

TSQ Series

Getting Connected Guide

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- TSQ Quantum Access MAX
- TSQ Quantum Ultra
- TSQ Vantage
- TSQ Quantum Access

TSQ Quantum Access MAX

EMC Directive 2004/108/EEC

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

EN 55011: 2007, A2: 2007	EN 61000-4-4: 2004
EN 61000-3-2: 2006	EN 61000-4-5: 2005
EN 61000-3-3: 1995, A1: 2001, A2: 2005	EN 61000-4-6: 2007
EN 61000-4-2: 1995, A1: 1999, A2: 2001	EN 61000-4-11: 2004
EN 61000-4-3: 2006	EN 61326-1: 2006

FCC Class A: CFR 47 Part 15: 2007

Low Voltage Safety Compliance

This device complies with European Union Directive 2006/95/EC implemented by 61010-1: 2001.



TSQ Quantum Ultra

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

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

Low Voltage Safety Compliance

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TSQ Vantage

EMC Directive 2004/108/EC

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EN 55011: 1998, A1: 1999, A2: 2002	EN 61000-4-4: 2004
EN 61000-3-2: 2006	EN 61000-4-5: 2006
EN 61000-3-3: 1995, A1: 2001, A2: 2005	EN 61000-4-6: 2001
EN 61000-4-2: 2001	EN 61000-4-11: 2004
EN 61000-4-3: 2006	EN 61326-1: 2006
FCC Class A, CFR 47 Part 15: 2007	CISPR 11: 1999, A1: 1999, A2: 2002

Low Voltage Safety Compliance

This device complies with the Low Voltage Directive 2006/95/EC and harmonized standard EN 61010-1.



TSQ Quantum Access

EMC Directive 89/336/EEC, 92/31/EEC, 93/68/EEC

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

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

Low Voltage Safety Compliance

This device complies with the Low Voltage Directive EN 61010-1:2001 and harmonized standard EN 61010-1: 2001.

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.



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Preface

About This Guide

Your TSQ[™] Series mass spectrometer is part of the Thermo Scientific family of mass spectrometers.

This guide provides information on how to connect a TSQ Series mass spectrometer to line power, the data system computer, the external vacuum system, and the waste exhaust system. In addition, this guide provides information on how to connect external devices, both those controlled from or independent of the Xcalibur[™] data system.

Related Documentation

In addition to this guide, Thermo Fisher Scientific provides the following documentation for TSQ Series mass spectrometers:

- A printed copy of the Safety and Regulatory Guide
- TSQ Series Preinstallation Requirements Guide
- TSQ Series Getting Started Guide
- TSQ Series Hardware Manual
- Ion Max and Ion Max-S API Source Hardware Manual
- H-ESI Probe User Guide
- HESI-II Probe User Guide
- *APPI Source Operator's Manual* (provided on the documentation CD that comes with the hardware)

The *Safety and Regulatory Guide* contains important safety information about Thermo Scientific mass spectrometry and liquid chromatography systems. This document is shipped with every Thermo Scientific mass spectrometer and liquid chromatography device.

To access the manuals for the mass spectrometer, from the Windows[™] taskbar, choose **Start > All Programs > Xcalibur > Manuals >** *Brand name of mass spectrometer*, and then click the listing for the PDF that you want to view. The software also provides Help. To access the Help, choose **Help** from the menu bar or click ? (Help) 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.



CAUTION Highlights electric shock hazards. Alerts you to the potential injury that could occur from electrical shock were you to come in contact with a specific instrument area or component.

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.

Safety Precautions for the H-ESI and ESI Modes

When operating the TSQ Series mass spectrometer in the H-ESI or ESI modes, ensure that you use the stainless steel grounding union supplied in the MS Accessory Kit to connect the inlet plumbing.



CAUTION To prevent an electric shock hazard, use the stainless steel grounding union supplied in the MS Accessory Kit. Do not use a grounding union made of a non-conductive material such as PEEK.

H-ESI mode

ESI mode





Contacting Us

There are several ways to contact Thermo Fisher 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.

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• Send an e-mail message to the Technical Publications Editor at techpubs-lcms@thermofisher.com.

Vacuum System, Gases, Ethernet Communication, and Line Power

This chapter describes how to connect a TSQ Series mass spectrometer to forepumps, necessary gases, the data system computer, and line power.

Contents

- Connecting the Forepumps to the Mass Spectrometer
- Connecting the Gases to the Mass Spectrometer
- Connecting the Mass Spectrometer to the Data System Computer
- Connecting the Mass Spectrometer to Line Power

Connecting the Forepumps to the Mass Spectrometer

Depending on the size of the ion transfer tube, the TSQ Series mass spectrometers require one or two forepumps. Table 1 lists the forepump requirement for the TSQ Series mass spectrometers.

 Table 1.
 Forepump requirement

One forepump	Two forepumps
TSQ Quantum [™] Access [™]	TSQ Quantum Ultra [™]
TSQ Quantum Access MAX	TSQ Quantum Ultra AM
	TSQ Quantum Ultra EMR
	TSQ Vantage™
	TSQ Vantage AM
	TSQ Vantage EMR

To connect the forepumps (also known as a mechanical pumps or rotary-vane pumps) to the mass spectrometer and the laboratory exhaust system, follow these procedures:

- Connecting One or Two Forepumps to the Mass Spectrometer
- Connecting the Forepumps to the Laboratory Exhaust System

Connecting One or Two Forepumps to the Mass Spectrometer

Follow these procedures to connect the forepump or forepumps to the vacuum port and then to line power:

- Connecting One or Two Forepumps to the Vacuum Port
- Connecting One or Two Forepumps to Line Power

Connecting One or Two Forepumps to the Vacuum Port

Figure 1 shows the vacuum hose assemblies used to connect one or two forepumps to the mass spectrometer. Table 2 lists the part numbers of these assemblies and their subcomponents. Table 3 lists the additional parts required to connect the appropriate vacuum hose assembly to one or two forepumps. These additional parts are supplied in the Mechanical Pump Kit.

Figure 1. Vacuum hose assemblies



Description		Part number
Single foreline vacuum hose assembly		70111-60480
Dual foreline vacuum hose assembly		70111-60481
Vacuum hose assembly subco	mponents:	
Vacuum hose, 1.5 in.	ID	00301-24163
	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 2.16 in. OD (adapter for the MS vacuum port)	97055-20714
	Adapter, 1.5 in. OD (adapter for the forepump)	70111-20210
	3-port manifold, 1.5 in.	97055-20222

Table 3. Parts required to connect the vacuum hose to the vacuum port of the forepump

Description		Part number
\bigcirc	Centering ring with O-ring, NW25, 26 mm ID, aluminum and Viton™	00108-02011
	Swing clamp, NW20/25, ISO-KF	00102-10020

* To connect the vacuum hose assembly to the mass spectrometer vacuum port

- 1. Connect the end of the vacuum hose assembly that has a 2.16 in. OD adapter to the mass spectrometer vacuum port:
 - a. Place the 41 mm (1.6 in.) ID centering ring on the flange of the mass spectrometer vacuum port. The vacuum port is located on the left side of the mass spectrometer (see Figure 2).
 - b. Using a NW32/40 swing clamp, secure the vacuum hose to the mass spectrometer vacuum port.



