

**Finnigan™**  
**LTO™**

Getting Connected

Revision A  
97055-97011

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- Pharmaceutical
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**Reader Survey...** Help us to improve the quality of our documentation by answering a few questions:

<i>Finnigan LTQ Getting Connected</i>	<i>Revision A 97055-97011</i>			
	Strongly Agree	Agree	Disagree	Strongly Disagree
The manual is well organized.	1	2	3	4
The manual is clearly written.	1	2	3	4
The manual contains all of the information I need.	1	2	3	4
The instructions are easy to follow.	1	2	3	4
The instructions are complete.	1	2	3	4
The technical information is easy to understand.	1	2	3	4
The figures are helpful.	1	2	3	4
I was able to make necessary connections by using this manual. (If not, please comment below.)	1	2	3	4

Additional Comments: (Attach additional sheets if necessary.)

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EN 61326	(1998)	EN 61000-4-5	(1995)
EN 61000-4-2	(1998)	EN 61000-4-6	(1996)
EN 61000-4-3	(1996)	EN 61000-4-11	(1994)
ENV 50204	(1995)	FCC Class A	

**EMC issues have been evaluated by EMC TECHNOLOGY SERVICES, A Subsidiary of UNDERWRITERS LABORATORY, INC (UL)**

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Making changes to your system includes replacing a part. Thus, to ensure continued compliance with EMC and safety standards, replacement parts should be ordered from Thermo Electron or one of its authorized representatives.

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In compliance with international regulations: If this instrument is used in a manner not specified by Thermo Electron San Jose, the protection provided by the instrument could be impaired.

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# Read This First

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Welcome to the Thermo Electron, Finnigan™ LTQ™ system!

This **Finnigan LTQ Getting Connected** manual provides you with information on how to connect your LTQ system.

This manual includes the following chapters:

**Chapter 1: Line Power, Vacuum System, Gases, and Ethernet Communication** describes how to connect the LTQ MS detector to line power, to the forepump, to the nitrogen gas, to the helium gas, and to the data system computer.

**Chapter 2: Connecting Probes** describes how to connect the LTQ MS detector to the ESI probe and APCI probe.

**Chapter 3: Control of Inlet Devices** describes how to connect external devices, how to connect devices that require contact closure, and how to trigger external devices.

**Chapter 4: Connecting the Thermo Electron Finnigan Surveyor® LC System** describes how to connect the LTQ MS detector to the Surveyor LC system.

**Chapter 5: Connecting the Thermo Electron Finnigan SpectraSYSTEM®** describes how to connect the LTQ MS detector to the SpectraSYSTEM equipped with an autosampler, pump, and UV detector.

**Chapter 6: Connecting the Agilent® 1100 Series LC** describes how to connect the LTQ MS detector to the Agilent 1100 Series LC system.

**Chapter 7: Upgrading the HP 1100 Series LC** describes how to upgrade the Hewlett-Packard® 1100 Series LC communication interface to an Ethernet interface so that the LC system can be controlled by the Xcalibur data system.

**Chapter 8: Connecting the Waters LC** describes how to connect the TSQ Quantum to the Waters Alliance® and Alliance HT Separations Modules and to the Waters 2487 Dual  $\lambda$  Absorbance Detector.

**Chapter 9: Connecting the SS420x Analog-to-Digital Interface Kit** describes how to install and configure the SS420x.

**Chapter 10: Connecting the 4-Port Serial PCB** describes how to install the 4-Port Serial PCB.

**Chapter 11: Making Plumbing Connections to Run Samples on the LTQ MS detector** describes how to connect plumbing for ESI/MS and APCI/MS sample introduction into the LTQ MS detector.

## **Changes to the Manual and Online Help**

To suggest changes to this manual or the online Help, please send your comments to:

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355 River Oaks Parkway  
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U.S.A.

You are encouraged to report errors or omissions in the text or index.  
Thank you.

## Abbreviations

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The following abbreviations are used in this and other manuals and in the online Help.

A	ampere
ac	alternating current
ADC	analog-to-digital converter
AP	acquisition processor
APCI	atmospheric pressure chemical ionization
API	atmospheric pressure ionization
ASCII	American Standard Code for Information Interchange
b	bit
B	byte (8 b)
baud rate	data transmission speed in events per second
°C	degrees Celsius
CD	compact disc
CD-ROM	compact disc read-only memory
cfm	cubic feet per minute
CI	chemical ionization
CIP	carriage and insurance paid to
cm	centimeter
cm <sup>3</sup>	cubic centimeter
CPU	central processing unit (of a computer)
CRC	cyclic redundancy check
CRM	consecutive reaction monitoring
<Ctrl>	control key on the terminal keyboard
<i>d</i>	depth
Da	dalton
DAC	digital-to-analog converter
dc	direct current
DDS	direct digital synthesizer
DEP™	direct exposure probe
DS	data system
DSP	digital signal processor

EI	electron ionization
EMBL	European Molecular Biology Laboratory
<Enter>	enter key on the terminal keyboard
ESD	electrostatic discharge
ESI	electrospray ionization
eV	electron volt
f	femto ( $10^{-15}$ )
°F	degrees Fahrenheit
.fasta file	extension of a SEQUEST search database file
FOB	free on board
ft	foot
FTP	file transfer protocol
g	gram
G	giga ( $10^9$ )
GC	gas chromatograph; gas chromatography
GC/MS	gas chromatograph / mass spectrometer
GND	electrical ground
GPIB	general-purpose interface bus
GUI	graphical user interface
h	hour
<i>h</i>	height
HPLC	high-performance liquid chromatograph
HV	high voltage
Hz	hertz (cycles per second)
ICIS™	Interactive Chemical Information System
ICL™	Instrument Control Language™
ID	inside diameter
IEC	International Electrotechnical Commission
IEEE	Institute of Electrical and Electronics Engineers
in.	inch
I/O	input/output
k	kilo ( $10^3$ , 1000)
K	kilo ( $2^{10}$ , 1024)
KEGG	Kyoto Encyclopedia of Genes and Genomes
kg	kilogram

<i>l</i>	length
L	liter
LAN	local area network
lb	pound
LC	liquid chromatograph; liquid chromatography
LC/MS	liquid chromatograph / mass spectrometer
LED	light-emitting diode
$\mu$	micro ( $10^{-6}$ )
m	meter
m	milli ( $10^{-3}$ )
M	mega ( $10^6$ )
M+	molecular ion
MB	Megabyte (1048576 bytes)
MH+	protonated molecular ion
min	minute
mL	milliliter
mm	millimeter
MS	mass spectrometer; mass spectrometry
MS	MS <sup>n</sup> power: where n = 1
MS/MS	MS <sup>n</sup> power: where n = 2
MS <sup>n</sup>	MS <sup>n</sup> power: where n = 1 through 10
<i>m/z</i>	mass-to-charge ratio
n	nano ( $10^{-9}$ )
NCBI	National Center for Biotechnology Information (USA)
NIST	National Institute of Standards and Technology (USA)
OD	outside diameter
$\Omega$	ohm
p	pico ( $10^{-12}$ )
Pa	pascal
PCB	printed circuit board
PID	proportional / integral / differential
P/N	part number
P/P	peak-to-peak voltage

ppm	parts per million
psig	pounds per square inch, gauge
RAM	random access memory
RF	radio frequency
RMS	root mean square
ROM	read-only memory
RS-232	industry standard for serial communications
s	second
SIM	selected ion monitoring
solids probe	direct insertion probe
SRM	selected reaction monitoring
SSQ <sup>®</sup>	single stage quadrupole
TCP/IP	transmission control protocol / Internet protocol
TIC	total ion current
Torr	torr
TSQ <sup>®</sup>	triple stage quadrupole
u	atomic mass unit
URL	uniform resource locator
V	volt
V ac	volts alternating current
V dc	volts direct current
vol	volume
w	width
W	watt
WWW	World Wide Web

**Note.** Exponents are written as superscripts. In the corresponding online Help, exponents are sometimes written with a caret (^) or with *e* notation because of design constraints in the online Help. For example:

MS<sup>n</sup> (in this manual)   Ms<sup>n</sup> (in the online Help)

10<sup>5</sup> (in this manual)   10<sup>5</sup> (in the online Help)

## Typographical Conventions

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Typographical conventions have been established for Thermo Electron San Jose manuals for the following:

- Data input
- Boxed information
- Topic headings

### Data Input

---

Throughout this manual, the following conventions indicate data input and output via the computer:

- Messages displayed on the screen are represented by capitalizing the initial letter of each word and by italicizing each word.
- Input that you enter by keyboard is represented in **bold face letters**. (Titles of topics, chapters, and manuals also appear in bold face letters.)
- For brevity, expressions such as “choose **File > Directories**” are used rather than “pull down the File menu and choose Directories.”
- Any command enclosed in angle brackets < > represents a single keystroke. For example, “press <F1>” means press the key labeled *F1*.
- Any command that requires pressing two or more keys simultaneously is shown with a plus sign connecting the keys. For example, “press <Shift> + <F1>” means press and hold the <Shift> key and then press the <F1> key.
- Any button that you click on the screen is represented in bold face letters and a different font. For example, “click on **Close**”.

## Boxed Information

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Information that is important, but not part of the main flow of text, is displayed in a box such as the one below.

**Note.** Boxes such as this are used to display information.

Boxed information can be of the following types:

- **Note** – information that can affect the quality of your data. In addition, notes often contain information that you might need if you are having trouble.
- **Tip** – helpful information that can make a task easier.
- **Important** – critical information that can affect the quality of your data.
- **Caution** – information necessary to protect your instrument from damage.
- **CAUTION** – hazards to human beings. Each CAUTION is accompanied by a CAUTION symbol. Each hardware manual has a blue CAUTION sheet that lists the CAUTION symbols and their meanings.
- **DANGER** – laser-related hazards to human beings. It includes information specific to the class of laser involved. Each DANGER is accompanied by the international laser radiation symbol.



## **Topic Headings**

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The following headings are used to show the organization of topics within a chapter:

# **Chapter 1**

## **Chapter Name**

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### **1.2 Second Level Topics**

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#### **Third Level Topics**

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#### **Fourth Level Topics**

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#### *Fifth Level Topics*

## **Reply Cards**

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Thermo Electron San Jose manuals contain one or two reply cards. All manuals contain a Customer Registration / Reader Survey card and some contain a Change of Location card. These cards are located at the front of each manual.

The Customer Registration / Reader Survey card has two functions. First, when you return the card, you are placed on the Thermo Electron San Jose mailing list. As a member of this list, you receive application reports and technical reports in your area of interest, and you are notified of events of interest, such as user meetings. Second, it allows you to tell us what you like and do not like about the manual.

The Change of Location card allows us to track the whereabouts of the instrument. Fill out and return the card if you move the instrument to another site within your company or if you sell the instrument. Occasionally, we need to notify owners of our products about safety or other issues.

# Chapter 1

## Line Power, Vacuum System, Gases, and Ethernet Communication

---

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

The following topics are discussed in this chapter:

- Connecting the LTQ MS Detector to Line Power
- Connecting the LTQ MS Detector to the Forepumps
- Connecting Gases to the LTQ MS Detector
- Connecting the LTQ MS Detector to the Data System Computer

## 1.1 Connecting the LTQ MS Detector to Line Power

---

To connect the LTQ MS detector to line power, proceed as follows:

1. Locate the MAIN POWER circuit breaker switch on the LTQ MS detector Power Entry Module.
2. Turn the circuit breaker switch to the Off (O) position.
3. Locate the Electronics switch and make sure that the switch is in the Service Mode position.
4. Connect the power cord from the POWER IN inlet located on the LTQ MS detector Power Entry Module, to the 230 V ac power source in your laboratory.

**Caution.** If your local area is subject to power fluctuations or power interruptions, a power conditioning device or an uninterruptible power supply (UPS) should be installed in your laboratory. (Refer to the topic **Power Conditioning Devices** in the LTQ MS detector **Preinstallation Requirements Guide**.)

## 1.2 Connecting the LTQ MS Detector to the Forepumps

To connect the LTQ MS detector to the forepumps, proceed as follows:

1. Using a hose clamp (P/N 00108-09001), connect the 3.8 cm (1.5 in.) ID reinforced vacuum hose to the LTQ MS detector vacuum inlet. (The vacuum hose inlet is located on the left side panel of the LTQ MS detector.)
2. Connect the 3.8 cm (1.5 in.) Tee (P/N 97055-20222) to the free end of the vacuum hose with a hose clamp (P/N 00108-09001).
3. Using hose clamps (P/N 00108-09001), connect the 3.8 cm (1.5 in.) ID reinforced vacuum hoses to the other branches of the Tee connector.
4. Connect a pump fitting adapter (P/N 00108-09005) to the free end of the vacuum hoses with a hose clamp (P/N 00108-09001).
5. Place a centering ring (P/N 00108-02011) on the flange of each forepump vacuum inlet.
6. Connect the vacuum hose (with the attached fitting adapter) to the pump vacuum inlet. Secure the hose to the pump using the KF20/25 vacuum hardware clamp (P/N 00102-10020).

