

LCQ Fleet

Getting Connected Guide

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EMC Directive 89/336/EEC as amended by 92/31/EEC and 93/68/EEC

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EN 55011	1998, A1; 1999, A2: 2002	EN 61000-4-3	2002
EN 61000-3-2	1995, A1; 1998, A2; 1998, A14; 2000	EN 61000-4-4	1995, A1; 2000, A2; 2001
EN 61000-3-3	1995; A1; 2001	EN 61000-4-5	1995, A1; 2001
EN 61326-1	1997; A1; 1998, A2; 2001, A3; 2003	EN 61000-4-6	1996, A1; 2001
EN 61000-4-2	2001	EN 61000-4-11	1994, A1; 2001
FCC Class A, CFR	47 Part 15 and Part 18, 2005	CISPR 11	1998, A1; 1999, A2; 2002

Low Voltage Safety Compliance

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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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Notice on the Proper Use of Thermo Scientific Instruments

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Your instrument is designed to work in a controlled electromagnetic environment. Do not use radio frequency transmitters, such as mobile phones, in close proximity to the instrument.

For manufacturing location, see the label on the instrument.



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Preface

This manual provides information on how to connect your LCQ Fleet[™] system.

Related Documentation

In addition to this guide, Thermo Scientific provides the following documentation for the LCQ Fleet MS detector:

- LCQ Fleet Preinstallation Requirements Guide
- LCQ Fleet Getting Started Guide
- LCQ Fleet Hardware Manual
- Ion Max and Ion Max-S API Source Hardware Manual

To access the manuals for the LCQ Fleet MS detector, from the Microsoft[™] Windows[™] taskbar, choose **Start > All Programs > Thermo Instruments > LTQ > Manuals > model** and then click the listing for the PDF that you want to view.

Note For Xcalibur version 2.0.7 or earlier, the path is **Start > All Programs > Xcalibur > Manuals > LTQ >** *model*.

To access the Help, choose **Help** from the menu bar or click the **?** button on the toolbar.

Safety and Special Notices

Make sure you follow the precautionary statements presented in this guide. The safety and other special notices appear in boxes.

Safety and special notices include the following:



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 may contain information that is critical for optimal performance of the system.

Note Highlights information of general interest.

Tip Helpful information that can make a task easier.

Contacting Us

There are several ways to contact Thermo Scientific for the information you need.

To contact Technical Support

Phone	800-532-4752
Fax	561-688-8736
E-mail	us.techsupport.analyze@thermofisher.com
Knowledge base	www.thermokb.com

Find software updates and utilities to download at mssupport.thermo.com.

To contact Customer Service for ordering information

Phone	800-532-4752
Fax	561-688-8731
E-mail	us.customer-support.analyze@thermofisher.com
Web site	www.thermo.com/ms

To copy manuals from the Internet

Go to mssupport.thermo.com and click **Customer Manuals** in the left margin of the window.

To suggest changes to documentation or to Help

- Send an e-mail message to the Technical Publications Editor at techpubs-lcms@thermofisher.com.
- Complete a brief survey about this document by clicking the link below. Thank you in advance for your help.



Line Power, Vacuum System, Gases, and Ethernet Communication

This chapter describes how to connect the LCQ Fleet MS detector to line power, the forepump, necessary gases, and the data system computer.

Contents

- Connecting the Forepump
- Connecting the Gases to the MS Detector
- Connecting the MS Detector to the Data System Computer

Connecting the MS Detector to Line Power

To connect the LCQ Fleet MS detector to line power

- 1. Turn the Main Power circuit breaker to the Off (O) position. See Figure 3 on page 5.
- 2. Make sure that the Electronics switch is in the Service Mode position.
- Connect the female plug of the power cord to the POWER IN receptacle of the power entry module.
- 4. Connect the male plug of the power cord to the 230 V ac power source in your laboratory.



CAUTION If your local area is subject to power fluctuations or power interruptions, you must install a power conditioning device or an uninterruptible power supply (UPS) in your laboratory. For more information, refer to the *LCQ Fleet Preinstallation Requirements Guide*. The UPS must be certified by both North American (UL, CSA) and European Agencies (TUV, UDE, SEMKO, DEMKO, and so on).

Connecting the Forepump

To connect the forepump (also known as a mechanical pump or rotary-vane pump) to the MS detector and the laboratory exhaust system, perform the following procedures:

• "Connecting the Vacuum Hose" on page 2

- "Connecting the Forepump to the Laboratory Exhaust System" on page 4
- "Connecting the Forepump to Line Power" on page 5

Connecting the Vacuum Hose

The vacuum hose accessory kit (P/N 97055-60135) contains the parts required to connect the forepump to the MS detector. Table 1 lists the components and Figure 1 shows the components of the vacuum hose assembly. The adapters at the two ends of the vacuum hose assembly are connected at the factory.

Table 1.Vacuum accessory kit (P/N 97055-60135)

Description	Part Number
Vacuum hose, 1.5 in. ID, 8 ft. length	00301-24163
Parts required to connect the vacuum port of the forepump	
Centering ring with O-ring, NW25, 26 mm ID, aluminum and Viton	00108-02011
Swing clamp, KF 20/25	00102-10020
Hose clamp, high-torque, 1.25 in. to 2.125 in., stainless steel	00201-99-00056
Adapter, 1.5 in. OD for the end that is inserted into the vacuum hose, 1.5 in. OD for the end that connects to the forepump	70111-20210
Parts required to connect the vacuum hose to the vacuum port of the MS de	tector
Centering ring with O-ring, NW40, 41 mm ID, aluminum and Nitrile	00108-02-00005
Swing clamp, NW32/40, aluminum	00108-02-00004
Hose clamp, high-torque, 1.25 in. to 2.125 in., stainless steel	00201-99-00056
Adapter, 1.5 in. OD for the end that is inserted into the vacuum hose, 2.16 in. OD for the end that connects to the detector,	97055-20714



To connect the LCQ Fleet MS detector to the forepump

- 1. To connect the vacuum hose to the MS detector
 - a. Place the 41 mm (1.6 in.) centering ring (P/N 00108-02-00005) on the flange of the vacuum port located on the back panel of the LCQ Fleet MS detector.
 - b. Using the NW 32/40 swing clamp (00108-02-00004), secure the end the vacuum hose that has the adapter for the LCQ Fleet MS detector to the vacuum port on the back of the LCQ Fleet MS detector.
- 2. To connect the other end of the vacuum hose to the forepump
 - a. Place the 26 mm (1.0 in.) centering ring (P/N 00108-02011) on the flange of the inlet port of the forepump.
 - b. Using the KF20/25 vacuum clamp (P/N 00102-10020), secure the vacuum hose assembly to the forepump.