Figure 2. Connecting the vacuum hose assembly to the mass spectrometer

- 2. To connect the vacuum hose assembly to each required forepump, do the following:
 - a. Place a 26 mm (1.0 in.) ID centering ring on the flange of the forepump inlet port.
 - b. Using a NW20/25 vacuum clamp, secure the vacuum hose assembly (foreline with a 1.5 in. OD adapter) to the forepump.

The appropriate vacuum hose assembly is supplied with the mass spectrometer (see Figure 1 on page 2). Figure 3 shows the vacuum hose assembly, centering rings, and clamps used to connect two forepumps to the TSQ Series mass spectrometer.

Figure 3. Connecting two forepumps to the mass spectrometer (view from the rear panel of the mass spectrometer)



Mass spectrometer (back panel)

Connecting One or Two Forepumps to Line Power

The forepumps get their line power from the mass spectrometer. The power outlets for the forepumps are located on the power panel of the mass spectrometer. Depending on the forepump requirement, the power panel contains one or two forepump outlets (see Figure 4 and Figure 5).



CAUTION Always plug the forepump power cords into the outlets labeled Forepump on the right side of the mass spectrometer. Never plug them directly into a wall outlet.

To connect the forepump to line power

- 1. On the power panel, switch the Main Power circuit breaker to the Off position (see Figure 4).
- 2. Connect the forepump power cord plug to the Forepump power receptacle on the mass spectrometer power panel. If the mass spectrometer requires two forepumps, its power panel contains two forepump receptacles.
- 3. Turn on the forepump power switch (see Figure 6).





receptacle



Main Power circuit breaker





Figure 6. View of the forepump power switch

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Connecting the Forepumps to the Laboratory Exhaust System

The proper operation of the forepumps 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 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.

Table 4 lists the parts required to connect the exhaust hose to the forepump.

Table 4. Parts required to connect the exhaust ho	ose
---	-----

Description		Part number
	Exhaust hose, blue, 1.0 in. ID, 10 ft length, supplied in the MS Ship Kit	00301-08301
PREZE	Hose clamps (2×)	00108-09001

- * To connect the exhaust port of the forepump to the laboratory exhaust system
 - 1. Using hose clamps, 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.

Allow the exhaust hose to 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 7 shows the blue exhaust hose connected to the optional oil mist filter. Figure 7 also shows the waste drain from the Ion Max API source connected to the solvent waste container.

For instructions on how to connect the Ion Max API source to the solvent waste bottle, see "Connecting the Source Housing Drain to the Waste Container" on page 19.



CAUTION Because the forepump exhaust is a health hazard, vent the forepump exhaust to an external exhaust system.

Figure 7. Exhaust and drainage systems



separate external exhaust system

Connecting the Gases to the Mass Spectrometer

This section describes how to connect the required gases to the TSQ Series mass spectrometer set up for the API mode. The TSQ Series mass spectrometer uses nitrogen for the API sheath gas, sweep gas, and auxiliary gas, and argon for the collision gas. The gas line connections are located on the lower-left side of the mass spectrometer. See Figure 8.



Figure 8. Left side of the TSQ Series mass spectrometer

To connect the gas lines, follow these procedures:

- Connecting the Nitrogen Source
- Connecting the Argon Source

Connecting the Nitrogen Source

The TSQ Series mass spectrometer requires high purity (99%) nitrogen for the API sheath gas, sweep gas, and auxiliary gas. Because nitrogen gas usage can be quite high, Thermo Fisher 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).

Terminate the nitrogen gas supply line with the connectors supplied in the MS Accessory Kit and listed in Table 5.

Table 5.	Nitrogen gas	line parts
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Description	Part number
Brass Swagelok [™] -type 1/4 in. nut	00101-12500
2-piece brass 1/4 in. ferrule	
• Front	00101-10000
• Back	00101-04000

* To connect the nitrogen source to the mass spectrometer

1. Connect an appropriate length of 1/4 in. ID Teflon[™] tubing with a brass Swagelok-type 1/4 in. nut and a 2-piece brass 1/4 in. ferrule to the nitrogen source regulator.

See Figure 9 on page 12 for the proper orientation of the fitting and ferrule.

2. Connect the opposite end of the Teflon tubing to the press-in fitting labeled NITROGEN IN and located on the left side of the mass spectrometer (Figure 8). 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 Argon Source

The argon for the 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 135 ± 70 kPa (20 ±10 psi). Because particulate filters can be a source of contamination, Thermo Fisher Scientific does not recommend their use.

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

Whether you choose copper or stainless steel gas lines for the argon, use gas lines that are free of oil and preferably flame dried. Run the gas lines on the left side of the TSQ Series mass spectrometer. Terminate the argon gas supply line with the connectors supplied in the MS Accessory Kit and listed in Table 6.

Description	Part number
Brass Swagelok-type 1/8 in. nut	00101-15500
2-piece brass 1/8 in. ferrule	
• Front	00101-08500
• Back	00101-02500

 Table 6.
 Argon gas line parts

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

* To connect the argon source to the TSQ Series mass spectrometer

1. Connect an appropriate length of 1/8 in. ID copper or stainless steel tubing with a brass Swagelok-type 1/8 in. nut and a 2-piece brass 1/8 in. ID ferrule to the ARGON IN gas inlet located on the left side of the mass spectrometer (Figure 8).

See Figure 9 for the proper orientation of the fitting and ferrule.

2. Connect the opposite end of the tubing to the argon gas source, using an appropriate fitting.





Connecting the Mass Spectrometer to the Data System Computer

The data system for the mass spectrometer consists of a computer, a monitor, and an optional printer. The mass spectrometer communicates with the data system computer through an Ethernet connection (see Figure 10).

Table 7 lists the parts required to connect the data system computer to the mass spectrometer. These parts are supplied in the MS Ship Kit.