**Note.** An efficient fume exhaust system is required for the proper operation of your forepumps. Most API applications will contribute to the accumulation of solvents in the forepumps. These solvents must be purged from the mechanical pump oil periodically by opening the ballast valve located on the top of the pump. When the ballast valve is opened, a large volume of volatile solvent waste might enter the fume exhaust system. Therefore, your fume exhaust system must be able to accommodate the effluent resulting from periodic purging. The frequency of the purging is dependent on the throughput of your system.

7. Use hose clamps (P/N 00108-09001) to connect the 2.5 cm (1 in.) ID blue exhaust hoses from the forepump exhaust ports to the pump exhaust system in your laboratory. **The exhaust hoses should travel at floor level and should extend no more than two meters (78.5 in.) above the level of the forepumps.**
8. Connect the forepumps to line power, as follows:
  - a. Locate the Main Power circuit breaker switch on the Power Entry Module and switch the circuit breaker to the Off (O) position.
  - b. Connect the power cords attached to the forepumps to the forepump outlets located on the Power Entry Module.

## 1.3 Connecting Gases to the LTQ MS Detector

---

This topic describes how to connect the required gases to the LTQ MS detector. The following topics are included:

- Connecting nitrogen gas to the LTQ MS detector
- Connecting helium gas to the LTQ MS detector

### Connecting Nitrogen Gas to the LTQ MS Detector

---

the LTQ MS detector requires high-purity (99%) nitrogen for the API sheath gas and auxiliary gas. Nitrogen gas usage can be quite high. Therefore, it is recommended that nitrogen gas be supplied from one of three sources as follows: a large, sealed, thermally insulated cylinder containing liquid nitrogen, from which the nitrogen gas is boiled off from the liquid; the largest nitrogen cylinder that can be practically used; or a nitrogen generator. The required gas pressure is  $690 \pm 140$  kPa ( $100 \pm 20$  psi).

Connect nitrogen gas to the LTQ MS detector, as follows:

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 1-1 for the proper orientation of the fitting and ferrule.
2. Connect the opposite end of the Teflon tubing to the LTQ MS detector press-in fitting labeled NITROGEN IN located on the left side panel of the LTQ MS detector. Connect the tubing by aligning the Teflon tubing with the opening in the fitting and firmly pushing the tubing into the fitting until the fitting holds the tubing securely.

### Helium

---

The **helium** for LTQ 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  $275 \pm 70$  kPa ( $40 \pm 10$  psi). Particulate filters can be a source of contamination, they are not recommended.

Helium can be dispensed from a tank containing 245 ft<sup>3</sup> of gas using a Matheson 3120 Series<sup>1</sup> regulator or equivalent tank and regulator.

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

The gas lines for helium can be copper or stainless steel. All gas lines need to be free of oil and preferably flame dried. Run the gas lines to the left side of the LTQ MS detector system. Terminate the helium gas supply lines with 1/8-in., female, Swagelok-type connectors.

1. 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 LTQ I/O panel. (See Figure 1-1 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.

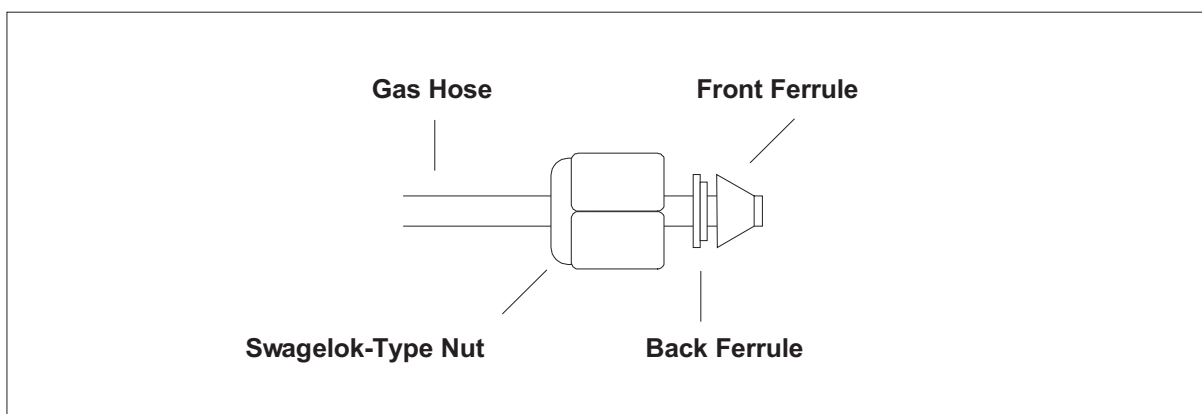


Figure 1-1. Proper orientation of the Swagelok-type nut and two-piece ferrule

## **1.4 Connecting the LTQ MS Detector to the Data System Computer**

---

The LTQ MS detector data system consists of a computer, a monitor, and an optional printer. The LTQ MS detector communicates with the data system computer through an Ethernet cable. To connect the Ethernet cable, proceed as follows:

1. Connect a category five network (Ethernet) cable (P/N 00302-01838) to the ETHERNET 100 BASE T connector located on the LTQ MS detector Power Entry Module.
2. Connect the opposite end of the Ethernet cable to the 10/100BaseT Ethernet switch (P/N 00825-01015) provided with the LTQ 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 LC and LTQ*.
4. Plug in the power supply for the Ethernet switch.



# Chapter 2

## Connecting Probes

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

The following topics are discussed in this chapter:

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

## 2.1 Connecting the ESI Probe to the LTQ MS Detector

---

Connect liquid lines to the ESI probe as follows:

1. Install the Ion Max source housing and ESI probe onto the LTQ MS detector as described in the **Finnigan Ion Max API Source Hardware Manual**.
2. Install liquid lines, as necessary, between the divert/inject valve, the LC system, the syringe pump, and the grounding union, as is appropriate for your application, in accordance with the associated drawing in the topic **Plumbing Connections for ESI/MS** on page 11-4.
3. Connect the 1-in. ID Tygon<sup>®</sup> tubing (P/N 00301-22922) to the source housing drain fitting. Insert the exit end of the tubing into a waste container. Ideally, the waste container should be vented 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.

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

Your laboratory must be equipped with at least two fume exhaust systems. Route the (blue) exhaust tubing from the forepumps 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.

## 2.2 Connecting the APCI Probe to the LTQ MS Detector

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Connect liquid lines to the APCI probe as follows:

1. Install the Ion Max source housing and APCI probe onto the LTQ MS detector as described in the **Finnigan Ion Max API Source Hardware Manual**.
2. Install liquid lines, as necessary, 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, in accordance with the associated drawing in the topic **Plumbing Connections for APCI/MS** on page 11-11.
3. Connect the 1-in. ID Tygon<sup>®</sup> tubing (P/N 00301-22922) to the source housing drain fitting. Insert the exit end of the tubing into a waste container. Ideally, the waste container should be vented 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.

**Caution.** Do **not** vent the PVC drain tubing (or any vent tubing connected to the waste container) to the same fume exhaust system to which you have connected the forepumps.

**Note.** If you need to install or replace the APCI sample tube, refer to the topic **API Source Maintenance** in the LTQ MS detector **Hardware Manual** for instructions.



# Chapter 3

## Control of External Devices

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This chapter describes how to connect the LTQ MS detector to external devices.

This chapter contains the following sections:

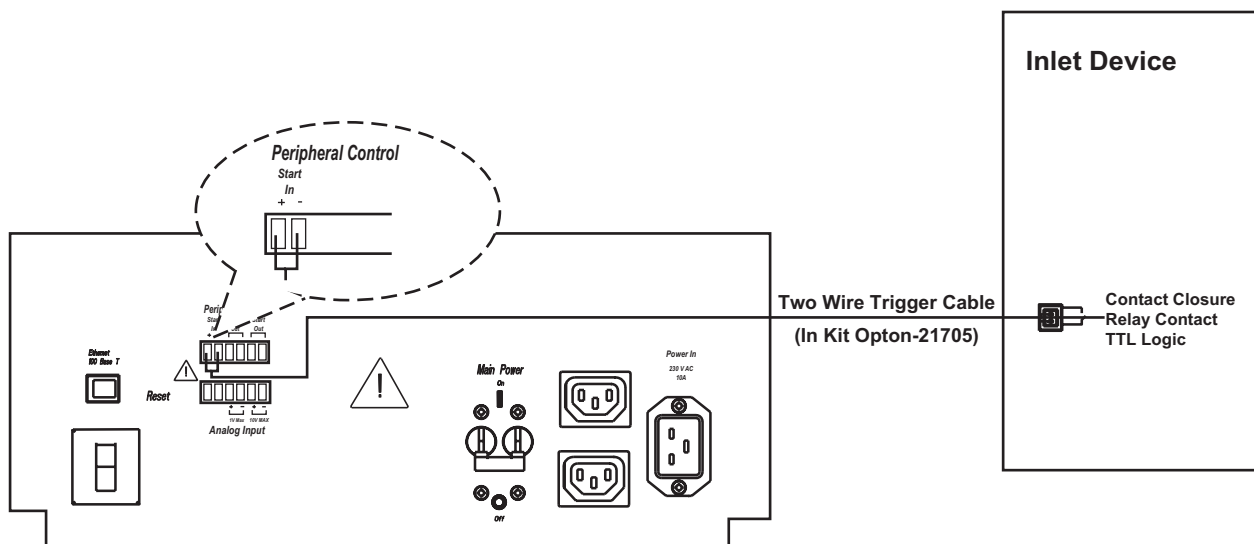
- External devices controlled by the Xcalibur<sup>®</sup> data system
- External devices not controlled by the Xcalibur data system

### 3.1 External Devices Controlled by the Xcalibur Data System

The Xcalibur data system allows for the control of external devices (e.g., autosamplers, pumps, and detectors) from several manufacturers including Thermo Electron, Agilent<sup>1</sup>, and Waters. The LTQ MS detector can start data acquisition from an external device upon receiving a contact closure (closed contact or open contact) signal from the device. The LTQ MS detector receives contact closure signals through a 2-wire trigger cable (in kit P/N OPTON-21705) connected to the LTQ MS detector START IN port. Figure 3-1 shows a simplified block diagram of the LTQ MS detector contact closures to an external device.

**Note.** The external device providing the start signal must have a good ground. Ground loops can cause problems.

**Caution.** Care must be taken with the CMOS that resides on the LTQ MS detector PLL PCB. The CMOS will fail if more than 5 V or 5 mA is applied to the system.



**Figure 3-1.** Portion of the power entry module showing contact closures for the LTQ MS detector and an external device

<sup>1</sup> Formerly Hewlett-Packard® (HP)

Table 3-1 lists the Xcalibur kits for various external devices.

**Table 3-1. Xcalibur kits for various external devices**

<b>Part Number</b>	<b>Description of Kit</b>
OPTON-21705	<b>Xcalibur Contact Closure Kit</b> (for devices not controlled by Xcalibur) 2-wire trigger cable 8-position screw connector
OPTON-21706	<b>Xcalibur SpectraSYSTEM Interface Kit</b> SpectraSYSTEM 9.05 EPROM for SN4000 EPROM removal tool Contact Closure Wiring Harness 2-wire trigger cable (contact closure)
OPTON-21709	<b>Xcalibur Additional 4-Port Serial Kit</b> 4-Port Serial PCB (PCI) and software Quad DB9 male adapter
OPTON-21710	<b>Xcalibur Waters Interface Kit</b> Waters serial I/F cable 2-wire trigger cable (contact closure)
OPTON-21721	<b>Xcalibur SS420x Interface Kit</b> SS420x main unit serial cable 2-wire trigger cable (contact closure) power supply Xcalibur Additional 4-Port Serial Kit
OPTON-30018	<b>Xcalibur JetDirect® Ethernet Control Kit</b> Contact closure PCB External contact closure cable Ethernet 10 Base-T cable (2) 10/100 Autosensing 8-port Ethernet switch HP JetDirect 400N PCB

## 3.2 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 configured in the Xcalibur Run Sequence dialog box as follows:

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

1. Connect the 2-wire trigger cable (in kit P/N OPTON-21705) from the LTQ MS detector power entry module to the contact closure terminal of the external device following the wiring scheme shown in Table 3-2.