Figure 2 shows the connection between the vacuum port of the MS detector and the exhaust port of the forepump.

Connecting the Forepump to the Laboratory Exhaust System

The proper operation of your forepump requires an efficient fume exhaust system. Most atmospheric pressure ionization (API) applications contribute to the accumulation of solvents in the forepump. While it is recommended that you periodically open the ballast valves (on the top of the pumps) to purge the accumulated solvents, opening the valves might allow a large volume of volatile solvent waste to enter the fume exhaust system. Choose an exhaust system that can accommodate the periodic purging of these solvents. The frequency of the purging depends on the throughput of your system.

* To connect the exhaust port of the forepump to the laboratory exhaust system

- 1. Use hose clamps (P/N 00108-09001) to secure the 2.5 cm (1 in.) ID blue exhaust hose to the forepump exhaust port.
- 2. Vent the free end of the blue exhaust hose to an external exhaust system in your laboratory.

The exhaust hose should travel at floor level for a minimum of two meters (78.5 in.) before it reaches the external exhaust system. This tubing acts as a trap for exhaust fumes that would otherwise recondense in the forepump oil.

Figure 2 shows the blue exhaust hose connected to the optional oil mist filter, which is connected to the exhaust port of the forepump.





Connecting the Forepump to Line Power

The forepump (also known as a mechanical pump, rotary pump, backing pump, or roughing pump) gets its line power from the LCQ Fleet MS detector. The power outlet for the forepump is located on the power entry module of the MS detector. As Figure 3 shows, the power entry module is located on the lower-right side of the LCQ Fleet MS detector.

- * To connect the forepump to line power (the forepump outlet of the MS detector):
- 1. On the power entry module, switch the Main Power circuit breaker to the Off (O) position.
- 2. Connect the power cord plug of the forepump to the Mechanical Pump power receptacle of the MS detector.
- 3. Turn on the power switch of the forepump.





Connecting the Gases to the MS Detector

This section describes how to connect the required gases to the LCQ Fleet MS detector. The LCQ Fleet MS detector uses nitrogen for the API sheath gas, auxiliary gas, and sweep gas, and helium for the collision gas. The gas line connections for the LCQ Fleet MS detector are located on its back panel as shown in Figure 4.



Figure 4. Back panel of the LCQ Fleet MS detector

Connecting the Nitrogen Source

The LCQ Fleet MS detector requires high purity (99%) nitrogen for the API sheath gas, auxiliary gas, and sweep gas. Because nitrogen gas usage can be quite high, Thermo Scientific recommends one of three nitrogen sources: a large, sealed, thermally insulated cylinder containing liquid nitrogen from which the nitrogen gas is boiled off; the largest nitrogen cylinder that can be practically used; or a nitrogen generator. The required gas pressure is 690 ± 140 kPa (100 ± 20 psi).

* To connect the nitrogen source to the LCO Fleet MS detector

1. Connect an appropriate length of 1/4 in. ID Teflon[™] tubing with a brass Swagelok[™]-type 1/4 in. nut (P/N 00101-12500) and a 2-piece brass 1/4 in. ferrule [P/N 00101-10000 (front), P/N 00101-04000 (back)] to the nitrogen source.

See Figure 5 for the proper orientation of the fitting and ferrule.

2. Connect the opposite end of the Teflon tubing to the LCQ Fleet MS detector press-in fitting labeled, Nitrogen In, and located on the back panel of the LCQ Fleet MS detector. To connect the tubing, align the Teflon tubing with the opening in the fitting and firmly push the tubing into the fitting until the tubing is secure.

Connecting the Helium Source

The helium for the LCQ Fleet MS detector collision gas must be ultra-high purity (99.999%) with less than 1.0 ppm each of water, oxygen, and total hydrocarbons. The required gas pressure is 275 ± 70 kPa (40 ± 10 psi). Because particulate filters can be a source of contamination, Thermo Scientific does not recommend their use.

You can dispense helium from a tank containing 245 ft^3 of gas, using a Matheson 3120 Series¹ regulator or equivalent tank and regulator.

Whether you choose copper or stainless steel gas lines for the helium, use gas lines that are free of oil and preferably flame dried. Run the gas lines to the back of the LCQ Fleet MS detector system. Terminate the helium gas supply lines with 1/8 in., female, Swagelok-type connectors.

* To connect the helium source to the LCQ Fleet MS detector

- Connect an appropriate length of 1/8 in. ID copper or stainless steel tubing with a brass Swagelok-type 1/8 in. nut (P/N 00101-15500) and a 2-piece brass 1/8 in. ID ferrule [P/N 00101-08500 (front), P/N 00101-2500 (back)] to the HELIUM IN gas inlet located on the back panel. See Figure 5 for the proper orientation of the fitting and ferrule.
- 2. Connect the opposite end of the tubing to the helium gas source, using an appropriate fitting.

Figure 5. Proper orientation of the Swagelok-type nut and two-piece ferrule



Connecting the MS Detector to the Data System Computer

The data system hardware for the LCQ Fleet MS detector consists of a computer, a monitor, and an optional printer. The LCQ Fleet MS detector communicates with the data system computer through an Ethernet cable.