 Table 7.
 Parts required to connect the data system computer to the mass spectrometer

Description	Part number
Category 5 network Ethernet cable (2×)	00302-01838
10/100 Base-T Ethernet switch, 5-port, 100 to 240 V	00825-01-00024

* To connect the mass spectrometer to the data system computer

- 1. Connect a category 5 network Ethernet cable to the ETHERNET 100 BASE-T connector located on the TSQ Series power panel.
- 2. Connect the opposite end of the Ethernet cable to the 10/100 Base-T Ethernet switch provided with the mass spectrometer.
- 3. Connect a second category 5 network Ethernet cable from the Ethernet switch to the Ethernet card on the data system computer labeled Surveyor MS.



Figure 10. Ethernet connections

Connecting the Mass Spectrometer to Line Power

The mass spectrometer power panels of the TSQ Vantage and TSQ Quantum Ultra include the Main Power circuit breaker, the Electronics switch, and the POWER IN receptacle. In addition to these controls, the TSQ Quantum Access and TSQ Quantum Access MAX have a Vacuum switch. The power panel is located on the right side of the mass spectrometer.

* To connect the mass spectrometer to line power

- 1. Turn the Main Power circuit breaker to the Off (O) position.
- 2. Ensure that the Electronics switch is in the Service Mode position. For the TSQ Quantum Access or TSQ Quantum Access MAX, also ensure that the Vacuum switch is in the Service Mode position.

Figure 11. Main Power circuit breaker, Electronics switch, and Vacuum switch

TSQ Vantage or TSQ Quantum Ultra



- 3. Connect the female plug of the power cord to the POWER IN receptacle on the power panel (Figure 12).
- 4. Connect the male plug of the power cord to the 230 V ac power source in your laboratory (Figure 12).
- 5. Connect the data system PC and the Ethernet switch to an appropriate wall outlet (Figure 12). Do **not** connect these system components to the same wall outlet as the mass spectrometer.



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 *TSQ Series Preinstallation Requirements Guide*. The UPS must be certified by both North American (UL, CSA) and European Agencies (TUV, UDE, SEMKO, DEMKO, and so on).

Figure 12. Connecting the mass spectrometer, data system PC, and Ethernet switch to line power



Right side of the TSQ Quantum Access or TSQ Quantum Access MAX

Connecting Probes

This chapter describes how to connect an ion source probe to the TSQ Series mass spectrometer equipped with an Ion Max or Ion Max-S API source.

Contents

- Connecting the ESI, H-ESI, or HESI-II Probes
- Connecting the APCI Probe
- Connecting the Source Housing Drain to the Waste Container

Connecting the ESI, H-ESI, or HESI-II Probes

- To connect liquid lines to the electrospray ionization (ESI) or heated electrospray ionization (H-ESI or HESI-II) probes
- 1. Install the Ion Max source housing as described in the *Ion Max and Ion Max-S API Source Hardware Manual.*
- 2. Depending on the type of probe, do one of the following:
 - Install the ESI probe on the Ion Max source housing as described in the *Ion Max and Ion Max-S API Source Hardware Manual.*
 - Install the H-ESI probe on the Ion Max housing as described in the *H-ESI Probe User Guide*.
 - Install the HESI-II probe on the Ion Max housing as described in the *HESI-II Probe* User Guide.
- 3. 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 4, "Connecting the Inlet Plumbing."
- 4. Connect the source housing drain to the solvent waste container, and vent the waste container to a fume exhaust system (see "Connecting the Source Housing Drain to the Waste Container" on page 19).

Connecting the APCI Probe

- * To connect liquid lines to the atmospheric chemical ionization (APCI) probe
- 1. Install the Ion Max or Ion Max-S source housing and APCI probe 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 4, "Connecting the Inlet Plumbing."
- 3. Connect the source housing drain to the solvent waste container, and vent the waste container to a fume exhaust system (see "Connecting the Source Housing Drain to the Waste Container" on page 19).

Note If you need to install or replace the APCI sample tube, refer to the *Ion Max and Ion Max-S API Source Hardware Manual*.

Connecting the Source Housing Drain to the Waste Container

When you reinstall the Ion Max or Ion Max-S API source, reconnect the drain at the bottom of the source housing to the solvent waste container (see Figure 13).





When you reconnect the drain tubing to the drain at the bottom of the Ion Max or Ion Max-S API source, ensure that you connect the Teflon source drain adapter, which can withstand the high temperatures produced by the H-ESI or APCI source, to the source drain. In addition, ensure that the tubing assembly includes at least 1 m (3 ft) of 1 in. ID Tygon tubing.

IMPORTANT Do **not** connect Tygon tubing directly to the source drain. At high temperatures, Tygon releases volatile contaminates.

IMPORTANT Do not connect silicone tubing to the API source outlet drain. If silicone tubing is connected to the outlet drain, you might observe background ions at m/z 536, 610, and 684. Use the silicone tubing that is provided with the filling/venting cap to connect 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.

IMPORTANT Your laboratory must be equipped with at least two fume exhaust systems:

The analyzer optics can become contaminated if the API source drain tube and the (blue) exhaust tubing from the forepumps are connected to the same fume exhaust system. Route the (blue) exhaust tubing from the forepumps to a dedicated fume exhaust system.

Do **not** vent the PVC drain tube (or any vent tubing connected to the waste container) to the same fume exhaust system that you have connected the forepumps to. Vent the waste container to a dedicated fume exhaust system.

Excessive draw from the fume exhaust system to the API source drain line can affect the system performance. Thermo Fisher Scientific recommends a maximum flow rate of 30 L/min.

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

Table 8.	Solvent waste system parts
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Part description	Part number	Kit location
Source drain adapter, Teflon	70111-20971	MS Accessory Kit
Reducing connector, single barbed fitting, 1 in.×0.5 in.	00101-03-00001	MS Ship Kit
Tubing, Tygon [™] PVC, 1 in. ID×1.1875 in. OD	00301-22922	MS Ship Kit
Tubing, Tygon, 0.5 in. ID×0.75 in. OD	00301-22920	MS Ship Kit
Cap, filling/venting	00301-57022	MS Ship Kit
Heavy-duty, 4 L Nalgene™ bottle	00301-57020	MS Ship Kit

Connecting 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 9 lists the Xcalibur kits for various external devices.

For additional information on connecting LC devices controlled from the Xcalibur data system, refer to the appropriate manual provided on the LC Devices software CD.

Contents

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

Table 9. Xcalibur kits for various external devi
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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-30012	 Ethernet Communication Kit Ethernet switch Cable, trigger external contact, 2-wire DB15 Cable, patch, 3 m (10 ft) CAT5 RJ45, straight shield

3

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 Fisher Scientific Inc., Agilent Technologies, and Waters Corporation. Contact your Thermo Fisher Scientific sales representative for information on the liquid chromatography systems compatible with your TSQ Series mass spectrometer.