**Table 3-2. Wiring the LTQ MS detector and an external device (not controlled by the Xcalibur data system) for contact closure**

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

2. Use the Xcalibur data system Run Sequence dialog box to configure the data system for the external device:
  - a. On the Xcalibur Home Page, choose **View > Info View** to open the Status Page (if it is not already open).
  - b. In the Sequence Setup window make sure there is an active method and then choose **Actions > Run Sequence** or **Actions > Run This Sample** to open the Run Sequence dialog box. See Figure 3-2.
  - c. Click on **Change Instruments** to open the Change Instruments In Use dialog box. See Figure 3-3.

The LTQ MS detector should **not** be in the *Start Instrument: Yes* mode. Observe the Acquisition Options group box.

- If the LTQ MS detector is in the *Start Instrument: Yes* mode, go to step d.
- If the LTQ MS detector is not in the *Start Instrument: Yes* mode, click on **OK** to close the dialog box and go on to step 3.



- d. In the LTQ MS detector row of the Start Instrument column, click on **Yes** to change the mode to Off (field is blank), then click on **OK** to save the setting and close the dialog box.
3. In the Acquisition Options group box select the Start When Ready check box, then click on **OK** to save the settings, close the dialog box, and start the sequence or queue it. The instrument method is downloaded to the LTQ MS detector and the Status Page displays *Waiting - Contact Closure*.
4. Push the start button on the external device to start the external device, the LTQ MS detector, and the acquisition of data.

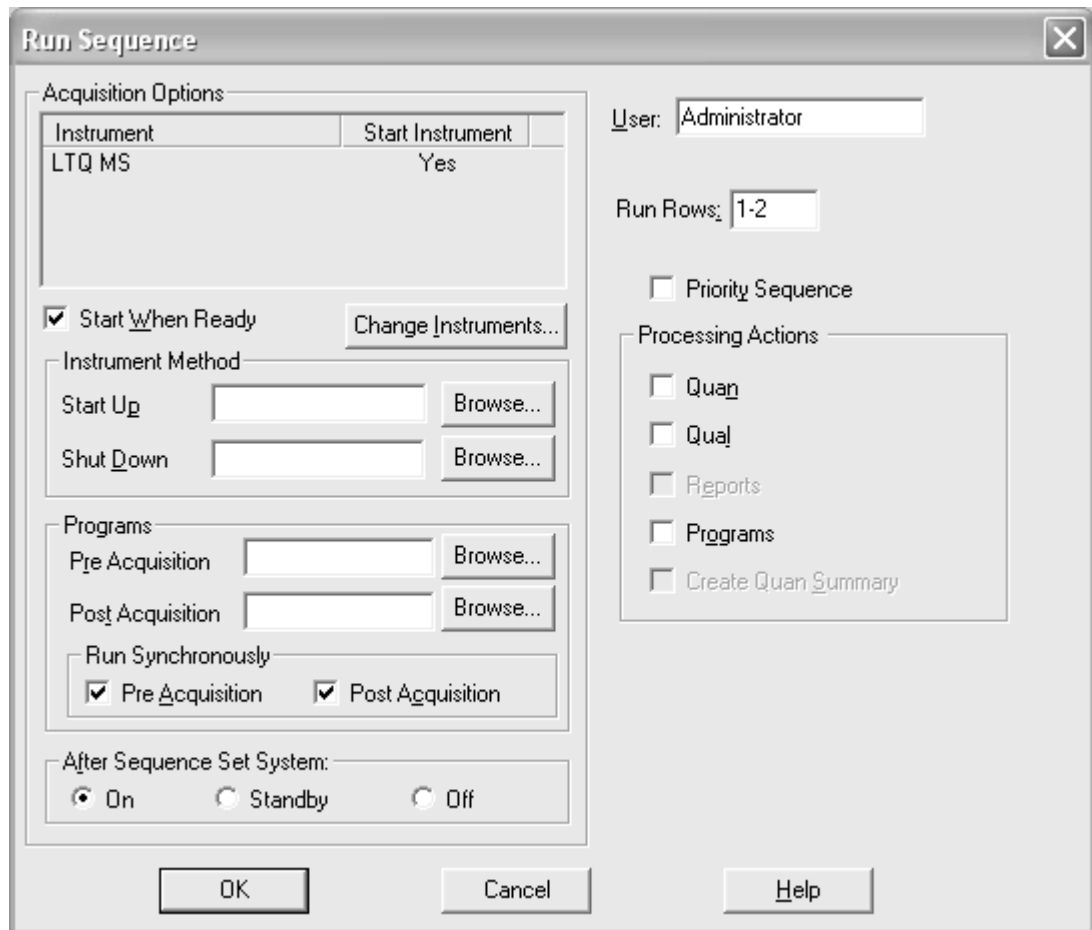
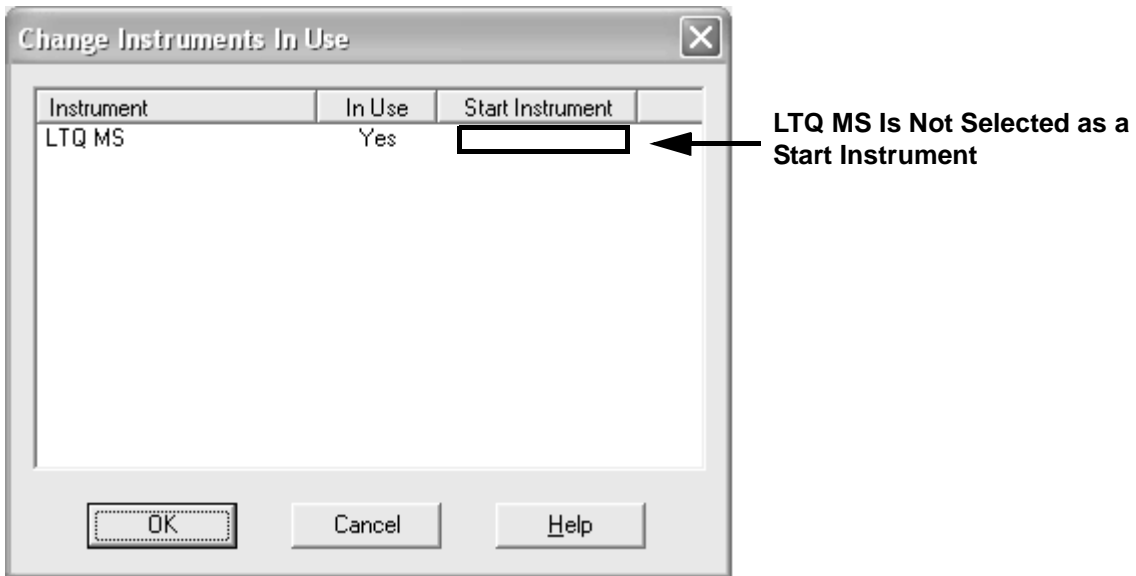


Figure 3-2. Run Sequence dialog box



**Figure 3-3. Change Instruments In Use dialog box**

# Chapter 4

## Connecting the Thermo Electron Finnigan Surveyor LC System

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This chapter describes how to connect the LTQ MS Detector to the Thermo Electron Finnigan Surveyor LC System.

This chapter contains the following sections:

- Connecting the Hardware
- Connecting the Plumbing

Table 4-1 lists the Xcalibur supported firmware for the Surveyor LC system.

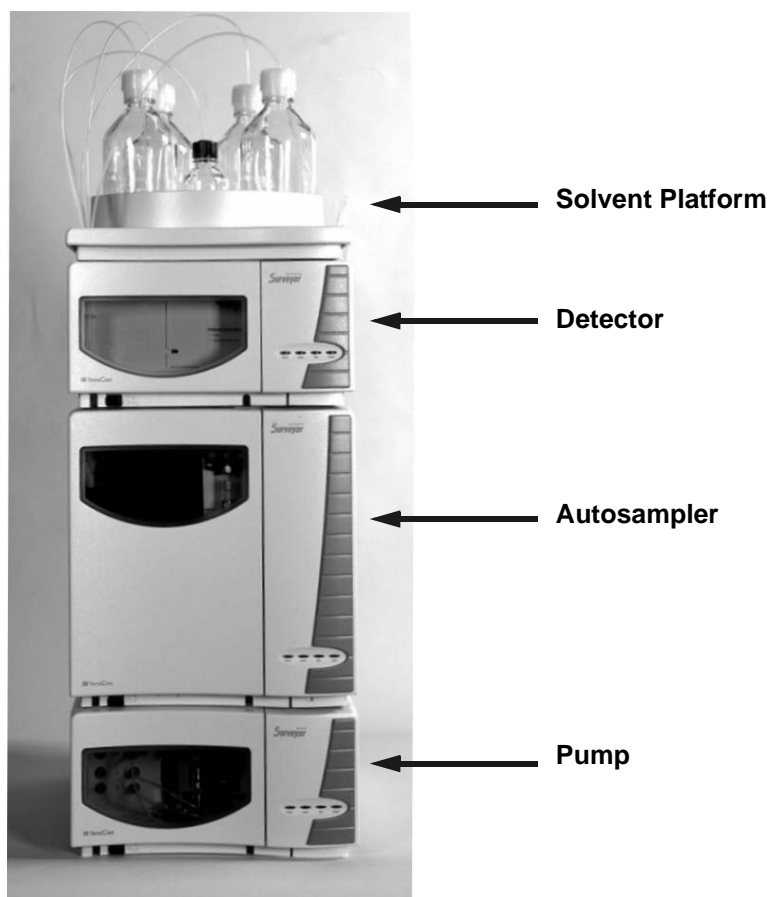
**Table 4-1. Xcalibur supported firmware versions for the Surveyor LC**

Module	Firmware Version
<b><i>LC pump</i></b>	
Converter board ROM	1.08
Converter board RAM	1.15
Main pump board	1.00
<b><i>Autosampler</i></b>	
Autosampler ROM	1.08
Autosampler RAM	2.13
<b><i>PDA detector</i></b>	
Converter board ROM	1.07
Converter board RAM	1.17
Main PDA board RAM	1.8
Main PDA board ROM (Mon960)	0.2
Main PDA board PIC processor	7.00
<b><i>UV/Vis detector</i></b>	
Converter board ROM	1.07
Converter board RAM	1.06
Main detector board	3.12

## 4.1 Connecting the Hardware

To connect the LTQ MS Detector and data system to a Surveyor LC system equipped with a PDA or UV/Vis detector, proceed as follows:

1. Stack the Surveyor modules in the following order from bottom to top: Surveyor Pump, Surveyor Autosampler, Surveyor Detector, and Surveyor Solvent Platform. See Figure 4-1.



**Figure 4-1. Surveyor LC system, with MS Pump and PDA Detector**

2. Interconnect the Surveyor modules with the System Synchronization Wiring Harness (P/N F5049-010). The connectors on the System Synchronization Wiring Harness are labeled appropriately. See Figure 4-2 or Figure 4-3.

When the System Synchronization Wiring Harness is properly connected, one connector is not used. If you are using the MS Pump, the connector labeled *LC Pump* is not used; if you are using the LC Pump, the connector labeled *MS Pump* is not used.

3. Connect the two pin end of the (P/N 70111-63136) cable to the START IN connection on the LTQ MS Detector power entry module.
4. Connect the other end of the Adapter LC/MS Interconnect to the System Synchronization Wiring Harness from step 2.
5. Connect the communication cable for the pump:
  - a. If you are using the Surveyor MS Pump, connect the 9-pin serial cable (P/N 72011-63008) from the pump RS-232 connector to the computer COM1 serial communication port (or another available port). See Figure 4-2.

**Note.** If your data system computer does not have a sufficient number of COM ports available, you might need to install the 4-port serial PCB as discussed in **Chapter 10: Connecting the 4-Port Serial PCB**.

- b. If you are using the Surveyor LC Pump, connect an Ethernet cable (P/N F5048-020) from the Surveyor LC Pump ENET connector to the Ethernet switch (P/N 00825-01015). See Figure 4-3.

**Note.** Use only the standard ports on the Ethernet switch for the Surveyor connections.

6. If you are using the Surveyor MS Pump, configure the COM1 serial port as follows. Otherwise, go to step 7.
  - a. Choose **Start > Settings > Control Panel**, then click on the System icon to open the System Properties dialog box.
  - b. Click on the Hardware tab, and then click on **Device Manager**.
  - c. Double-click on **Ports (COM & LPT)**. The available ports are displayed below Ports (COM & LPT) in the Device Manager list.
  - d. Double-click on **Communication Port (COM1)** to display the Communication Port (COM1) Properties dialog box.
  - e. Click on the Port Setting tab.
  - f. Set the configuration parameters:

Bits per Second	19200
Data Bits	8
Parity	none
Stop Bits	1
Flow Control	none
  - g. Click on **OK** to save the changes and close the Communication Port (COM1) Properties dialog box.
  - h. Close the Device Manager window by clicking on the Close button in the title bar.