¹For more information, visit: http://www.matheson-trigas.com

***** To connect the MS detector to the data system computer

- 1. Connect a category five network (Ethernet) cable (P/N 00302-01838) to the ETHERNET 100 BASE T connector located on the LCQ Fleet MS detector Power Entry Module.
- 2. Connect the opposite end of the Ethernet cable to the 10/100Base-T Ethernet switch (P/N 00825-01015) provided with the LCQ Fleet MS detector.
- 3. Connect a second Ethernet cable (P/N 00302-01838) from the Ethernet switch to the Ethernet card on the data system computer labeled Surveyor MS.
- 4. Connect the Ethernet switch to line power.

Connecting Probes

This chapter describes how to connect an ion source probe to the LCQ Fleet MS detector.

Contents

- Connecting the ESI Probe to the MS Detector
- Connecting the APCI Probe to the MS Detector

Connecting the ESI Probe to the MS Detector

- To connect liquid lines to the electrospray ionization (ESI) probe
- 1. Install the Ion Max source housing and ESI probe onto the LCQ Fleet MS detector as described in the *Ion Max and Ion Max-S API Source Hardware Manual*.
- 2. Install liquid lines between the divert/inject valve, the LC system, the syringe pump, and the grounding union, as appropriate for your application. For more information, see Chapter 6, "Connecting the Inlet Plumbing."
- 3. Connect the 1 in. ID Tygon[™] tubing (P/N 00301-22922) to the source housing drain.
- 4. Insert the other end of the tubing into a waste container, and vent the waste container to a fume exhaust system.

CAUTION Prevent solvent waste from backing up into the API source and mass spectrometer. Always ensure that the PVC drain tubing is above the level of liquid in the waste container.



Do **not** vent the PVC drain tube connected to the waste container to the same fume exhaust system to which you have connected the forepump. Connecting the API source drain tube and the forepump exhaust to the same fume exhaust system is likely to contaminate the analyzer optics.

Equip your laboratory with at least two independent fume exhaust systems. Route the (blue) exhaust tubing from the forepump to a dedicated fume exhaust system. Route the PVC drain tube from the API source to the waste container. Vent the waste container to a dedicated fume exhaust system that is independent from that used for exhausting the forepump.

Connecting the APCI Probe to the MS Detector

- * To connect liquid lines to the atmospheric chemical ionization (APCI) probe
- 1. Install the Ion Max source housing and APCI probe onto the LCQ Fleet MS detector as described in the *Ion Max and Ion Max-S API Source Hardware Manual*.
- 2. Install liquid lines between the divert/inject valve, the LC system, the syringe pump, and the sample inlet fitting on the APCI probe, as is appropriate for your application. For more information, see Chapter 6, "Connecting the Inlet Plumbing."
- 3. Connect the 1 in. ID Tygon tubing (P/N 00301-22922) to the source housing drain.
- 4. Insert the other end of the tubing into a waste container, and vent the waste container to a fume exhaust system.

CAUTION Prevent solvent waste from backing up into the API source and mass spectrometer. Always ensure that the PVC drain tubing is above the level of liquid in the waste container.



Do **not** vent the PVC drain tube connected to the waste container to the same fume exhaust system to which you have connected the forepump. Connecting the API source drain tube and the forepump exhaust to the same fume exhaust system is likely to contaminate the analyzer optics.

Equip your laboratory with at least two independent fume exhaust systems. Route the (blue) exhaust tubing from the forepump to a dedicated fume exhaust system. Route the PVC drain tube from the API source to the waste container. Vent the waste container to a dedicated fume exhaust system that is independent from that used for exhausting the forepump.

Note If you need to install or replace the APCI sample tube, refer to the *LCQ Fleet Hardware Manual* for instructions.

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Connecting to External Devices

This chapter describes how to make the contact closure connection to external devices. External devices include devices controlled or not controlled from the Xcalibur[™] data system. Table 2 lists the Xcalibur kits for various external devices.

Contents

- External Devices Controlled by the Xcalibur Data System
- External Devices Not Controlled by the Xcalibur Data System

Table 2. Xcalibur kits for various external devices

Part Number / Kit	Description of Kit
OPTON-21705	Xcalibur contact closure kit (for devices not controlled by Xcalibur) 2-wire trigger cable 8-position screw connector
OPTON-21709	Xcalibur Additional 4-Port Serial Kit 4-Port Serial PCB (PCI) and software Quad DB9 male adapter
OPTON-21710	Xcalibur Waters Interface Kit Waters serial I/F cable 2-wire trigger cable (contact closure)
OPTON-21721	Xcalibur SS420x Interface Kit SS420x main unit serial cable 2-wire trigger cable (contact closure) power supply Xcalibur Additional 4-Port Serial Kit
OPTON-30018	Xcalibur JetDirect [®] Ethernet Control Kit Contact closure PCB External contact closure cable Ethernet 10 Base-T cable (2) 10/100 Autosensing 8-port Ethernet switch HP JetDirect 400N PCB

External Devices Controlled by the Xcalibur Data System

The Xcalibur data system controls external devices (for example, autosamplers, pumps, and detectors) from several manufacturers including Thermo Scientific, Agilent¹, and Waters. The MS detector can start data acquisition upon receiving a contact closure signal from an external device, typically an autosampler. The LCQ Fleet MS detector receives contact closure signals through a 2-wire trigger cable that you connect to its START IN port.



CAUTION The external device providing the start signal must have a good ground. Ground loops can cause problems and create a safety hazard. Care must be taken with the CMOS integrated circuits that reside on the LCQ Fleet MS detector I/O PCB. These integrated circuits will fail if more than 5 V or 5 mA are applied to the system.

The LCQ Fleet can be connected to any device supported by LC Devices 2.0.2. LC Devices 2.0.2 contains the instrument control software for the devices listed in Table 3.