The mass spectrometer can start data acquisition upon receiving a contact closure signal from an external device, typically an autosampler. The TSQ Series mass spectrometer receives contact closure signals through a trigger cable connected 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 TSQ Series mass spectrometer I/O PCB. These integrated circuits fail if more than 5 V or 5 mA are applied to the system.

To connect an external device such as a liquid chromatography system to your TSQ Series mass spectrometer, follow these procedures:

- Making Contact Closure with Devices Controlled by Xcalibur
- Selecting the Appropriate Start Instrument

Making Contact Closure with Devices Controlled by Xcalibur

Thermo Fisher Scientific provides instructions for connecting supported liquid chromatography systems to a Thermo Scientific mass spectrometer. You can access the appropriate instruction guide from the data system computer.

* To connect the contact closure cable

1. Connect the appropriate contact closure cable to the Start In pins located on the power entry panel of the mass spectrometer.

Figure 14 shows the contact closure connection between an Accela LC system and a TSQ Series mass spectrometer. For more information on how to connect an Accela LC system to a TSQ Series mass spectrometer, refer to the *Accela Getting Connected Guide*.




Not drawn to scale

2. To connect the external device, follow the instructions in the appropriate manual.

The LC Devices CD contains manuals for the LC devices controlled from the Xcalibur data system. If these manuals were downloaded during the installation of the LC device drivers, you can access them by choosing the following from the Windows taskbar:

Start > All Programs > Xcalibur > Manuals > LC Devices > Product name

Note For LC Devices versions higher than 2.2.0, the manuals link location is subject to change.

Selecting the Appropriate Start Instrument

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

* To ensure that Xcalibur lists the appropriate device as the start instrument

1. On the Roadmap view of the Xcalibur Home Page, click i (Sequence Setup).

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 close 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. See Figure 15. The Yes in the Start Instrument column indicates that the Accela Autosampler is set up as the default start instrument once the sequence run begins.

Run Sequence	
Acquisition Options Instrument Start Instrument Accela AS Yes Accela PUMP Accela PDA TSQ Quantum Change Instruments Instrument Method Browse Start Up Browse Shut Down Browse Programs Pre Acquisition Run Synchronously Instrument Acquisition Acquisition Prost Acquisition	User: cook Run Rows: 1 Priority Sequence Processing Actions Quan Qual Reports Programs Create Quan Summary
© On C Standby C Off	
OK Cancel	Help

Figure 15. Run Sequence dialog box with the Accela AS selected as the start instrument

- 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 Accela Autosampler selected as the start instrument. See Figure 16.

С	hange Instruments In L	Jse		X
	Instrument Accela AS Accela Pump Accela PDA TSQ Quantum	In Use Yes Yes Yes Yes	Start Instrument Yes	
	0K	Cancel	Help	

Figure 16. Change Instruments In Use dialog box

- 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.

To connect an external device, such as a liquid chromatography system, to your TSQ Series mass spectrometer, follow these procedures:

- Making Contact Closure with Devices Not Controlled by Xcalibur
- Starting a Sequence Run from Xcalibur

Making Contact Closure with Devices Not Controlled by Xcalibur

To connect the contact closure cable

Note To start data acquisition on the TSQ Series mass spectrometer, 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 TSQ Series mass spectrometer.

- 1. Connect the 2-wire trigger cable (in kit P/N OPTON-21705) to the Start In pins on the power entry panel of the TSQ Series mass spectrometer.
- 2. Connect the cable to the contact closure terminal of the external device, following the wiring scheme listed in Table 10.
- Table 10. Wiring the TSQ Series mass spectrometer for contact closure with an external device not controlled by the Xcalibur data system

TSQ Series mass spectrometer power entry panel	External device contact closure terminal
TTL IN 1	Output (start) terminal
DIGITAL GROUND	Ground terminal

Figure 17 shows a block diagram of the contact closure connection to an external device.

Figure 17. Schematic of the contact closure connection between the mass spectrometer 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 TSQ Series mass spectrometer as the start instrument for a sequence run. When you are ready to inject a set of samples, ensure that the TSQ Series mass spectrometer is **not** listed as the start instrument in Xcalibur.

To start the sequence run *

- 1. On the Roadmap view of the Xcalibur Home Page, click (Sequence Setup) 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.
- с. Click **Open** to open the sequence and close the Open dialog box.

Sequence files have an .sld file extension.

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

The Run Sequence dialog box appears (see Figure 18).

Run Sequence	
Acquisition Options Instrument Start Instrument TSQ Quantum ✓ Start When Ready Change Instruments Instrument Method Browse Start Up Browse Shut Down Browse	User: cook Run Rows: 1 Priority Sequence Processing Actions Quan Qual Reports Programs
Pre Acquisition Browse Post Acquisition Browse Run Synchronously Image: Pre Acquisition Image: Pre Acquisition Image: Post Acquisition After Sequence Set System: Image: On the other standard stan	Create Quan <u>S</u> ummary

Figure 18. Run Sequence dialog box

4. Click Change Instruments.

The Change Instruments In Use dialog box appears. See Figure 19.

Figure 19. Change Instruments In Use dialog box with no start instrument specified

С	hange Instruments In l	lse			
	Instrument TSQ Quantum	In Use Yes	Start Instrument	_	The mass spectrometer is not selected as the start instrument
	OK	Cancel	<u>H</u> elp		

- 5. In the Start Instrument column, ensure that the TSQ Series mass spectrometer is not specified as the start instrument:
 - If **Yes** appears in the Start Instrument column, click **Yes** to change the mode to Off (field becomes blank), and then click **OK** to save the setting and close the dialog box.
 - If **Yes** does not appear in the Start Instrument column, click **OK** to close the dialog box.
- 6. In the Acquisition Options area of the Run Sequence dialog box, select the **Start When Ready** check box, and click **OK**. The settings are saved, the dialog box closes, and the sequence starts or gets appended to the queue.

The instrument method downloads to the TSQ Series mass spectrometer, and the Status page displays the following message:

Waiting - Contact Closure

If the Roadmap view of the Home Page does not display the Info view, click []. (Information View) to display it, and then click the **Status** tab to display the Status page.

7. Start the external device.

An acquisition from the TSQ Series mass spectrometer begins after the external device sends the "Contact Closure" signal that the mass spectrometer is waiting for.

In situations where the Xcalibur data system does not have any control of external devices such as autosamplers, control might be through a third-party data system or a built-in control system. For example, you can control the SpectraSYSTEM[™] AS3000 autosampler from its front panel command center. See Figure 20.

Note Because LC Devices does not include support for the Thermo Scientific SpectraSYSTEM LC modules, the SpectraSYSTEM autosampler is considered an external device outside Xcalibur data system control.

Figure 20. SpectraSYSTEM LC system



Connecting the Inlet Plumbing

This chapter describes how to make the plumbing connections to introduce sample into the atmospheric pressure ionization (API) source of the mass spectrometer.