- i. Click on **OK** to close the System Properties dialog box.
  - j. Restart the computer to enable the new settings.
7. Connect a Category 5 network (Ethernet) cable (P/N 00302-01838) from the Surveyor PDA ENET connector to one of the standard ports on the Ethernet switch (P/N 00825-01015). See Figure 4-2 or Figure 4-3 for a wiring diagram.
  8. Connect an Ethernet cable (P/N 00302-01838) from the Surveyor Autosampler ENET connector the Ethernet switch.
  9. Connect an Ethernet cable (P/N 00302-01838) from the Ethernet switch to the computer 3Com 3C900B-TX Ethernet card labeled *Surveyor*.
  10. Connect an Ethernet cable (P/N 00302-01838) from the Ethernet switch to the LTQ MS Detector Ethernet connection on the power entry module.
  11. Confirm that the 3Com 3C905B-TX Ethernet card is assigned to the LTQ MS Detector and the Surveyor LC System:
    - a. Choose **Start > Settings > Control Panel**, then double-click on the Network and Dial-up Connections icon to open the Network and Dial-up Connections dialog box.
    - b. Right-click on the Local Area Connection 3 icon and then choose **Properties** from the shortcut menu. The Local Area Connection Properties dialog box opens.
    - c. Select *Internet Protocol (TCP/IP)* from the Components Checked Are Used By This Connection list box. Click on **Properties** to open the Internet Protocol (TCP/IP) Properties dialog box.
    - d. Confirm that the IP address for the 3Com 3C905B-TX Ethernet card is 172.16.0.101 as in Table 4-2.
    - e. Click on **OK** to close the Internet Protocol (TCP/IP) Properties dialog box, and then click on **OK** to close the Network dialog box.

**Table 4-2. Data system computer configured with three (3) Ethernet cards**

Slot	Ethernet Card	Use	IP Address	Subnet mask
1	3Com 3C900B-TPC	LCQ Series Instruments	10.0.0.101	255.255.255.0
2	3Com 3C905B-TX	User's Network	192.x.x.x	255.255.255.0
3	3Com 3C905B-TX	LTQ MS Detector and Surveyor LC System	172.16.0.101	255.255.0.0

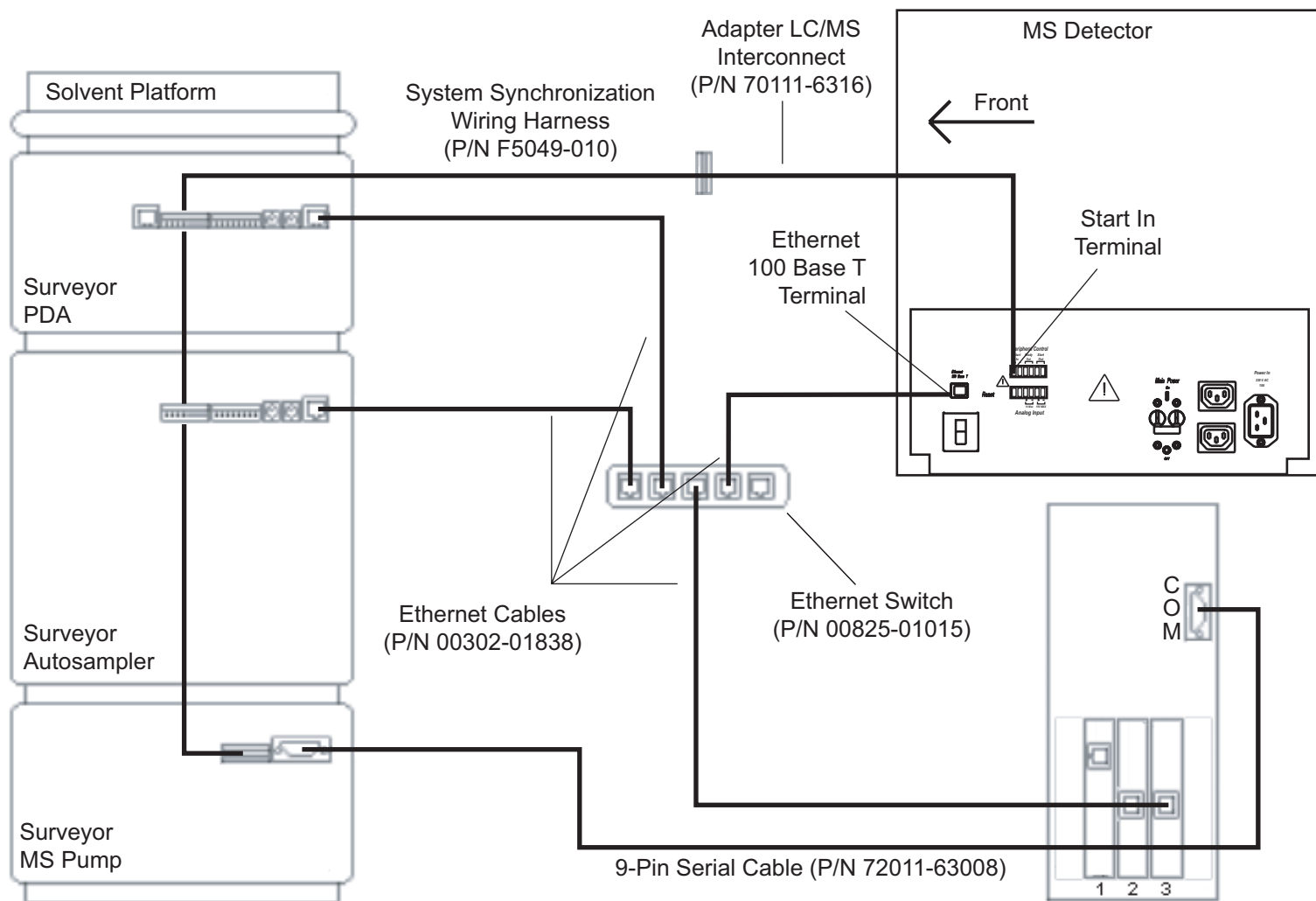


Figure 4-2. Cable diagram for the Surveyor LC system with an MS Pump, LTQ MS Detector, and data system computer

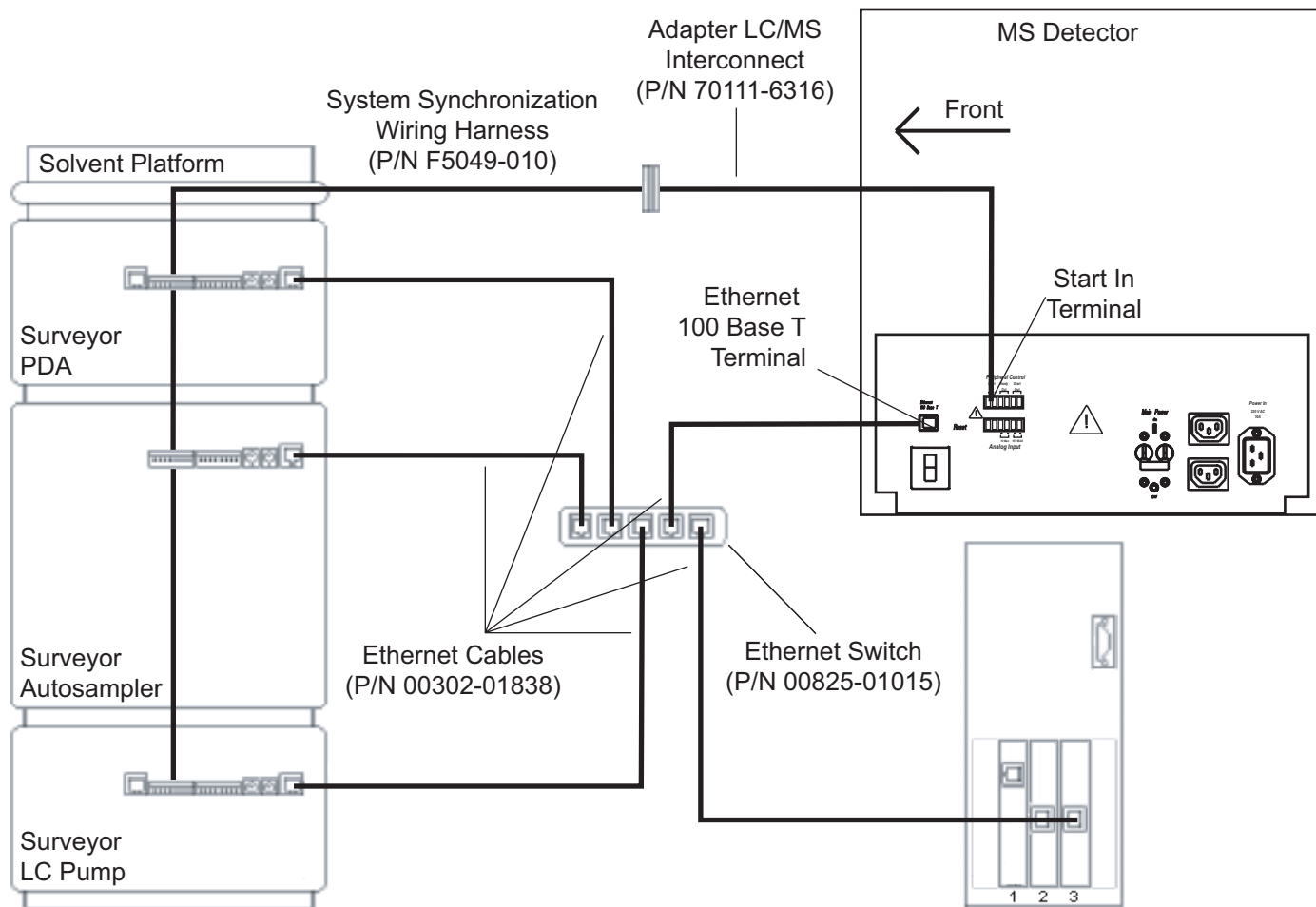


Figure 4-3. Cable diagram for the Surveyor LC system with an LC Pump, LTQ MS Detector, and data system computer



## 4.2 Connecting the Plumbing

The following procedure assumes that a Thermo Electron service representative has set up your Surveyor LC system and has done the following:

- Mounted the syringe drive assembly to the front of the Surveyor Autosampler
- Installed the flowcell in the optional Surveyor PDA detector or Surveyor UV/Vis detector
- Assembled the solvent reservoir bottles
- Connected the Super Flangeless™ fittings to the four solvent lines.

For more detailed instructions on connecting a Surveyor LC system, refer to the **Finnigan Surveyor Getting Connected manual**.

Plumb the Surveyor modules as follows:

**Note.** Each numbered step in the procedure corresponds to a highlighted number in Figure 4-4.

1. Connect the Teflon tubing (with fitting and ferrule) from the wash bottle to the left side of the syringe valve. See Figure 4-5.
2. Connect the solvent reservoir tubing to the analytical pump:
  - a. Feed the Teflon tubing from the solvent bottles through the guide slots located on the left side of the Surveyor modules.
  - b. Connect the Super Flangeless fittings to the inlets of the degassing chamber located on the MS Pump or LC Pump.

A Super Flangeless fitting properly swaged onto the end of a 1/8-in OD solvent reservoir tubing is shown in Figure 4-6.
  - c. Use the (black) tubing clamps located on the inside left of the Surveyor Autosampler to secure the tubing.
3. Connect the autosampler to the pump:
  - a. Depending on your autosampler model, do one of the following:
    - For the Surveyor Autosampler Lite, use the bushing (P/N 2522-0066) and the ferrule (P/N 2522-3830) that come in the autosampler accessory kit to attach the 12-in. l, 0.010-in. ID, stainless steel tubing (P/N A0941-010) that also comes in the kit to port 5 of the Rheodyne injection valve. See Figure 4-7.
    - For the Surveyor Autosampler, pull the stainless steel tubing that exits the column oven of the autosampler forward and then downward through the access port in the bottom of the autosampler as shown in Figure 4-8.

**Tip.** If you need to decrease the gradient delay volume of your system, bypass the tubing behind the column oven. This tubing allows the mobile phase to equilibrate to the requested column oven temperature, but it also adds 250  $\mu$ L of gradient delay volume to your system. To bypass this tubing, disconnect it from port 5 of the Rheodyne injection valve. After you disconnect the column oven tubing, use another piece of tubing to connect the outlet of the pulse dampener directly to port 5 of the injection valve.