Device	Firmware version
Accela Autosampler	2.15
Accela PDA Detector	2.02
Accela Pump	12.47c
Agilent 1100 Autosampler	A.06.01 (012)
Agilent 1100 Binary pump	A.06.01 (012)
Agilent 1100 Quaternary pump	A.06.01 (012)
Agilent 1100 DAD (PDA detector)	A.06.01 (012)
Agilent 1100 Heater	
Agilent 1100 MWD (multiple wavelength detector)	A.06.01 (012)
Agilent 1100 VWD (variable wavelength detector)	A.06.01 (012)
Agilent 1100 Thermostatted autosampler	A.06.01 (012)
Agilent 1100 Well Plate autosampler	A.06.01 (012)
Surveyor Autosampler or Surveyor Autosampler Plus	2.15
Surveyor LC Pump Plus	2.0
Surveyor MS Pump	2.47
Surveyor MS Pump Plus	2.47
Surveyor PDA Plus Detector	ROM 1.08
Surveyor UV/Vis Plus Detector	

 Table 3.
 Devices supported by LC Devices 2.0.2 (Sheet 1 of 2)

¹ Formerly Hewlett-Packard[®] (HP)

Device	Firmware version			
SS420x Analog to Digital Converter board				
Thermo Micro AS	1.03			
Thermo PAL (autosampler)				
Waters 2795 Separations Module	2.02			

 Table 3.
 Devices supported by LC Devices 2.0.2 (Sheet 2 of 2)

This section contains the following topics:

- "Making Contact Closure with Devices Controlled by Xcalibur" on page 13
- "Selecting the Appropriate Start Instrument" on page 13

Making Contact Closure with Devices Controlled by Xcalibur

To connect the contact closure cable

- 1. Connect the appropriate contact closure cable to the Start In pins located on the power entry module of the MS detector.
- 2. To connect the external device, follow the instructions given in the manufacturer's documentation.

Selecting the Appropriate Start Instrument

By default, Xcalibur selects the configured autosampler as the start instrument for a sequence run.



- To ensure that the appropriate device is listed as the start instrument
- 1. On the Xcalibur Roadmap Home Page, click the Sequence Setup button.

The Sequence Setup window appears.

- 2. Open the sequence that you want to run:
 - a. Choose File > Open.

The Open dialog box appears.

- b. Browse to the appropriate folder, and then select a sequence file.
- c. Click **Open** to open the sequence and exit the Open dialog box.

Sequence files are identified by their .sld file extension.

3. Choose Actions > Run Sequence or Actions > Run This Sample.

The Run Sequence dialog box appears. Figure 6 shows the Run Sequence dialog box. The Yes in the Start Instrument column indicates that the Surveyor Autosampler will be used as the start instrument once the sequence run begins.

Figure 6.	Run Sequence	e dialog box	with the Survey	yor AS selecte	d as the start instrument
-----------	--------------	--------------	-----------------	----------------	---------------------------

Run Sequence	×
Acquisition Options Instrument Start Instrument Yes ✓ Start When Ready Change Instruments Instrument Method Start Up Browse Shut Down Browse Programs Pre Acquisition Post Acquisition Browse Run Synchronously ✓ Post Acquisition	Liser: B.A.Cook Run Rows: 1 Priority Sequence Processing Actions Quan Quan Qual Reports Programs Create Quan Summary
After Sequence Set System: On C Standby C Off	
OK Cancel	<u>H</u> elp

- 4. Verify that the appropriate device is listed as the start instrument in the Acquisition Options box.
- 5. If the appropriate device is not listed as the start instrument, change the starting device:
 - a. Click Change Instruments.

The Change Instruments In Use dialog box appears, with, for example, the Surveyor AS selected as the Start instrument. See Figure 7.

Figure 7. Change Instruments In Use dialog box with the Surveyor AS selected as the start instrument

Change Instruments In Use				
Instrument Surveyor PDA LCQ Fleet Surveyor AS Surveyor MS Pump	<mark>In Use</mark> Yes Yes Yes Yes	Start Instrument		
ОК	Cancel	Help		

- b. In the Start Instrument column, click the blank field to the right of the appropriate triggering device (typically an autosampler). The word **Yes** moves to this field.
- c. Click **OK** to save the setting and close the Change Instruments In Use dialog box.
- 6. Complete the remaining selections in the Run Sequence dialog box.
- 7. Click OK to save the settings, close the dialog box, and start the sequence or queue it.

External Devices Not Controlled by the Xcalibur Data System

External devices that are not controlled by the Xcalibur data system must be properly connected for contact closure, and the appropriate instrument must be selected as the start instrument in the Xcalibur Run Sequence dialog box.

This section contains the following topics:

- "Making Contact Closure with Devices Controlled by Xcalibur" on page 13
- "Starting a Sequence Run from Xcalibur" on page 16

Making Contact Closure with Devices Not Controlled by Xcalibur

To connect the contact closure cable

Note To start data acquisition on the LCQ Fleet MS detector, the output (start) signal from the external device must be *Normally Hi* (+5 V) and momentarily go to *Low*. If you cannot configure the external device to go from *Normally Hi* to *Low* momentarily, it cannot be used with the LCQ Fleet MS detector.

- 1. Connect the 2-wire trigger cable (in kit P/N OPTON-21705) to the Start In pins on the power entry module of the LCQ Fleet MS detector.
- 2. Connect the cable to the contact closure terminal of the external device, following the wiring scheme listed in Table 4.

Table 4. Wiring the LCQ Fleet MS detector and an external device (not controlled by the Xcalibur data system for contact closure

LCQ Fleet MS detector Power Entry Module	External Device Contact Closure Terminal
TTL IN 1	Output (start) terminal
DIGITAL GROUND	Ground terminal

Figure 8 shows a block diagram of the contact closure connection to an external device.

Figure 8. Schematic of the contact closure connection between the MS detector and an external device



Starting a Sequence Run from Xcalibur

When the Xcalibur data system does not control the autosampler you are using, Xcalibur selects the LCQ Fleet MS detector as the Start instrument for a sequence run. When you are ready to inject a set of samples, ensure that the LCQ Fleet MS detector is **not** listed as the start instrument in Xcalibur.

* To start the sequence run



- 1. On the Xcalibur Roadmap Home Page, click the **Sequence Setup** button to open the Sequence Setup window.
- 2. Open the sequence that you want to run:
 - a. Choose File > Open.

The Open dialog box appears.

b. Browse to the appropriate folder, and then select a sequence file.

c. Click **Open** to open the sequence and exit the Open dialog box.