In addition to the instructions provided in this chapter, the *TSQ Quick Reference Library* contains quick connections guides that describe the inlet plumbing.

Contents

- Introducing Sample
- Setting Up the Syringe Pump
- Setting Up the Inlet for Direct Infusion
- Setting Up the Inlet for High-Flow Infusion
- Setting Up the Inlet for Manual or Auto-Loop Injections
- Setting Up the Inlet for an LC/MS System with an Autosampler
- Connecting the Grounding Union to the ESI, H-ESI, or HESI-II Probe Sample Inlet

Introducing Sample

The following topics describe the hardware and the techniques used to introduce sample into the mass spectrometer ion source:

- Sample Introduction Techniques
- Divert/Inject Valve
- Divert/Inject Valve
- Fittings, Tubing, Unions, and Sample Loops

Sample Introduction Techniques

Technique	Use	Reference
Direct infusion	Automatic tuning and calibration in the ESI or H-ESI modes	"Setting Up the Inlet for Direct Infusion" on page 42
	Or tuning on a pure sample in the ESI, H-ESI, or APCI modes	
High-flow infusion	Tuning on an analyte of interest using the same flow rate and mobile phase composition that you plan to use for your LC/MS experiment	"Setting Up the Inlet for High-Flow Infusion" on page 45
Manual loop injection without chromatographic separation	Qualitative or quantitative analysis when you have a limited amount of a pure sample	"Setting Up the Inlet for Manual or Auto-Loop Injections" on page 51
Manual loop injection with chromatographic separation	Qualitative or quantitative analysis when you have a limited amount of a sample mixture	-
	Requires an LC column between the injection valve and the API source	
Auto-loop injection	Optimizing the mass spectrometer's sensitivity to a compound for an MS/MS experiment	-
High-performance liquid chromatography (HPLC) including an autosampler	Qualitative or quantitative analysis of a sample mixture	"Setting Up the Inlet for an LC/MS System with an Autosampler" on page 56

You can use the following techniques to introduce samples into the mass spectrometer.

A block schematic of these sample introduction techniques is shown in Figure 21. The connections from the LC outlet or from the syringe pump to the divert/inject valve are made with fingertight fittings and red PEEK tubing. The connection between the divert/inject valve and the waste container is made with a fingertight fitting and 0.03 in. ID \times 1/16 in. OD Teflon tubing.



Figure 21. Block schematic of sample introduction techniques

Divert/Inject Valve

The TSQ Series mass spectrometer includes a motorized, stainless steel, six-port, two-position, Rheodyne[™] valve, located on the front panel of the mass spectrometer above the API source. You can configure (plumb) the divert/inject valve as a loop injector for flow-injection analysis or as a divert valve for direct infusion, high-flow infusion, or LC/MS experiments.

You can control the divert/inject valve from the data system or by pressing the blue button above the valve (see Figure 22). The LEDs above the button indicate the valve position.



Figure 22. View of the divert/inject valve with its control button and LED indicators

In the divert valve configuration (Figure 23), the valve switches between these two positions:

- Detector. Solvent flow from the LC pump enters the valve through port 2 and exits the valve through port 3 toward the detector.
- Waste. Solvent flow from the LC pump enters the valve through port 2 and exits the valve through port 1 to waste.
- Figure 23. Divert valve positions



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In the injection valve configuration (Figure 24), the valve switches between these two positions:

- Load. The sample loop is isolated from the solvent stream. Solvent flow from the LC pump enters and exits the valve through ports 2 and 3, respectively. When you load the sample through port 5, the sample enters and exits the sample loop through ports 4 and 1, respectively. As you overfill the sample loop, the sample exits the valve through port 6 to waste.
- Inject. The sample loop is open to the solvent stream. The LC pump solvent flow flushes sample out of the sample loop, and then out of the valve through port 3 toward the API source.





Syringe Pump

The TSQ Series mass spectrometer includes an electronically-controlled, integrated syringe pump. See Figure 25. The syringe pump delivers sample solution from an installed syringe into the atmospheric pressure ionization (API) source. When the syringe pump is operating, a motor drives a pusher block that depresses the plunger of the syringe at a rate that is specified in the data system. (The default flow rate is $3 \mu L/min$.) Liquid flows out of the syringe needle and into the sample transfer line as the plunger is depressed. A syringe holder holds the syringe in place. To set up the syringe pump, see "Setting Up the Syringe Pump" on page 41.

You can start and stop the syringe pump from the Tune Master window. Refer to Tune Master Help for instructions on operating the syringe pump from the data system. You can also start and stop the syringe pump by pressing the syringe pump button. You can run the syringe pump in Purge mode, where the flow rate is five percent of the syringe volume per second, by holding down the button.

The syringe pump light-emitting diode (LED) illuminates green whenever the syringe pump is pumping. The LED illuminates yellow when the drive screw is at the end of its travel.

To connect the syringe needle to the inlet plumbing, use a short length of Teflon tubing (0.03 in. ID \times 1/16 in. OD) as an adapter and an LC union (Figure 25).





Fittings, Tubing, Unions, and Sample Loops

This topic provides guidelines and a replaceable parts list for connecting the inlet plumbing.

Making the Plumbing Connections

When you make the plumbing connections, ensure the following:

- The ends of the PEEK tubing are squarely cut (see Figure 26). For best results, use a polymeric tubing cutter to ensure square cuts. Poorly cut tubing can cause flow restrictions.
- The PEEK tubing makes contact with the bottom of the receiving port (see Figure 26). Tubing that is not properly seated can add dead volume to a chromatographic system.
- The fittings are not overtightened. Tighten PEEK fittings fingertight. Do not use a wrench to tighten PEEK fittings. Overtightening PEEK fittings can cause leaks.



Figure 26. Making a proper connection

The divert/inject valve, located on the front panel of the mass spectrometer above the API source, is a six-port, two-position, Rheodyne injection valve. The six ports use standard 10-32 fittings for high-pressure, 1/16 in. OD tubing. See Figure 27. To connect high-pressure tubing to the valve, use the one-piece fingertight fittings provided in the MS Accessory Kit.

Figure 27. Internal view of the divert/inject valve ports



Ordering Parts

Table 11 lists the parts such as fittings, tubing, and unions used to connect the inlet plumbing. The MS Accessory Kit (P/N 70111-62034) contains many of the parts you need.