- b. Place the fingertight nut and ferrule set (P/N 00101-18088) onto the free end of the stainless steel tubing. Then, attach the tubing to the pump.
  - For the **MS pump**, screw the fitting into the outlet port of the pulse dampener (Figure 4-7).
  - For the **LC pump**, screw the fitting into the in-line filter body on the top of the purge manifold (Figure 4-8).
4. Connect port 6 of the Rheodyne injection valve to the inlet of your LC column by using an appropriate length of tubing, a Rheodyne nut (P/N 3522-0066) and a Rheodyne ferrule (P/N 2522-3830). The six ports of the Rheodyne injection valve are labeled in Figure 4-9.
5. Connect the outlet of the LC column to the inlet of the flowcell.
  - a. If your system contains a detector with a LightPipe flowcell, the tubing connected to the inlet of the flowcell is red, insulated, 0.005-in. ID PEEK tubing. The connections to a Surveyor UV/Vis detector with a LightPipe flowcell are shown in Figure 4-10.
  - b. If your system contains a Surveyor UV/Vis detector with a standard 1 cm flowcell, connect the 0.010-in. ID stainless steel tubing from the flowcell inlet to the column outlet.

**Caution.** If your system contains a Surveyor UV/Vis detector with a LightPipe flowcell, never remove the LightPipe flowcell from the LightPipe mounting assembly without first removing the photodiode mounting assembly. If you want to remove the LightPipe flowcell from its mounting assembly, refer to the **Finnigan Surveyor Getting Connected** manual.

6. Connect the outlet of the flowcell to the inlet of the MS detector. Use 1/16-in. fittings and the red, 0.005-in. ID, PEEK tubing that is included in the MS accessory kit to connect a LightPipe flowcell. If the your system contains a Surveyor UV/Vis detector with a standard flowcell, connect the 0.010-in. ID stainless steel outlet tubing to the inlet of the MS detector. If necessary, use a connector and additional tubing.

**Note.** You need to configure the modules of your Surveyor LC System before you run samples. Refer to the **Finnigan Surveyor Getting Started with Xcalibur** manual for information on configuring the modules.

**Finnigan LTQ**

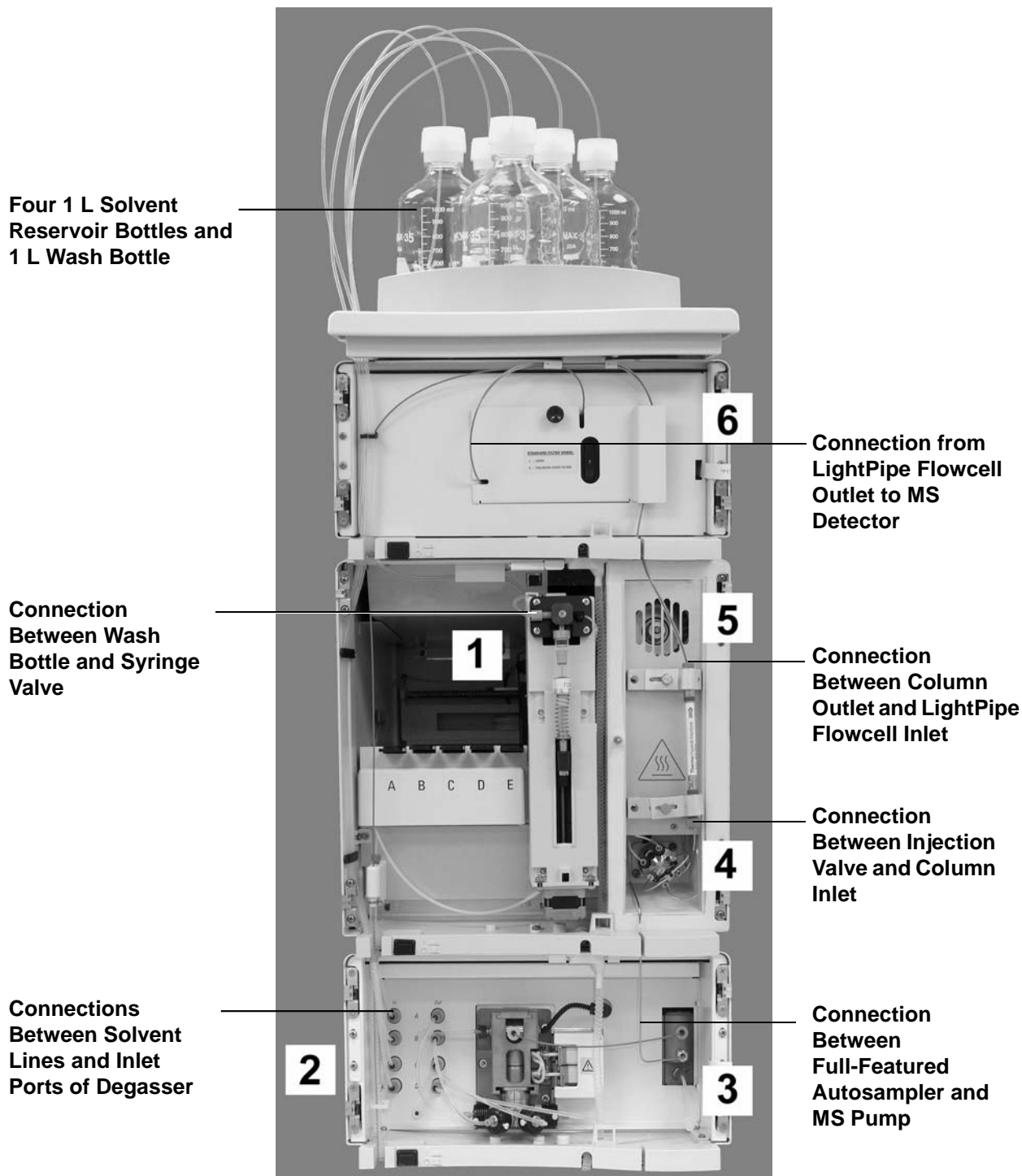
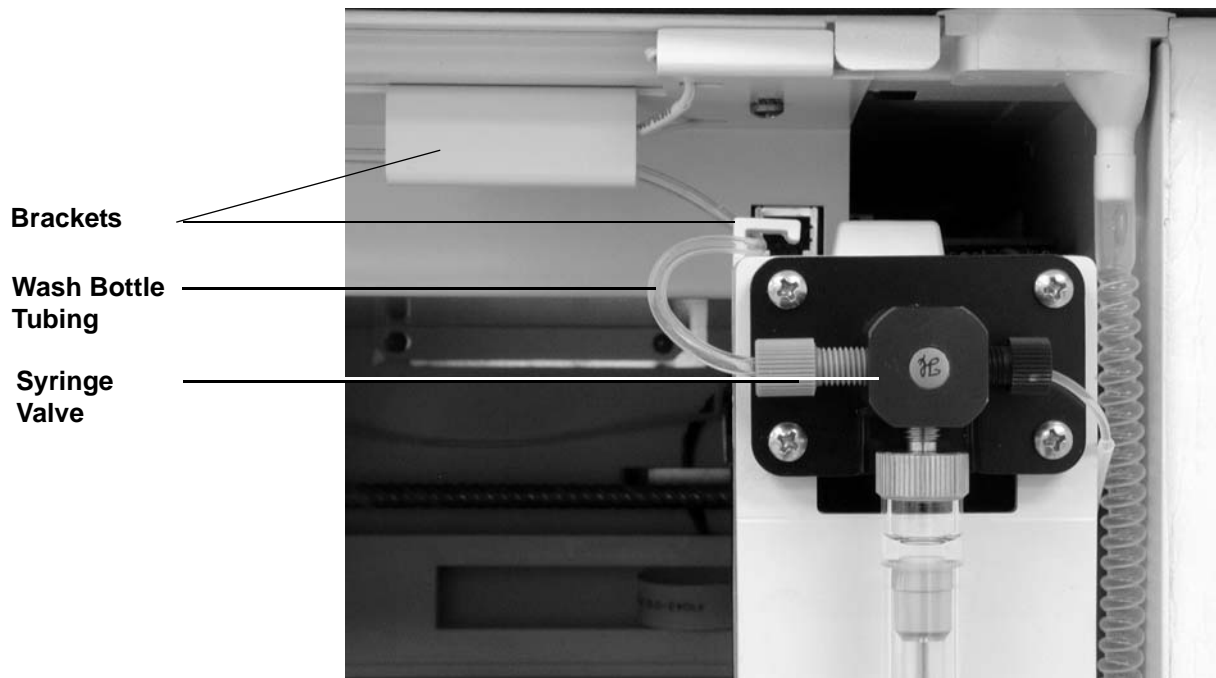
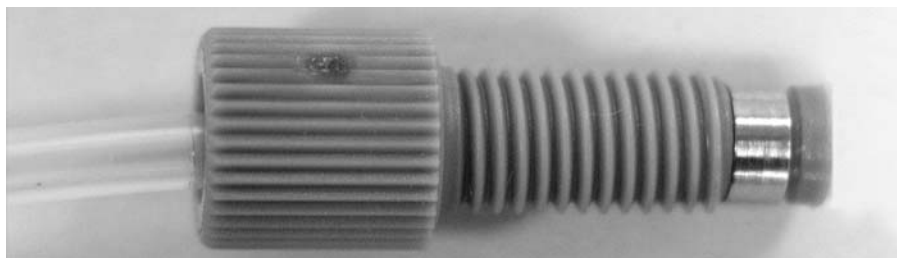