Sequence files are identified by their .sld file extension.

3. Choose Actions > Run Sequence or Actions > Run This Sample.

The Run Sequence dialog box shown in Figure 9 appears. Because the LCQ Fleet MS detector is the only configured instrument, it is listed as the start instrument for the sequence run.

Run Sequence	
Acquisition Options Instrument Start Instrument LCQ Fleet MS Yes	<u>U</u> ser: ∣acook Run Rows: 1 I Priority Sequence
✓ Start When Heady Change Instruments Instrument Method Browse Start Up Browse Shut Down Browse	Processing Actions Quan Qual Reports Programs
Pre Acquisition Browse Post Acquisition Browse Run Synchronously ✓ Pre Acquisition ✓ Post Acquisition	Create Quan <u>S</u> ummary
Atter Sequence Set System: On O Standby O Off OK Cancel	<u>H</u> elp

Figure 9. Run Sequence dialog box with the MS detector specified as the start instrument

4. Click Change Instruments.

The Change Instruments In Use dialog box appears. See Figure 10.

C	hange Instruments In U	lse		×	
	Instrument LCQ Fleet MS	In Use S Yes ◄	itart Instrument		 LCQ Fleet MS detector is not selected as a start instrument
	[0K	Cancel	<u>H</u> elp		

Figure 10. Change Instruments In Use dialog box with no start instrument specified

- 5. Check the status of the LCQ Fleet MS detector under Acquisition Options.
 - If the LCQ Fleet MS detector is in the *Start Instrument: Yes* mode, go to step 6.
 - If the LCQ Fleet MS detector is not in the *Start Instrument: Yes* mode, click **OK** to close the dialog box and go to step 7.
- 6. In the LCQ Fleet MS detector row of the Start Instrument column, click **Yes** to change the mode to Off (field is blank), and then click **OK** to save the setting and close the dialog box.
- 7. In the Acquisition Options area, select the **Start When Ready** check box, click **OK** to save the settings, close the dialog box, and start the sequence or queue it.

The instrument method downloads to the LCQ Fleet MS detector, and the Status page displays *Waiting - Contact Closure*.



- 8. If the Home page does not display the Info view, click the **Information View** button to display it, and then click the **Status** tab to display the Status page.
- 9. To start the external device, push the "Start" button on the external device.

Data acquisition from the LCQ Fleet MS detector begins after the external device sends the "Contact Closure" signal that the LCQ Fleet MS detector is waiting for.

Connecting a Thermo Scientific LC System

This chapter describes how to make the contact closure connections between a Surveyor[™] Plus or an Accela[™] LC system and the LCQ Fleet MS detector.

Contents

- Making Contact Closure with a Surveyor Plus LC System
- Making Contact Closure with an Accela LC System

For information on making the plumbing and back panel connections for a Thermo Scientific LC system, refer to its Getting Connected manual.

To make contact closure with a Thermo Scientific LC system, you must have the adapter cable shown in Figure 11.

Figure 11. LXQ/LTQ interconnect adapter cable (P/N 60053-63037)



Making Contact Closure with a Surveyor Plus LC System

Table 5 lists the firmware for the Surveyor Plus LC devices supported by the Xcalibur 2.0.5 data system. LC Devices 2.0.2 contains the instrument control software for these devices. For information on making contact closure between the modules of the LC system, refer to the *Surveyor Plus Getting Connected* manual.

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Device	Firmware version
Surveyor LC Pump Plus Pump Main Board and Pump Converter Board	2.01, 2.00
Surveyor MS Pump and Surveyor MS Pump Plus	2.47
Surveyor Autosampler	2.15
Surveyor PDA Plus Detector	2.01

Table 5. Firmware versions supported by Xcalibur 2.0.5

To connect an LCQ Fleet MS detector to a Surveyor Plus LC system with the 7-connector system interconnect cable

- 1. Connect the 8-pin connector (with hood and labeled MS/LC) end of the LXQ/LTQ interconnect adapter cable (P/N 60053-63037) to the M/S connector of the 7-connector system interconnect cable.
- 2. Plug the 6-pin end (labeled LTQ/TXQ) of the adapter cable into the START IN connection (green, 2-pin) on the lower-right side of the MS detector, as shown in Figure 12.

To connect the Surveyor MS Pump or Surveyor MS Pump Plus, you must use an additional adapter cable (P/N 60053-63038).

- 3. To connect a Surveyor MS Pump or Surveyor MS Pump Plus to the interconnect cable:
 - a. Connect the end of the adapter cable labeled PUMP to one of the PUMP connectors of the 7-connector interconnect cable.
 - b. Plug the end of the adapter cable labeled MS PUMP into the 8-pin socket on the back panel of the Surveyor MS Pump.



Figure 12. Surveyor Plus LC system connected to an LCQ Fleet MS detector

Making Contact Closure with an Accela LC System

Table 6 lists the firmware for the Accela LC devices supported by the Xcalibur 2.0.5 data system. LC Devices 2.0.2 contains the instrument control software for these devices. For information on making contact closure between the modules of the LC system, refer to the *Accela Getting Connected* manual.

	,		
Device		Firmware version	
Accela Pump		12.47c	
Accela Autosampler		2.15	
Accela PDA Detector		2.01	

Table 6. Firmware versions supported by Xcalibur 2.0.5

To connect an Accela system to the LCQ Fleet MS detector, you must have the adapter cable shown in Figure 11, in addition to the system interconnect cable.

* To connect an LCQ Fleet MS detector to the Accela LC system

- 1. Connect the 8-pin connector with hood (labeled MS/LC) end of the LXQ/LTQ interconnect adapter cable to the M/S connector of the system interconnect cable.
- 2. Connect the open, 6-pin end (labeled LTQ/TXQ) of the adapter cable to the START IN connection (green, 2-pin) on the lower-right side of the MS detector, as shown in Figure 13.

Figure 13. Accela LC connected to an LCQ Fleet MS detector



Not Drawn to Scale

5

Connecting the 4-Port Serial PCB

The 4-Port Serial PCB and Quad DB9 male cable (P/N OPTON-21709) provide four additional communication ports for the data system computer. See Figure 14.