 Table 11. Frequently used parts for making the inlet plumbing connections

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 \times 0.190 mm OD	00106-10499
	Tubing, red PEEK, 0.005 in. ID \times 1/16 in. OD	00301-22912
	Tube, Teflon, 0.03 in. ID \times 1/16 in. OD, precut 0.1 ft length	00301-22915
	Fitting, adapter, 10-32 to 1/4-28 PEEK, 0.040 in. (1.0 mm) thru-hole (for the ESI or H-ESI probe sample inlet)	00101-18080
	Fitting, two-piece, fingertight, natural PEEK, for 1/16 in. OD high-pressure tubing	00101-18081
	Ferrule, 0.016 in. ID, natural PEEK (for use with fused-silica infusion line)	00101-18120
	Fitting, grounding union, 1/16 in. orifice, stainless steel	00101-18182
	Fitting, fingertight, for 1/16 in. OD high pressure tubing	00101-18195
	Ferrule, Fingertight 2, natural PEEK, for 1/16 in. OD high-pressure tubing	00101-18196
(P)	Fitting, LC union, 0.010 in. thru-hole, black PEEK	00101-18202
	Fitting, union Tee, 0.020 in. thru-hole, black PEEK	00101-18204
	Fitting, one-piece fingertight, 10-32, high pressure, natural PEEK, for 1/16 in. OD tubing (Upchurch F-120)	00109-99-00016
	5 μL sample loop, stainless steel, Rheodyne	00110-22026

Setting Up the Syringe Pump

This section describes how to set up the syringe pump.

Note You can use the syringe pump to directly infuse sample into the source, to infuse sample into the solvent stream produced by an LC pump, or to automatically load sample into the divert/inject valve.

Table 12 lists the fittings and tubing required to connect the LC union to the syringe needle. The MS Accessory Kit contains the Syringe Adapter Kit (P/N 70005-62011) with these fittings and tubing.

Table 12. Fittings and tubing required to set up the syringe

Part	Description
(D)	LC union, PEEK, 10-32, for fingertight fittings and 1/16 in. OD tubing, 0.01 in. thru-hole
	Two-piece fingertight fitting for 1/16 in. OD tubing, PEEK, 10-32
	Teflon tubing, 4 cm (1.5 in.) length, 0.03 in. ID \times 1/16 in. OD

* To set up the syringe for infusion or high-flow infusion experiments

- 1. Fill a clean syringe with your sample solution.
- 2. Using a two-piece fingertight fitting, connect a 4 cm (1.5 in.) length of Teflon tubing (0.03 in. ID \times 1/16 in. OD) to the black PEEK LC union. See Figure 28.
- 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, use the needle tip to enlarge the opening slightly in the end of the tubing.





- 4. Place the syringe into the syringe holder of the syringe pump.
- 5. While squeezing the release button on the pusher block, lower the pusher block until it just contacts the syringe plunger (see Figure 25 on page 38).

Setting Up the Inlet for Direct Infusion

This section describes how to connect the inlet plumbing to introduce sample into the ion source by direct infusion.

Table 13 lists the fittings and tubing required to plumb the system for direct infusion, including the fittings and tubing required to set up the syringe pump.

For information on connecting the fused-silica capillary between the grounding union and the ESI or H-ESI sample inlet port, refer to the *Ion Max and Ion Max-S API Source Hardware Manual* or the *H-ESI Probe User Guide*, respectively.

Table 13. Fittings and tubing required to set up the system for a direct infusion experiment

Part	Description
	Grounding union, stainless steel, zero dead volume (ZDV), for 1/16 in. OD tubing, 0.01 in. thru-hole
	LC union, black PEEK, 10-32, for fingertight fittings and 1/16 in. OD tubing, 0.01 in. thru-hole
	Two-piece fingertight fitting for 1/16 in. OD tubing, natural PEEK, 10-32
	Teflon tubing, 4 cm (1.5 in.) length, 0.03 in. ID \times 1/16 in. OD
	Red PEEK tubing $(0.005 \text{ in. ID} \times 1/16 \text{ in. OD})$

Figure 29 shows a TSQ Series mass spectrometer set up to introduce sample by direct infusion in the ESI mode.



Figure 29. TSQ Series mass spectrometer set up for direct infusion in the ESI mode

* To connect an infusion line between the LC union and the grounding union

- 1. Set up the syringe pump (see "Setting Up the Syringe Pump" on page 41).
- 2. Connect the infusion line as follows:
 - Using a two-piece fingertight fitting, connect a section of red PEEK tubing (infusion line) to the free end of the LC union.
 - Using a two-piece fingertight fitting, connect the other end of the infusion line to the stainless steel grounding union.

Figure 30 shows the connection between the LC union and the grounding union made with red PEEK tubing and fingertight fittings. For the ESI probe, the grounding union is held by the Ion Max or Ion Max-S grounding bar (see Figure 40 on page 60). For the H-ESI or HESI-II probe, the grounding union is held by the grounding union holder connected to the probe (Figure 41 on page 61).



Figure 30. Connecting the infusion line to the LC union and the grounding union

3. Connect the grounding union to the ESI or H-ESI probe sample inlet. See "Connecting the Grounding Union to the ESI, H-ESI, or HESI-II Probe Sample Inlet" on page 59.

Setting Up the Inlet for High-Flow Infusion

The sections describes how to connect the inlet plumbing to introduce sample into the ion source by high-flow infusion.

Table 14 lists the fittings and tubing required to set up the system for high-flow infusion, including the fittings and tubing required to set up the syringe pump.

Part	Description
	Grounding union, stainless steel, zero dead volume (ZDV), for 1/16 in. OD tubing, 0.01 in. thru-hole
	LC union, PEEK, 10-32, for fingertight fittings and 1/16 in. OD tubing, 0.01 in. thru-hole
	Two-piece fingertight fitting for 1/16 in. OD tubing, PEEK, 10-32
	Fitting, union Tee, 0.020 in. thru-hole, black PEEK
	Fitting, one-piece fingertight, 10-32, high pressure, natural PEEK, for 1/16 in. OD tubing
	Teflon tubing, 0.03 in. ID \times 1/16 in. OD, sufficient length to connect port 1 of the divert/inject valve to a waste container
	Red PEEK tubing (0.005 in. ID×1/16 in. OD)

Table 14. Fittings and tubing required to plumb the system for high-flow infusion

Figure 31 shows a TSQ Series mass spectrometer set up to perform a high-flow infusion experiment in the ESI mode.



