESI), or nanospray ionization (NSI).

auxiliary gas The outer-coaxial gas (nitrogen) that assists the sheath (inner-coaxial) gas in dispersing and/or evaporating sample solution as the sample solution exits the APCI, ESI, or HESI nozzle.

C

collision gas A neutral gas used to undergo collisions with ions.

computer data system *See* data system.

contact closure connection The cable connection is from the external peripheral device to the mass spectrometer contact closure pins (Start In ±). The external device sends the contact closure (start) signal to the mass spectrometer.

D

damping gas Helium gas introduced into the ion trap mass analyzer that slows the motion of ions entering the mass analyzer so that the ions can be trapped by the rf voltage fields in the mass analyzer.

data system Consists of a computer, a monitor, a keyboard, a mouse, an Ethernet switch, and an optional printer.

E

electrospray (ESI) A type of atmospheric pressure ionization that is currently the softest ionization technique available to transform ions in solution into ions in the gas phase.

electrospray ionization (ESI) *See* electrospray (ESI).

F

forepump The pump that evacuates the foreline. A rotary-vane pump is a type of forepump. It might also be referred to as a backing, mechanical, rotary-vane, roughing, or vacuum pump.

H

heated-electrospray (H-ESI) A type of atmospheric pressure ionization that converts ions in solution into ions in the gas phase by using electrospray ionization (ESI) in combination with heated auxiliary gas.

heated-electrospray ionization (H-ESI) *See* heated-electrospray (H-ESI).

I

ion source A device that converts samples to gas-phase ions.

N

nanoelectrospray (nanoNSI or NSI) A type of electrospray (ESI) that accommodates very low flow rates of sample and solvent at 1–20 nL/min (for static nanospray) or 100–1000 nL/min (for dynamic nanospray).

S

sheath gas The inner coaxial gas (nitrogen), which is used in the API source to help nebulize the sample solution into a fine mist as the sample solution exits the ESI or APCI nozzle.

source *See* API source.

sweep gas Nitrogen gas that flows out from behind the sweep cone in the API source. Sweep gas aids in solvent declustering and adduct reduction.

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