Table 7 lists the Xcalibur kit used with the 4-port serial PCB.

Table 7. Xcalibur Kit used with the 4-Port Serial PCB

Part number	Contents
OPTON-21709	Xcalibur Additional 4-Port Serial Kit: 4-Port Serial PCB (PCI) and software and quad DB (male adapter)

Figure 14. 4-Port Serial PCB and Quad DB9 male cable



* To install the 4-port serial PCB in the data system computer

- 1. Turn off the data system computer.
- 2. Remove the computer cover to expose the PCBs.
- 3. Remove the cover plate from the computer slot where you want to install the 4-port serial PCB.



CAUTION Wear a grounding strap to avoid electrostatic discharge (ESD) damage to the 4-port serial PCB.

- 4. Carefully remove the 4-port serial PCB from its protective shipping bag. Wear a grounding strap to avoid damaging the 4-Port Serial PCB.
- 5. Hold the 4-port serial PCB by its edges and position it so that the 78-pin (small computer system interface [SCSI]) connector faces the back of the computer.
- 6. Plug the 4-port serial PCB into the slot of the computer by firmly pushing the edge of the card into the connector until the card is seated.
- 7. To secure the 4-port serial PCB in place, use the screw from the slot cover plate.
- 8. Replace the computer cover.
- 9. To connect the quad DB9 male cable
 - a. Connect the SCSI port connector of the quad DB9 male cable to the connector located on the 4-port serial PCB.
 - b. Connect one or more of the DB9 connectors to the appropriate inlet devices.
- 10. Restart the data system computer.

The 4-port serial PCB is a Plug and Play device. When Windows starts, it automatically detects and configures the new 4-port serial PCB and loads the appropriate drivers.

Connecting the Inlet Plumbing

This chapter describes how to make the appropriate plumbing connections to introduce sample into the Ion Max-S[™] ion source of the MS detector.

Contents

- Sample Introduction
- Fittings, Tubing, Unions, and Sample Loops
- Setting Up the Inlet for Direct Infusion
- Setting Up the Inlet for High-Flow Infusion
- Setting Up the Inlet for Loop Injections (Flow Injection Analyses)
- Setting Up the Inlet for an LC/MS System with an Autosampler
- Connecting the Grounding Union to the ESI Probe Sample Inlet

Sample Introduction

With the LCQ Fleet MS detector, which has a divert/inject valve and a syringe pump, you can introduce sample into the Ion Max-S API ion source as follows:

- For direct infusion, connect the syringe pump on the front of the MS detector directly to the Ion Max ion source. To push sample into the ion source, set the rate at which the syringe pump depresses the plunger of the syringe.
- For high-flow infusion, connect the syringe pump and the outlet of an LC pump to two legs of a union tee, and then connect the third leg of the union tee to the ion source. To introduce sample into the ion source, set the rate at which the syringe pump depresses the plunger of the syringe and the flow rate of the solvent stream produced by the LC pump.
- For loop injection (flow injection analyses), connect the solvent flow from an LC pump to port 2 of the divert/inject valve, a sample loop to ports 1 and 4 of the valve, and a loop filler to port 5 of the valve. To introduce sample into the ion source, load sample into the sample loop through the loop filler, and then switch the position of the injection valve, allowing the solvent stream to backflush the contents of the sample loop into the ion source.

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• For automated injections using an autosampler, connect the outlet from a liquid chromatography system that contains an autosampler to port 2 of the divert/inject valve. Then set up an autosampler to make automated injections into the solvent flow produced by the LC pump.

Table 8 summarizes the sample introduction and analytical techniques for ESI/MS and APCI/MS.

Sample Introduction into LCQ Fleet Mass Spectrometer	ESI Analytical Technique	APCI Analytical Technique	Procedure for connecting the plumbing
Direct Infusion	Analysis of a pure analyte Automatic calibration and tuning		"Setting Up the Inlet for Direct Infusion" on page 29
High-Flow Infusion (syringe pump injection into LC solvent flow)	Analysis of a pure analyte	Analysis of a pure analyte	"Setting Up the Inlet for High-Flow Infusion" on page 31
Loop injection into LC solvent flow	Analysis of a pure analyte Automatic optimization of tuning using an analyte	Analysis of a pure analyte Automatic optimization of tuning using an analyte	"Setting Up the Inlet for Loop Injections (Flow Injection Analyses)" on page 36

Table 8.	Sample intro	duction and a	analytical tecl	hniques for ES	I/MS and APCI/MS

Fittings, Tubing, Unions, and Sample Loops

The divert/inject valve, located in the upper front of the LCQ Fleet MS detector, is a 6-port, two-position, Rheodyne[™] injection valve. The six ports use standard 10-32 fittings for high-pressure 1/16 in. OD tubing. The LC union and union tee that you use to connect the syringe pump to the ion source also use standard 10-32 fittings for 1/16 in. OD tubing.

IMPORTANT When cutting PEEK tubing, ensure that you make square cuts. Thermo Scientific recommends that you use a tubing cutter to cut the PEEK tubing used to make the inlet plumbing connections.

Table 9 lists the frequently used parts for making plumbing connections for ESI/MS and APCI/MS.