Figure 31. TSQ Series mass spectrometer set up to perform a high-flow infusion experiment in the ESI mode

To set up the system for a high-flow infusion experiment, make the following six connections in any order:

Connection	What to connect	Reference
#1	Connect the syringe to the union Tee.	"Connecting the Syringe to the Union Tee" on page 47
#2	Connect the union Tee to the divert/inject valve.	"Connecting the Syringe to the Union Tee" on page 47
#3	Connect the outlet of the LC pump to the divert/inject valve.	"Connecting the LC Pump to the Divert/Inject Valve" on page 48
#4	Connect port 1 of the divert /inject valve to a waste container.	"Connecting the Divert/Inject Valve to a Waste Container" on page 49
#5	Connect the union Tee to the grounding union for the ESI and H-ESI modes, or directly to the sample inlet for the APCI mode.	"Connecting the Union Tee to the API Source" on page 49
#6	For the ESI and H-ESI modes, connect the grounding union to the probe sample inlet.	"Connecting the Grounding Union to the ESI, H-ESI, or HESI-II Probe Sample Inlet" on page 59

For instructions on connecting the grounding union to the sample inlet of the ESI or APCI, H-ESI, or HESI-II probe, refer to the *Ion Max and Ion Max-S API Source Hardware Manual*, the *H-ESI User Guide*, or the *HESI-II Probe User Guide*, respectively.

Connecting the Syringe to the Union Tee

✤ To connect the syringe to the union Tee

- 1. Set up the syringe (see "Setting Up the Syringe Pump" on page 41).
- 2. Connect a length of red PEEK tubing between the LC union and the union Tee:
 - Using a two-piece fingertight fitting, connect a red PEEK infusion line to the free end of the LC union that is connected to the syringe.
 - Using a two-piece fingertight fitting, connect the other end of the red PEEK infusion line to the union Tee.

Figure 32 shows the fittings required to connect the LC union to the union Tee.



Figure 32. Connecting 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

- Using a one-piece fingertight fitting, connect a length of red PEEK tubing to port 3 of the divert/inject valve (see Figure 33).
- Using a two-piece fingertight fitting, connect the other end of the tubing to the free end of the union Tee (see Figure 33).

Figure 33. Connecting the union Tee to the divert/inject valve



Connecting the LC Pump to the Divert/Inject Valve

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

- Using a one-piece fingertight fitting, connect a length of PEEK tubing to port 2 of the divert/inject valve. Figure 33 shows the ports of the divert/inject valve.
- Using an appropriate fitting, connect the other end of the tubing to the outlet of the LC system.

Connecting the Divert/Inject Valve to a Waste Container

- * To connect the divert/ inject valve to a waste container
- 1. Using a one-piece fingertight fitting, connect a length of 0.03 in. $ID \times 1/16$ in. OD, Teflon tubing to port 1 of the divert/inject valve. Figure 33 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 API Source

✤ To connect the union Tee to the API source

- 1. Using a fingertight fitting and a ferrule, connect one end of a length of red PEEK tubing to the union Tee (see Figure 34).
- 2. Depending on whether you are connecting the ESI, H-ESI, HESI-II, or APCI probe, connect the other end of the red PEEK tubing as follows:
 - For the APCI probe, connect the other end of the red PEEK tubing directly to the sample inlet of the APCI probe with a two-piece fingertight fitting.

Note Do not use the grounding bar of the Ion Max or Ion Max-S API 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 mode.

• For the ESI probe, use a two-piece fingertight fitting to connect the other end of the red PEEK tubing to the grounding union (see Figure 34). The grounding union is held by the grounding bar of the Ion Max-S API source.

The grounding union slides into the grounding bar on the Ion Max or Ion Max-S API source (see Figure 40 on page 60). 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*.

• For the H-ESI or HESI-II probes, use a two-piece fingertight fitting to connect the other end of the red PEEK tubing to the grounding union (see Figure 34). The grounding union is held by the H-ESI or HESI-II probe grounding union holder.



Figure 34. Connecting the union Tee to the grounding union

Setting Up the Inlet for Manual or Auto-Loop Injections

This section describes how to connect the inlet plumbing to introduce sample into the ion source by manual or auto-loop injection.

Table 14 lists the fittings and tubing required to set up the system for manual or auto-loop injections, including the fittings and tubing required to set up the syringe pump for auto-loop injections.

Part	Description
	(For the ESI, HESI-II, or H-ESI probes only) Grounding union, stainless steel, zero dead volume (ZDV), for 1/16 in. OD tubing, 0.01 in. thru-hole
	(For auto-loop injections only) LC union, PEEK, 10-32, for fingertight fittings and 1/16 in. OD tubing, 0.01 in. thru-hole
	Two-piece fingertight fitting for 1/16 in. OD tubing, PEEK, 10-32
	Fitting, one-piece fingertight, 10-32, high pressure, natural PEEK, for 1/16 in. OD tubing, Upchurch F-120
Teflon tube, precut 4 cm (1.5 in.) length,	
	0.03 in. ID×1/16 in. OD
	Used to make the loop filler fitting for manual injections, or to connect the syringe needle to the LC union for auto-loop injections
	Teflon tubing (of sufficient length) to connect port 6
	of the divert/inject valve to a waste container
	0.03 in. ID×1/16 in. OD
	Red PEEK tubing (0.005 in. ID×1/16 in. OD)
	(Optional for manual injections) Rheodyne PEEK needle port can be ordered from Rheodyne (Rheodyne part number 9013)

Table 15. Fittings and tubing required to plumb the system for manual or auto-loop injections

Figure 35 and Figure 36 show a TSQ Series mass spectrometer set up to introduce sample by manual loop injection and auto-loop injection, respectively.



Figure 35. TSQ Series mass spectrometer set up to introduce sample by manual loop injection in the ESI mode





* To set up the inlet for loop injections

- 1. Depending on whether you want to load the sample loop manual with a hand-held syringe or automatically with the syringe pump, do one of the following:
 - To load sample with a hand-held syringe, connect a loop filler fitting to port 5 of the divert/inject valve (see Figure 37).

You can create a loop filler fitting by inserting the 0.1 ft (3 cm) length of 0.03 in. ID Teflon tubing into a one-piece fingertight fitting, or you can order a loop filler fitting from Rheodyne LLC (PEEK needle port 9013).



Figure 37. Divert/inject valve set up for manual loop injections

- To load sample automatically with the syringe pump, set up the syringe pump ("Setting Up the Syringe Pump" on page 41), and then make the following connections:
 - a. Using a two-piece fingertight fitting, connect a red PEEK infusion line to the free end of the LC union that is connected to the syringe.
 - b. Using a one-piece fingertight fitting, connect the other end of the red PEEK infusion line to port 5 of the divert/inject valve.
- 2. Connect a sample loop to ports 1 and 4 of the divert/inject valve.
- 3. 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 backpressure 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 backpressure of 3 bar (43 psi), or connect an in-line backpressure regulator between the LC pump outlet and the divert/inject valve.

b. Using a one-piece fingertight fitting, connect the other end of the tubing to port 2 of the divert/inject valve.