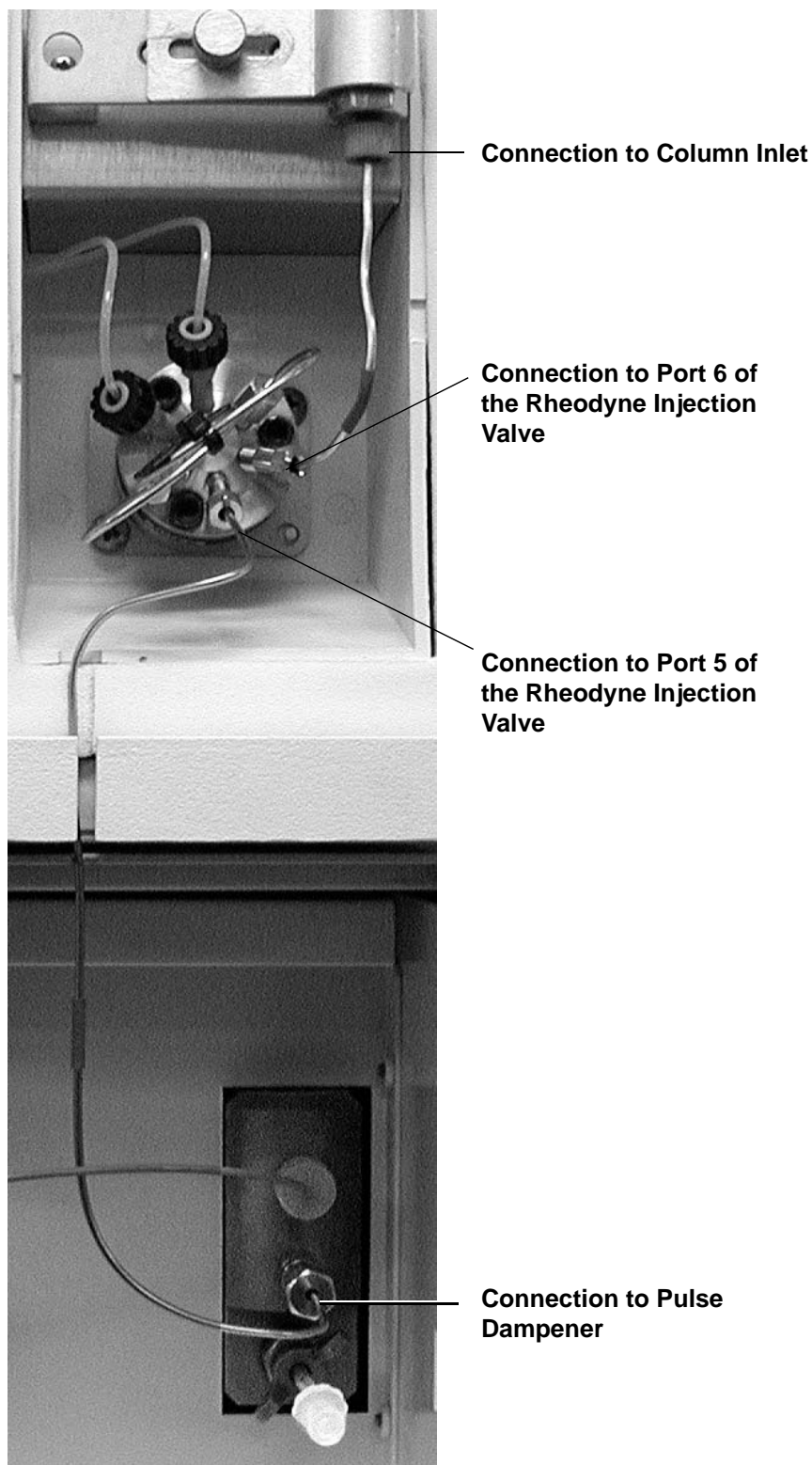
Figure 4-4. Plumbed Surveyor Stack



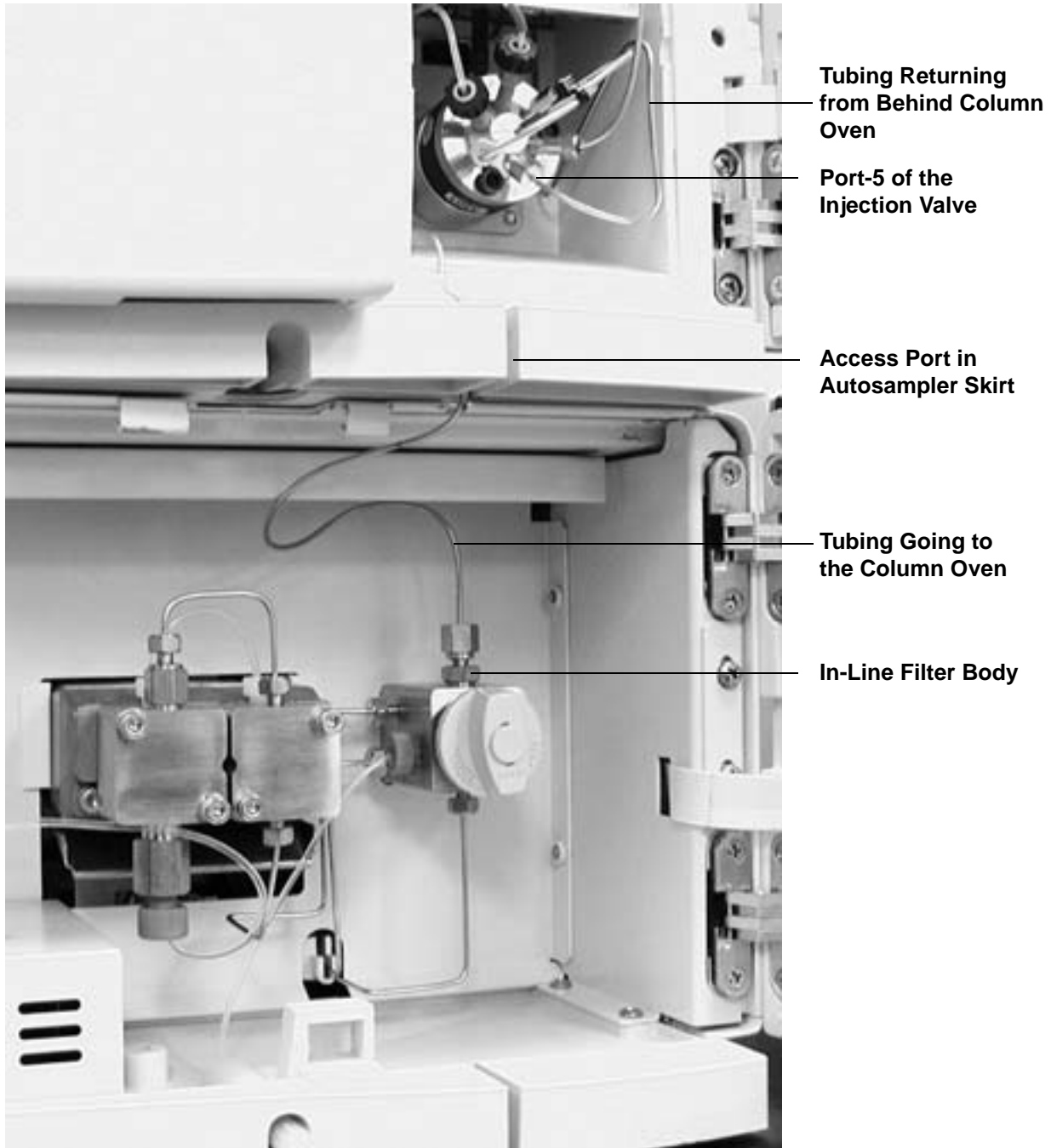
**Figure 4-5.** Wash bottle tubing connection to syringe valve, showing brackets



**Figure 4-6.** Solvent reservoir tubing with Super Flangeless fitting



**Figure 4-7. Connection between Surveyor Autosampler Lite and MS Pump**

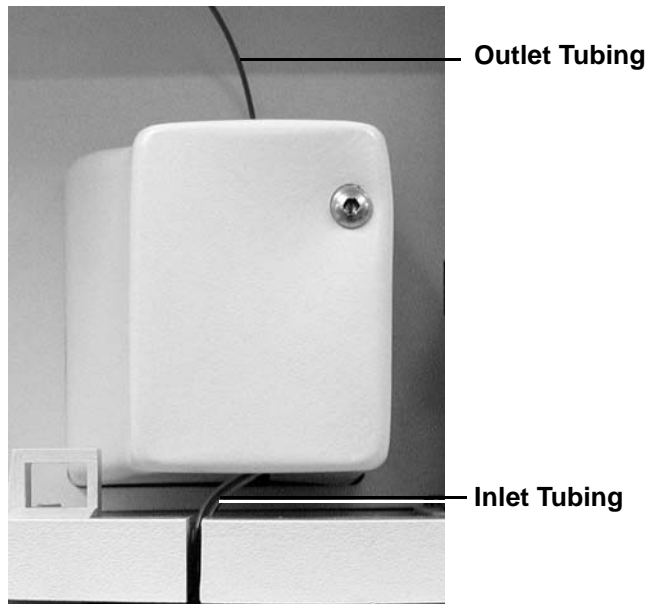


**Figure 4-8. Surveyor LC Pump connected to Full Featured Surveyor Autosampler**

**Finnigan LTQ**



**Figure 4-9. Six-Port Rheodyne Injection Valve (7739)**



**Figure 4-10. Surveyor UV/Vis detector showing LightPipe flowcell cover and tubings**





# Chapter 5

## Connecting the Thermo Electron Finnigan SpectraSYSTEM

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The Xcalibur data system allows control of the Thermo Electron Finnigan SpectraSYSTEM<sup>® 1</sup> with autosampler (AS3000, AS3500), pump (P2000, P4000), and UV detector (UV2000, UV6000LP).

This chapter contains the following sections:

- Connecting to a SpectraSYSTEM with a UV2000 Detector
- Connecting to a SpectraSYSTEM with a UV6000LP Detector
- Configuring the Autosampler and Pump

Table 5-1 lists the Xcalibur kit used with the SpectraSYSTEM.

**Table 5-1. Xcalibur kit used with the SpectraSYSTEM**

Part Number	Description of Kit
OPTON-21706	<b>Xcalibur SpectraSYSTEM Interface Kit</b> SpectraSYSTEM 9.05 EPROM for SN4000 EPROM removal tool Contact Closure Wiring Harness 2-wire trigger cable (contact closure)

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<sup>1</sup> Formerly Thermo Separation Products (TSP) SpectraSYSTEM

Table 5-2 lists the Xcalibur supported firmware for the SpectraSYSTEM.

**Table 5-2. Xcalibur supported firmware versions for the SpectraSYSTEM**

Module	Model Number	Firmware Version*
Binary pump	P2000	4.03
Quaternary pump	P4000	4.04
Autosampler	AS3000/3500	3.44
UV/VIS detector	UV2000	3.13
Photo diode array detector	UV6000LP	1.00
Serial interface	SN4000	9.05

\*To obtain the firmware version for a module, push the <MENU> key on the keypad, then use the <\_> key to select TESTS. Press the <ENTER> key twice to display the Software Version.

Table 5-3 lists the reference manuals for the SpectraSYSTEM.

**Table 5-3. SpectraSYSTEM reference manuals**

Module	Model Number	Reference Manual
Binary pump	P2000	SpectraSYSTEM & SpectraSERIES Gradient Pump Reference Manual
Quaternary pump	P4000	SpectraSYSTEM & SpectraSERIES Gradient Pump Reference Manual
Autosampler	AS3000/3500	SpectraSYSTEM & SpectraSERIES Autosampler Reference Manual
UV/VIS detector	UV2000	SpectraSYSTEM UV/VIS Detector Reference Manual
Photo diode array detector	UV6000LP	UV6000LP Detector Reference Manual

## 5.1 Connecting to a SpectraSYSTEM with a UV2000 Detector

For additional information about your SpectraSYSTEM modules refer to the manuals listed in Table 5-3.

To connect the LTQ MS detector to a SpectraSYSTEM equipped with a UV2000 detector, proceed as follows:

1. Interconnect the pump, autosampler, and the UV2000 detector with the Contact Closure Wiring Harness. Follow the wiring scheme shown in Figure 5-1.
2. Connect the SN4000 (P/N A3625-073) to the pump, autosampler, UV2000 detector, and the data system computer: (Figure 5-1)

**Caution.** Before you remove the top cover of the SN4000, turn the power switch located on the rear of the SN4000 to Off, and disconnect the 12 V dc power supply.

- a. Turn the SN4000 power switch to Off and disconnect the 12 V dc power supply.
- b. Turn the SN4000 upside down to access the four Phillips-head screws that secure the top cover to the case.
- c. Remove the screws and slide the top cover off to expose the SN4000 PCB and the RJ11 and RJ45 ports.
- d. Verify that the EPROM firmware version 9.05 (P/N A4636-129) is installed in socket U12 located on the SN4000 PCB. Sockets U11, U28, and U29 should be empty. Verify that the correct firmware is installed in the pump, autosampler, and UV detector. (Refer to Table 5-2 on page 5-2.)
- e. Connect one RJ11 6-pin, 4-wire cable from the PUMP port located on the SN4000 PCB to the COM port located on the rear of the pump. (Route all cables through the access hole located in the rear panel of the SN4000.)
- f. Connect another RJ11 6-pin, 4-wire cable from the A/S port located on the SN4000 PCB to the COM port located on the rear of the autosampler.
- g. Connect a third RJ11 6-pin, 4-wire cable from the DET 1 port located on the SN4000 PCB to the COM port located on the rear of the UV2000 detector.

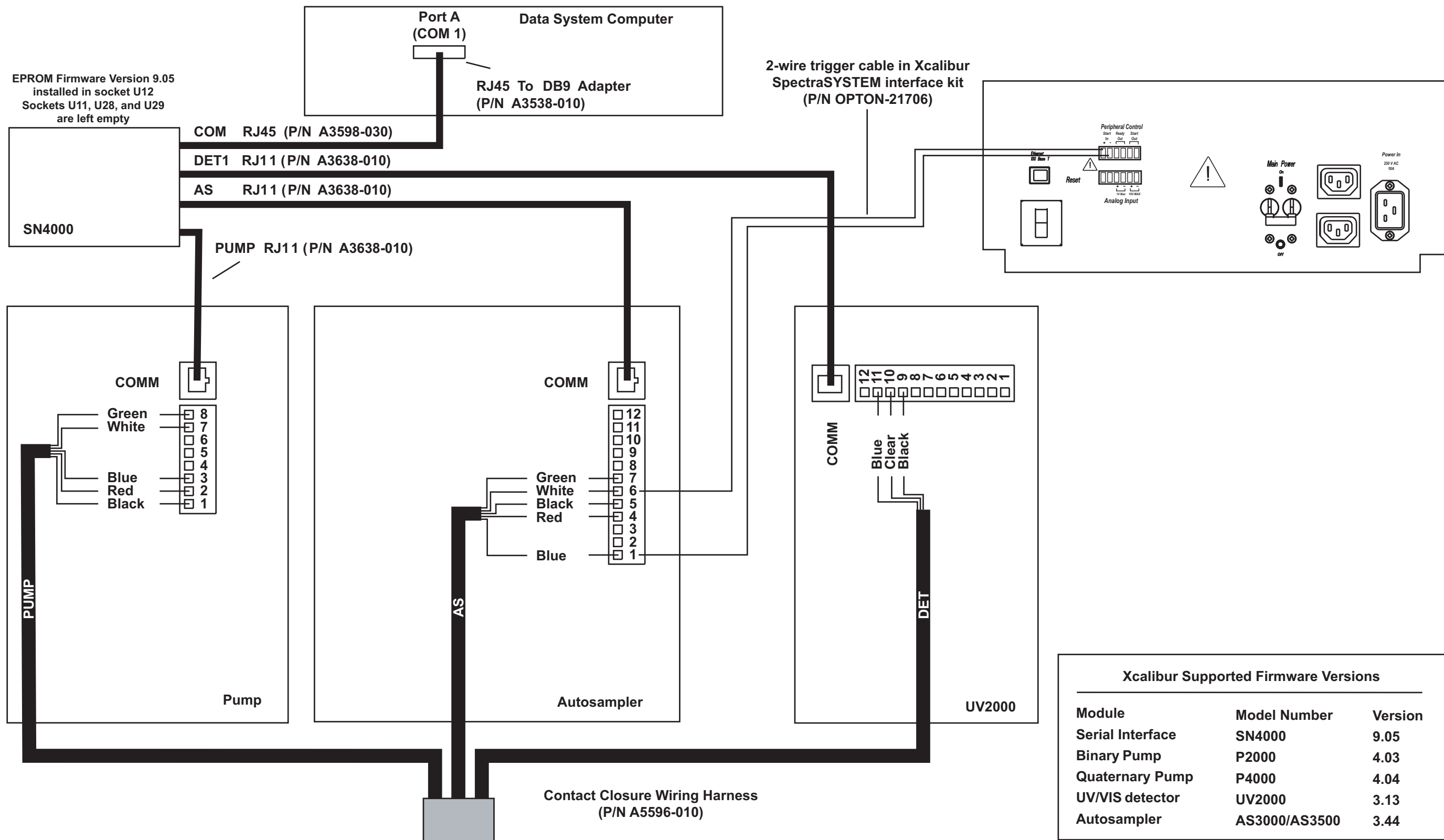
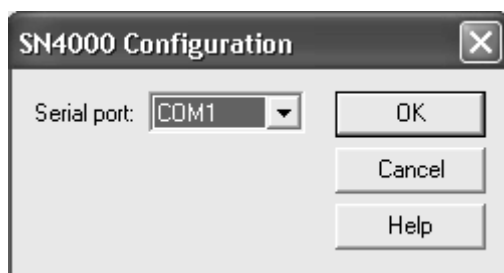