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Part	Part Description	Part Number
	Metal Needle Kit (contains a blunt-tip, 32-gauge stainless steel needle; ferrules; PEEK™ adapter union; and ZDV 1/4-28 union)	OPTON-20014
	Metal Needle Kit (contains a blunt-tip, 34-gauge stainless steel needle; ferrules; PEEK adapter union; and ZDV 1/4-28 union)	OPTON-20015
	Tubing, fused-silica, 0.1 mm ID × 0.4 mm OD (infusion line)	00106-10504
	Tubing, fused-silica, 0.1 mm ID × 0.190 mm OD (fused-silica sample tube and fused-silica capillary tube)	00106-10499
	Tubing, PEEK, 0.005 in. ID \times 1/16 in. OD (red)	00301-22912
	Tube, Teflon [™] , 0.03 in. ID × 1/16 in. OD (for use with syringe needle and LC union)	00301-22915
	Tubing, PVC, unreinforced, 3/8 in. ID (clear) (API probe drain tube)	00301-22895
4	Fitting, Adapter, Kel-F™, Upchurch Scientific™ (connects directly to ESI probe inlet)	00101-18080
	Fitting, Fingertight, Upchurch Scientific (natural) (used with (red) PEEK tubing)	00101-18081
	Ferrule, Kel-F, 0.008 in. ID, Upchurch Scientific (clear) (used with fused-silica tubing and the blunt-tip, 34-gauge stainless steel needle included in Metal Needle Kit)	00101-18114
	Ferrule, Kel-F, 0.012 in. ID, Upchurch Scientific (clear) (used with blunt-tip, 32-gauge stainless steel needle included in Metal Needle Kit)	00101-18116

Part	Part Description	Part Number
	Ferrule, 0.016 in. ID, PEEK, Upchurch Scientific (natural) (for use with fused-silica infusion line)	00101-18120
4	Ferrule, LC, 1/16 in., stainless steel, (used to connect red PEEK tubing to the divert/inject valve)	2522-3830
THE REAL PROPERTY OF	Fitting, grounding union, 1/16 in. orifice, stainless steel	00101-18182
4	Fitting, Fingertight, Upchurch Scientific (red) (used with (red) PEEK tubing)	00101-18195
1	Ferrule, Fingertight 2, Upchurch Scientific (natural) (used with the Teflon tubing and (red) PEEK tubing)	00101-18196
•	Fitting, LC union, 0.010 in. orifice, PEEK (black)	00101-18202
*	Fitting, union tee, 0.020 in. orifice, PEEK (black)	00101-18204
16	Fitting, adapter union, PEEK, Upchurch Scientific (natural) (used with blunt-tip 32- or 34-gauge stainless steel needle, included in Metal Needle Kit)	00101-18206
-Em	Nut, LC 1/16 in. stainless steel, Rheodyne	2522-0066
4	Ferrule, LC 1/16 in. stainless steel, Rheodyne (used to connect the (red) PEEK tubing and the sample loop to the divert/inject valve)	2522-3830
	5 μL sample loop, stainless steel, Rheodyne	00110-22026
	10 μL sample loop, stainless steel, Rheodyne	00110-22012
for 10-32,	20 μL sample loop, stainless steel, Rheodyne	00110-22028
30° ports	50 μL sample loop, stainless steel, Rheodyne	00110-22016
	100 μL sample loop, stainless steel, Rheodyne	00110-22018
	500 μL sample loop, stainless steel, Rheodyne	00110-22020
	1 mL sample loop, stainless steel, Rheodyne	00110-22022

Table 9.	Frequently used	parts for making plumbing	connections for ESI/MS	and APCI/MS (Sheet 2 of 2)
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Setting Up the Inlet for Direct Infusion

To tune and calibrate the LCQ Fleet MS detector, use the syringe pump to infuse a sample solution into the ion source that is set up for the ESI mode.

To introduce sample solution with the syringe pump, you must connect an infusion line between the syringe pump and the grounding union that is held by the grounding bar of the Ion Max-S API ion source. See Figure 15.

To connect the syringe to the grounding union, perform the following procedures:

- "Setting Up the Syringe" on page 30
- "Connecting an Infusion Line to the Grounding Union" on page 30

Figure 15. Connection between the ESI probe and the syringe pump



Setting Up the Syringe

* To fill the syringe, connect it to the LC union, and insert it into the syringe pump

- 1. Fill a clean, 500-µL Unimetrics syringe with your sample solution.
- 2. Connect a 4 cm (1.5 in.) length of Teflon tubing (0.03 in. ID \times 1/16 in. OD) with a fingertight fitting (for a 10-32 receiving port and 1/16 in. OD tubing) and a ferrule to the LC union. See Figure 16.
- 3. Insert the needle of the syringe into the segment of Teflon tube. Check that the needle tip of the syringe fits readily into the opening in the free end of the Teflon tubing. If necessary, you can enlarge the opening in the end of the tubing slightly.



Figure 16. Connecting the syringe and the LC union

- 4. Place the syringe into the syringe holder of the syringe pump.
- 5. While squeezing the blue release buttons on the syringe pump handle, push the handle forward until it just contacts the syringe plunger.

Connecting an Infusion Line to the Grounding Union

- * To connect an infusion line between the LC union and the grounding union
- 1. Connect a section of red PEEK tubing (infusion line) with a fingertight fitting and ferrule (for a 10-32 conical receiving port and 1/16 in. OD tubing) to the free end of the LC union.
- 2. Connect the other end of the infusion line with a fingertight fitting (for a 10-32 port and 1/16 in. OD tubing) and a ferrule to the grounding union.





Setting Up the Inlet for High-Flow Infusion

For high-flow infusion analyses, you connect the syringe pump and the outlet of an LC pump to two legs of a union tee. You connect the third leg of the union tee to the ion source.

To make the plumbing connections for sample introduction from the syringe pump into solvent flow from an LC pump, perform the following procedures in any order:

- "Connecting the Syringe to the Union Tee" on page 32
- "Connecting the Union Tee to the Divert/Inject Valve" on page 32
- "Connecting the LC Pump to the Divert/Inject Valve" on page 34
- "Connecting the Divert/Inject Valve to a Waste Container" on page 34
- "Connecting the Union Tee to the Ion Source" on page 34

Connecting the Syringe to the Union Tee

Use red PEEK tubing and fingertight fittings with ferrules to connect the syringe to the LC union tee.

* To connect the syringe to the LC union tee

- 1. Set up the syringe as described in "Setting Up the Syringe" on page 30.
- 2. Using a fingertight fitting and a ferrule, connect a red PEEK infusion line to the free end of the LC union that is connected to the syringe.
- 3. Using a fingertight fitting and a ferrule, connect the other end of the red PEEK infusion line to the union tee.

Figure 18 shows the fittings required to connect the LC union to the union tee.