- 4. Connect port 3 of the divert/inject valve to the ion source:
 - a. Using a one-piece fingertight fitting, connect a length of red PEEK tubing to port 3 of the divert/inject valve.
 - b. Depending on whether you are using the APCI probe or the ESI probe, do one of the following:
 - For the APCI probe, go to step 4c.
 - For the ESI, H-ESI, or HESI-II probes go to step 4d.
 - c. For the APCI probe, connect the other end of the red PEEK tubing to the sample inlet of the APCI probe (see Figure 38). Go to step 5.





d. For the ESI, H-ESI, or HESI-II probe, use a two-piece fingertight fitting to connect the other end of the red PEEK tubing that is connected to port 3 of the divert/inject valve to the grounding union.

For instructions on how to connect the other end of the grounding union to the sample inlet of the ESI, H-ESI, or HESI-II probes, refer to the *Ion Max and Ion Max-S API Ion Source Hardware Manual*, the *H-ESI User Guide*, or the *HESI-II Probe User Guide*, respectively.

- 5. Connect the divert /inject valve to a waste container:
 - a. Using a Rheodyne fitting, connect one end of a length of 0.03 in. $ID \times 1/16$ in. OD Teflon tubing to port 6 of the divert/inject valve.
 - b. Place the other end of the Teflon tubing in an appropriate waste container.

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

This section describes how to connect the inlet plumbing to introduce sample into the ion source with a liquid chromatography system that includes an autosampler.

Table 16 lists the fittings and tubing required to connect an LC system to the mass spectrometer.

Table 16. Fittings and tubing required to plumb the system for an LC/MS experiment

Part	Description
	(For the ESI, H-ESI, and HESI-II probes) Grounding union, stainless steel, zero dead volume (ZDV), for 1/16 in. OD tubing, 0.01 in. thru-hole
	Two-piece fingertight fitting for 1/16 in. OD tubing, PEEK, 10-32
	Fitting, one-piece fingertight, 10-32, high pressure, natural PEEK, for 1/16 in. OD tubing, Upchurch F-120
	Red PEEK tubing
	$(0.005 \text{ in. ID} \times 1/16 \text{ in. OD})$
	Teflon tubing 0.03 in. $ID \times 1/16$ in. OD, sufficient length to connect port 1 of the divert/inject valve to a waste container

Figure 39 shows a TSQ Series mass spectrometer set up to perform an LC/MS experiment in the ESI mode.



Figure 39. TSQ Series mass spectrometer set up to perform an LC/MS experiment in the ESI mode

* To connect the inlet plumbing for an LC/MS system with an autosampler

- 1. Connect the outlet of the LC system 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 your LC system.
 - b. Using a one-piece fingertight fitting, connect the other end of the red PEEK tubing to port 2 of the divert/inject valve.
- 2. Connect the divert /inject valve to a waste container:
 - a. Using a Rheodyne fitting, connect one end of a length of 0.03 in. $ID \times 1/16$ in. OD Teflon tubing to port 1 of the divert/inject valve.
 - b. Route the other end of the Teflon tubing to an appropriate waste container.

- 3. To connect port 3 of the divert/inject valve to the ion source, do one of the following:
 - For the ESI probe, go to step 4.
 - For the H-ESI or HESI-II probes, go to step 6.
 - For the APCI probe, go to step 8.
- 4. To connect the divert/inject valve to the grounding union held by the grounding bar used for the ESI probe:
 - a. Using a one-piece fingertight fitting, connect a length of red PEEK tubing to port 3 of the divert/inject valve.
 - b. Using a two-piece fingertight fitting, connect the other end of the red PEEK tubing to the grounding union.
- 5. To connect the other end of the grounding union held by the grounding bar to the ESI probe sample inlet, refer to the *Ion Max and Ion Max-S API Source Hardware Manual*.

You have finished connecting the inlet plumbing for the ESI probe.

- 6. To connect the divert/inject valve to the grounding union held by the grounding union holder attached to the H-ESI or HESI-II probe:
 - a. Using a one-piece fingertight fitting, connect a length of red PEEK tubing to port 3 of the divert/inject valve.
 - b. Using a two-piece fingertight fitting, connect the other end of the red PEEK tubing to the grounding union.
- 7. To connect the other end of the grounding union to the H-ESI or HESI-II probe sample inlets, follow the instructions in the *H-ESI Probe Operator's Guide* or the *HESI-II Probe User Guide*, respectively.

You have finished connecting the inlet plumbing for the H-ESI or HESI-II probe.

- 8. To connect the divert/inject valve to the APCI probe sample inlet:
 - a. Using a one-piece fingertight fitting, connect a length of red PEEK tubing to port 3 of the divert/inject valve.
 - b. Using a two-piece fingertight fitting, connect the other end of the red PEEK tubing to the APCI probe sample inlet.

You have finished connecting the inlet plumbing for the APCI probe.
Connecting the Grounding Union to the ESI, H-ESI, or HESI-II Probe Sample Inlet

For instructions on connecting the PEEK safety sleeve and fused-silica sample tube from the grounding union to the ESI, H-ESI, or HESI-II probe sample inlet, refer to the *Ion Max and Ion Max-S API Source Hardware Manual*, *H-ESI Probe User Guide*, or *HESI-II Probe User Guide* respectively.

Note The standard sample tube for the HESI-II probe is a metal needle.

Figure 40 shows the connection between the grounding union and the ESI probe sample inlet.



CAUTION Ensure that the grounding union is made of stainless steel. Do not use a grounding union made of a non-conductive material such as PEEK, as doing so creates an electric shock hazard.



Figure 40. Connection between the grounding union and the ESI probe sample inlet

Figure 41 shows the connection between the grounding union and the H-ESI probe sample inlet.



Figure 41. Connection between the grounding union and the H-ESI probe sample inlet

Figure 42 shows the connection between the grounding union and the HESI-II probe sample inlet.

Figure 42. Connection between the grounding union and the HESI-II probe sample inlet



5

Connecting the 4-Port Serial PCB

This chapter describes how to install a 4-port serial PCB for systems that require additional communication ports.

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 43.

Table 17 lists the kit and its contents used with the 4-port serial PCB.

Table 17. Kit used with the 4-port serial PCB

Part number	Description of kit
OPTON-21709	Xcalibur Additional 4-Port Serial Kit4-port serial PCB (PCI) and softwareQuad DB (male adapter)

Figure 43. 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. Wearing a grounding strap, carefully remove the 4-port serial PCB from its protective shipping bag.
- 5. Hold the 4-port serial PCB by its edges and position it so that the 78-pin 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 male connectors to the appropriate inlet devices.
- 10. Restart the data system computer.

The 4-port serial PCB is a plug-and-play device. When the operating system starts, it automatically detects and configures the new 4-port serial PCB and loads the appropriate drivers.

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