Figure 5-1. Schematic diagram showing the cable connections for the LTQ MS detector and a SPECTRASYSTEM equipped with a pump, autosampler, and UV2000 detector

- h. Connect an RJ45 8-pin, 8-wire cable from the COM port located on the SN4000 PCB to an RJ45 to DB9 adapter.
        - i. Connect the DB9 adapter and the attached cable to the RS-232 port (labeled A) located on the rear of the data system computer.
        - j. Reinstall the SN4000 top cover and mounting screws.
        - k. Reconnect the power cable from the 12 V dc power supply to the Power In inlet located on the rear of the SN4000.
3. Connect the 2-wire trigger cable (in kit P/N OPTON-21706) from the LTQ MS detector power entry module to the contact closure terminal located on the rear of the autosampler following the wiring scheme shown in Figure 5-1.
4. Use the Xcalibur data system Instrument Configuration dialog box to assign the RS-232 connection from the SN4000 to COM1 (port A) of the data system computer:
  - a. Choose **Start > Programs > Xcalibur > Instrument Configuration** to open the Instrument Configuration dialog box.
  - b. Scroll through the Available Devices group box and double-click on the TSP SN4000 button. The TSP SN4000 button is copied to the Configured Devices group box and is displayed as a Configured Devices button.
  - c. Double-click on the TSP SN4000 button in the Configured Devices group box. Xcalibur opens the TSP SN4000 Configuration dialog box. See Figure 5-2.
  - d. Select *COM1* in the Serial Port list box, then click on **OK** to save the setting and close the dialog box.



**Figure 5-2. SN4000 Configuration dialog box**

Go to **Configuring the Autosampler and Pump** on page 5-10.

## 5.2 Connecting to a SpectraSYSTEM with a UV6000LP Detector

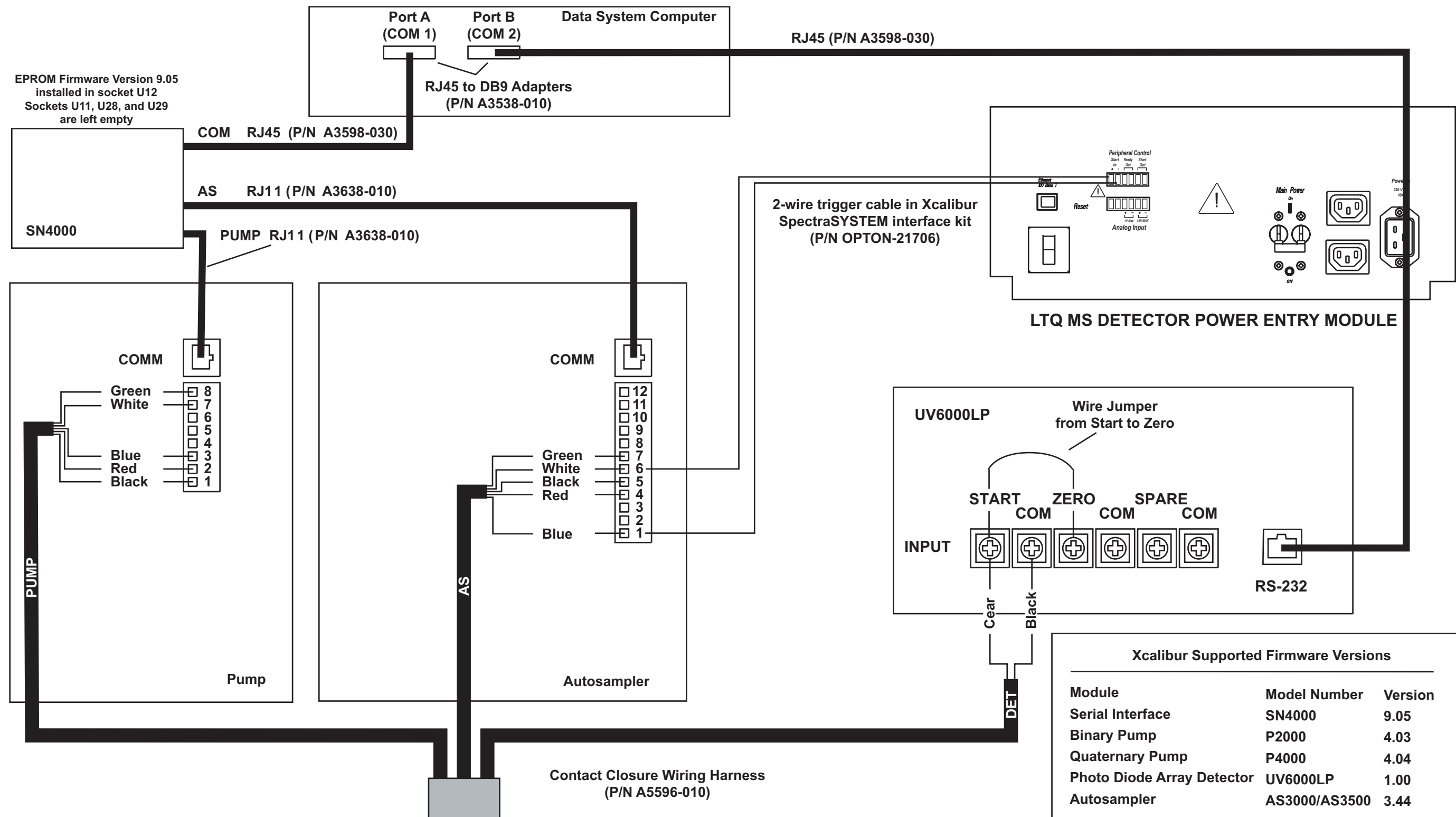
For additional information about your SpectraSYSTEM modules, refer to the manuals listed in Table 5-3.

To connect the LTQ MS detector to a SpectraSYSTEM equipped with a UV6000LP detector, proceed as follows:

1. Interconnect the pump, autosampler, and UV6000LP with the Contact Closure Wiring Harness. Follow the wiring scheme shown in Figure 5-3.
2. Connect the SN4000 (P/N A3625-073) to the pump, autosampler, and data system computer: (Figure 5-3)

**Caution.** Before you remove the top cover of the SN4000, turn the power switch to Off, and disconnect the 12 V dc power supply.

- a. Turn the SN4000 power switch located on the rear of the module to Off and disconnect the 12 V dc power supply.
- b. Turn the SN4000 upside down to access the four Phillips-head screws that secure the top cover to the case.
- c. Remove the screws and slide the top cover off to expose the SN4000 PCB and the RJ11 and RJ45 ports.
- d. Verify that the EPROM firmware version 9.05 (P/N A4636-129) is installed in socket U12 located on the SN4000 PCB. Sockets U11, U28, and U29 should be empty. Verify that the correct firmware is installed in the pump, autosampler, and UV detector. (Refer to 5-2.)
- e. Connect one RJ11 6-pin, 4-wire cable from the PUMP port located on the SN4000 PCB to the COM port located on the rear of the pump. (Route all cables through the access hole located in the rear panel of the SN4000.)
- f. Connect another RJ11 6-pin, 4-wire cable from the A/S port located on the SN4000 PCB to the COM port located on the rear of the autosampler.
- g. Connect the RJ45 8-pin, 8-wire cable from the COM port located on the SN4000 PCB to an RJ45 to DB9 adapter.
- h. Connect the DB9 adapter and the attached cable to the RS-232 port (labeled A) located on the rear of the data system computer.
- i. Reinstall the SN4000 top cover and mounting screws.



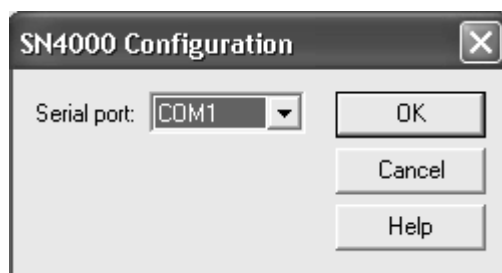
Xcalibur Supported Firmware Versions		
Module	Model Number	Version
Serial Interface	SN4000	9.05
Binary Pump	P2000	4.03
Quaternary Pump	P4000	4.04
Photo Diode Array Detector	UV6000LP	1.00
Autosampler	AS3000/AS3500	3.44

Figure 5-3. Schematic diagram showing the cable connections for the LTQ MS detector and a SPECTRASystem equipped with a pump, autosampler, and UV6000LP detector

- j. Reconnect the power cable from the 12 V dc power supply to the Power In inlet located on the rear of the SN4000.
3. Connect the UV6000LP detector to the data system computer: (See Figure 5-3.)
  - a. Connect an RJ45 8-pin, 8-wire cable to the RS-232 port located on the rear of the UV6000LP detector.
  - b. Connect the other end of the RJ45 8-pin, 8-wire cable to an RJ45 to DB9 adapter.
  - c. Connect the DB9 adapter and the attached cable to the RS-232 port (labeled A) located on the rear of the data system computer.

**Note.** If your data system computer has too few serial ports for your needs, you might need to install the 4-port serial PCB as discussed in **Chapter 10: Connecting the 4-Port Serial PCB.**

4. Connect the 2-wire trigger cable (in kit P/N OPTON-21706) from the LTQ MS detector power entry module to the contact closure terminal located on the rear of the autosampler following the wiring scheme shown in Figure 5-3.
5. Use the Xcalibur data system Instrument Configuration dialog box to assign the RS-232 connection from the SN4000 to COM1 (port A) or another available port of the data system computer:
  - a. Choose **Start > Programs > Xcalibur > Instrument Configuration** to open the Instrument Configuration dialog box.
  - b. Scroll through the Available Devices group box and double-click on the TSP SN4000 button. The TSP SN4000 button is copied to the Configured Devices group box and is displayed as a Configured Devices button.
  - c. Double-click on the TSP SN4000 button in the Configured Devices group box. Xcalibur opens the SN4000 Configuration dialog box. See Figure 5-4.
  - d. Select *COM1* (or the port that you used) in the Serial Port list box, then click on **OK** to save the setting and close the dialog box.



**Figure 5-4. SN4000 Configuration dialog box**



6. Use the Xcalibur data system Instrument Configuration dialog box to assign the RS-232 connection from the UV6000LP to an empty COM port, such as COM3, of the data system computer:
  - a. Choose **Start > Programs > Xcalibur > Instrument Configuration** to open the Instrument Configuration dialog box.
  - b. Scroll through the Available Devices group box and double-click on the TSP UV6000 button. The TSP UV6000 button is copied to the Configured Devices group box and is displayed as a Configured Devices button.
  - c. Double-click on the TSP UV6000 button in the Configured Devices group box. Xcalibur opens the UV6000 Configuration dialog box. See Figure 5-5.
  - d. Select the port to which the UV6000LP is attached (in this case COM3) in the Serial Port list box, then click on **OK** to save the setting and close the dialog box.