Connecting the Union Tee to the Divert/Inject Valve

***** To connect the union tee to the divert/Inject valve

- 1. Using a fingertight fitting and a ferrule, connect a length of red PEEK tubing to port 3 of the divert/inject valve. Alternatively, use a stainless steel nut and ferrule to connect the tubing to the divert/inject valve.
- 2. Using a fingertight fitting and a ferrule, connect the other end of the tubing to the free end of the union tee. See Figure 19 and Figure 20.



Figure 19. Six-port divert/inject valve connections





Connecting the LC Pump to the Divert/Inject Valve

* To connect the LC pump to the divert/inject valve

- 1. Using a fingertight fitting and a ferrule, connect a length of PEEK tubing to port 2 of the divert/inject valve. Figure 19 shows the ports of the divert/inject valve.
- 2. Using an appropriate fitting and ferrule, connect the other end of the tubing to the outlet of the LC.

Connecting the Divert/Inject Valve to a Waste Container

* To connect the divert/ inject valve to a waste container

- 1. Using a fingertight fitting and a ferrule, connect a length of red PEEK tubing to port 1 of the divert/inject valve. Figure 19 shows the ports of the divert/inject valve.
- 2. Insert the other end of the tubing into a suitable waste container.

Connecting the Union Tee to the Ion Source

To connect the union tee to the ion source

- 1. Using a fingertight fitting and a ferrule, connect the one end of a length of red PEEK tubing to the union tee. Figure 21 shows the connections to the union tee.
- 2. Depending on whether you are using the ESI probe or the APCI probe, do one of the following:
 - For the APCI probe, using a fingertight fitting and a ferrule to connect the other end of the tubing directly to the sample inlet of the APCI probe. Figure 21 shows the connection between the union tee and the sample inlet of the APCI probe.

Note You do not use the grounding bar of the Ion Max-S ion source for the APCI probe. A knurled nut secures the grounding bar to the Ion Max-S ion source. You do not need to remove the grounding bar to run the system in the APCI ionization mode.



Figure 21. Plumbing diagram showing APCI/MS sample introduction with high-flow infusion

• For the ESI probe, use a fingertight fitting and a ferrule to connect the other end of the tubing to the grounding union that is held by the grounding bar of the Ion Max-S ion source. See Figure 22 and Figure 23.

The grounding union slides into the grounding bar on the Ion Max-S ion source as shown in Figure 28 on page 40. For instructions on connecting the grounding union to the ESI probe sample inlet, refer to the *Ion Max and Ion Max-S API Source Hardware Manual*.

Figure 22. Connecting the union tee to the grounding union used for the ESI probe





Figure 23. Plumbing diagram showing ESI/MS sample introduction with high-flow infusion

Setting Up the Inlet for Loop Injections (Flow Injection Analyses)

* To set up the inlet for loop injections

1. Connect a loop filler to port 5 of the divert/inject valve. See Figure 24.





- 2. Connect a sample loop to ports 1 and 4.
- 3. To connect the LC pump to port 2 of the divert/inject valve
 - a. Using an appropriate fitting and ferrule, connect one end of a length of red PEEK tubing to the outlet of the LC pump.

To produce a stable solvent flow, the Surveyor MS Pump Plus requires a minimum back pressure of 3 bar (43 psi). To connect the Surveyor MS Pump Plus, use a length of 0.005 in. ID PEEK tubing sufficient to exert a back pressure of 3 bar, or connect an in-line back pressure regulator between the LC pump outlet and the divert/inject valve.

- b. Using a fingertight fitting and a ferrule, connect the other end of the tubing to port 2 of the divert/inject valve.
- 4. Depending on whether you are using the APCI probe or the ESI probe, do one of the following to connect port 3 of the divert/inject valve to the ion source:
 - For the APCI probe, use two fingertight fittings and two ferrules to connect a length of red PEEK tubing between port 3 of the divert/inject valve and the sample inlet of the APCI probe. See Figure 25.





Setting Up the Inlet for Loop Injections (Flow Injection Analyses)

• For the ESI probe, use two fingertight fittings and two ferrules to connect a length of red PEEK tubing between port 3 of the divert/inject valve and the grounding union. See Figure 26. To connect the other end of the grounding union to the ESI probe sample inlet, follow the instructions in the *Ion Max and Ion Max-S API Ion Source Hardware Manual*.





- 5. To connect the divert /inject valve to a waste container:
 - a. Use a fingertight fitting and a ferrule to connect one end of a length of red PEEK tubing to port 6 of the divert/inject valve.
 - b. Place the other end of the tubing to an appropriate waste container.

Setting Up the Inlet for an LC/MS System with an Autosampler

- * To connect the inlet plumbing for an LC/MS system with an autosampler
 - 1. Using an appropriate fitting and ferrule, connect one end of a length of red PEEK tubing to the outlet of your LC system.
 - 2. Using a fingertight fitting and a ferrule, connect the other end of the tubing to port 2 of the divert/inject valve. See Figure 27.





- 3. To connect port 3 of the divert/inject valve to the ion source, do one of the following:
 - For the ESI probe, use two fingertight fittings and two ferrules to connect a length of red PEEK tubing between port 3 of the divert/inject valve and the grounding union. To connect the other end of the grounding union to the ESI probe sample inlet, follow the instructions in the *Ion Max and Ion Max-S API Source Hardware Manual*.
 - For the APCI probe, use two fingertight fittings and two ferrules to connect a length of red PEEK tubing between port 3 of the divert/inject valve and the APCI probe sample inlet.
- 4. To connect the divert /inject valve to a waste container:
 - a. Using a fingertight fitting and a ferrule, connect one end of a length of red PEEK tubing to port 1 of the divert/inject valve.
 - b. Place the other end of the tubing to an appropriate waste container.

Connecting the Grounding Union to the ESI Probe Sample Inlet

For instruction on connecting the PEEK safety sleeve and fused-silica sample tube from the grounding union to the ESI probe sample inlet, refer to the *Ion Max and Ion Max-S API Source Hardware Manual*.

Figure 28. Connecting the grounding union to the sample inlet of the ESI probe



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