Figure 5-5. UV6000 Configuration dialog box

Go to the next section: **Configuring the Autosampler and Pump.**

## 5.3 Configuring the Autosampler and Pump

---

To configure the autosampler and pump, proceed as follows:

1. Configure the autosampler for SpectraNet communication:
  - a. Turn on the pump, autosampler, and UV detector.
  - b. Turn on the SN4000.
  - c. After the autosampler power-up sequence is complete, press <MENU> on the autosampler keypad, then select /OPTIONS/Configurations/ to access the Configurations Menu.
  - d. Move the cursor to the Mode field, and use the <+> and the <-> keys to select *SpectraNet*. Then, press <ENTER> to accept the field value and exit the Configuration Menu.
2. Configure the autosampler for contact closure:
  - a. Press <MENU> on the autosampler keypad, then select /OPTIONS/Input Polarity/ to access the Input Polarity Menu.
  - b. Move the cursor to the Pump Ready Active field, and use the <+> and the <-> keys to select *Hi* or *Lo*. Both the autosampler and the pump must have the same polarity. Then, press <ENTER> to accept the field value and exit the Configuration Menu.
3. Configure the pump for contact closure:
  - a. Press <MENU> on the pump keypad, then select /OPTIONS/More/ to access the More Menu.
  - b. Move the cursor to the Ready Output Active field, and use the <+> and the <-> keys to select *Hi* or *Lo*. Both the autosampler and the pump must have the same polarity. Then press <ENTER> to accept the field value and exit the Configuration Menu.
4. Use the Xcalibur data system Instrument Configuration dialog box to configure the autosampler and pump:
  - a. Choose **Start > Programs > Xcalibur > Instrument Configuration** to open the Instrument Configuration dialog box.
  - b. Scroll through the Available Devices group box and double-click on the TSP Autosampler button. The TSP Autosampler button is copied to the Configured Devices group box and is displayed as a Configured Devices button.
  - c. Double-click on the TSP Autosampler button in the Configured Devices group box. Xcalibur opens the TSP Autosampler Configuration dialog box. See Figure 5-6.

- d. Click on **Autoconfigure** to configure the autosampler, and then click on **OK** to save the settings and close the dialog box.
- e. Scroll through the Available Devices group box and double-click on the TSP P4000 (or TSP P2000) button. The TSP P4000 button is copied to the Configured Devices group box and is displayed as a Configured Devices button.
- f. Double-click on the TSP P4000 button in the Configured Devices group box. Xcalibur opens the Pump Configuration dialog box. See Figure 5-7.
- g. Click on **Autoconfigure** to configure the pump, and then click on **OK** to save the settings and close the dialog box.

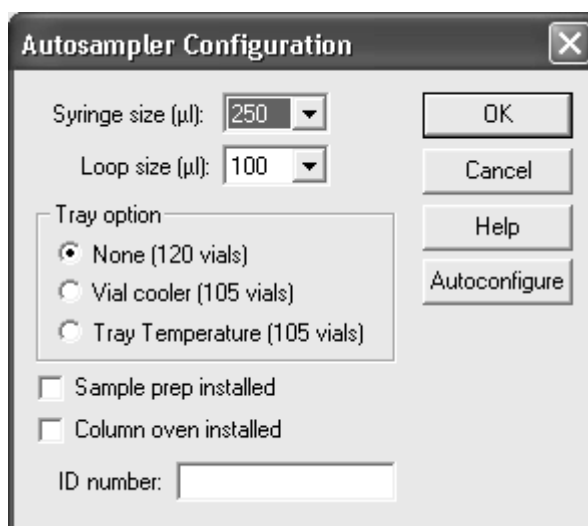


Figure 5-6. Autosampler Configuration dialog box

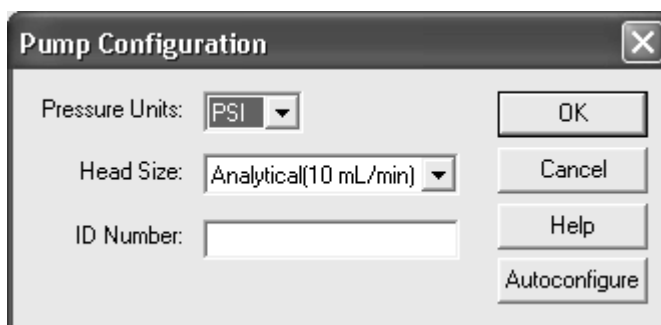


Figure 5-7. Pump Configuration dialog box



# Chapter 6

## Connecting the Agilent 1100 Series LC

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The Xcalibur data system allows control of the Agilent®<sup>1</sup> 1100 Series LC.

For additional information about the Agilent 1100 Series LC refer to the Agilent 1100 Series LC reference manuals.

Table 6-1 lists the Xcalibur supported firmware versions for the Agilent 1100 Series LC.

**Table 6-1. Xcalibur supported firmware versions for the Agilent 1100 Series LC**

Module	Model Number	Firmware Version*
Isocratic pump	G1310A	5.04
Binary pump	G1312A	5.04
Quaternary pump	G1311A	5.04
Capillary pump	G1376A	5.05
Autosampler	G1313A	5.04
Micro-sampler	G1387A	5.04
Thermostatted autosampler	G1329A	5.04
Well-plate autosampler	G1367A	5.04
Micro well-plate auttosampler	G1377A	5.04
Thermostatted column compartment	G1316A	5.04
Variable wavelength detector	G1314A	5.04
Diode-array detector	G1315A	5.04
Multiple wavelength detector**	G1365B	5.04

\*To obtain the firmware versions for the Agilent 1100 modules, verify that the Agilent 1100 Series modules are connected by CAN communication cables, all the modules are turned on, and the Agilent 1100 Control Module is connected. Push the <ESC> key on the Control Module until *System* is displayed in the upper left corner of the display, and then push the <F4> key to access the Records and display the firmware version.

\*\*Only works with version B of the control module

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<sup>1</sup> Formerly Hewlett-Packard® (HP)

Agilent 1100 Series LC systems with JetDirect® interface cards must have revision 2 mainboards to function properly with LAN communications. Table 6-2 shows the required revision level for each module; the serial number listed in the table and all serial numbers after that number are supported.

**Table 6-2. Agilent 1100 modules with JetDirect Cards and the supported version serial number**

Module	P/N (Mainboard)	Supported Version Serial Numbers*
G1310A Isocratic	G1311-65520	DE64300355 US64400233
G1311A Quad	G1311-65520	DE64301137 US64401134
G1312A Bin	G1312-65520	DE64300703 US64400425
G1313A ALS	G1313-65520	DE64302092 US64400886
G1314A VWD	G1314-65520	JP64201926 JP64201926
G1315A DAD	G131-65520	DE64301532 US64400333

\* All serial numbers above the listed number in numeric order are supported.

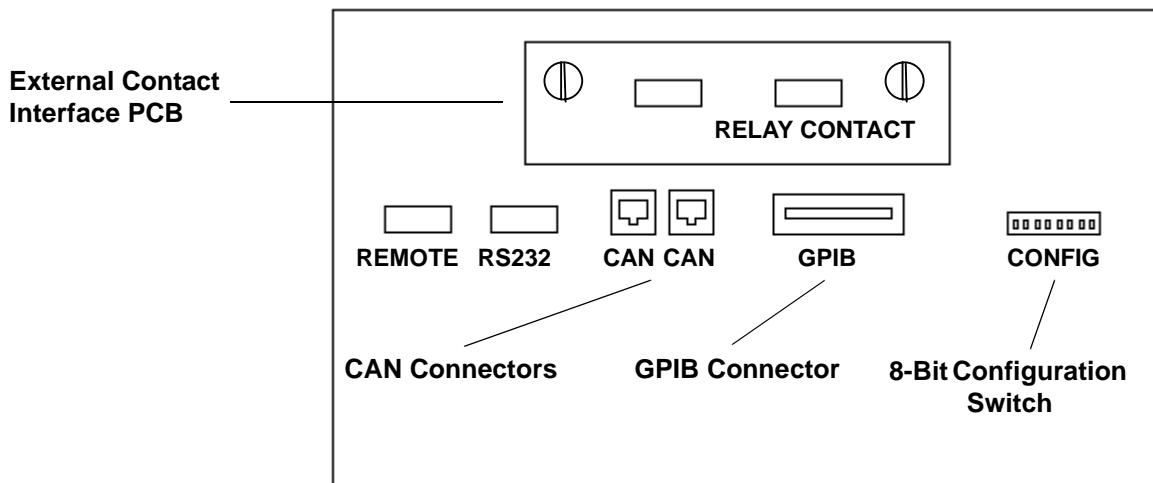
**Note.** The Agilent 1100 Series devices query the PC for the stack IP address only during their start up procedure. Therefore, complete the following procedure and ensure that the Xcalibur Home Page window is open before turning on the Agilent 1100 Series devices.

Connect the LTQ MS Detector to an Agilent 1100 Series LC as follows:

1. Interconnect the modules of your Agilent 1100 Series LC with the CAN cables following the instructions in the Agilent 1100 Series LC reference manuals.
2. Locate the 8-bit configuration switch (labeled *CONFIG*) on the rear of each Agilent 1100 Series module. Make sure that the third DIP switch is in the 0 position (down) to specify the use of the Ethernet interface.
3. If your Agilent 1100 Series Autosampler is not equipped with an External Contact Interface PCB (P/N 00012-27714), you need to install the PCB:
  - a. Make sure that the autosampler is Off.

**Finnigan LTQ**

- b. Remove the cover plate from the slot where you will install the External Contact Interface PCB by loosening the two screws that fasten the plate to the chassis of the autosampler.
  - c. Insert the External Contact Interface PCB into the slot and tighten the two screws to fasten the PCB to the chassis of the autosampler. See Figure 6-1.
4. Connect the 2-wire DB15 trigger cable (PCB P/N 00012-27716) from the LTQ MS Detector I/O panel to the RELAY CONTACT connector located on the External Contact Interface PCB of the Agilent 1100 Series Autosampler following the wiring scheme shown in Table 6-3. (Figure 6-1)



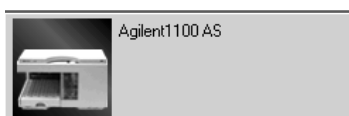
**Figure 6-1. Agilent 1100 Series Autosampler (G1313A) rear panel**

**Table 6-3. Wiring the LTQ MS Detector and the Agilent 1100 Series Autosampler for contact closure**

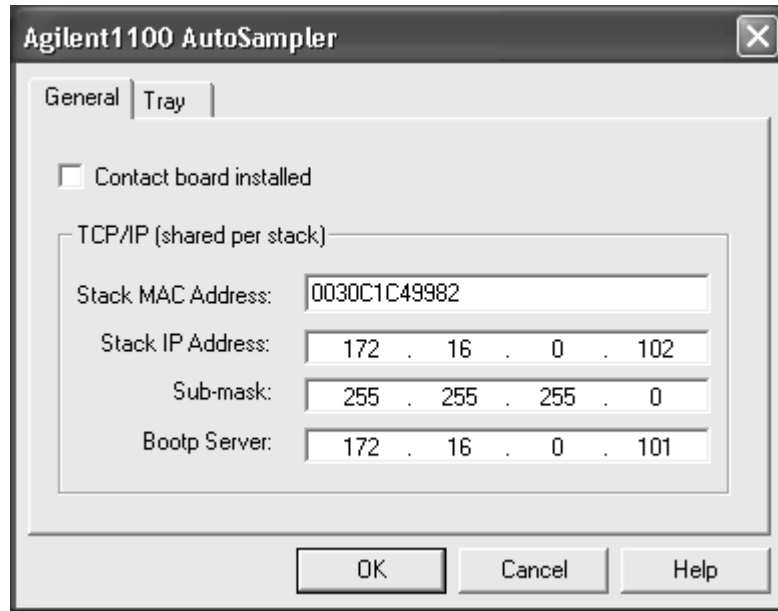
Cable Wire	Agilent 1100 Series Autosampler Contact Closure Pin	LTQ MS Detector I/O Panel
White	1	Start In (+)
Brown	2	Start In (-)

**Important.** An HP JetDirect 400N network card must be installed in one module in the Agilent 1100 Series LC stack. If your LC stack contains a detector (e.g., diode-array detector, variable wavelength detector, multiple wavelength detector), the HP JetDirect 400N network card should be installed in the detector. Otherwise, it can be installed in any module with an open slot.

5. If you need to install the HP JetDirect 400N network card, do the following:
  - a. Make sure that the module is Off.
  - b. Remove the cover plate from the slot where you will install the HP JetDirect 400N network card by loosening the two screws that fasten the plate to the chassis of the module.
  - c. Insert the HP JetDirect 400N network card into the slot and tighten the two screws to fasten the PCB to the chassis of the module.
6. Connect an Ethernet cable from the JetDirect 400N network card to the Ethernet hub.
7. Connect an Ethernet cable from the Ethernet hub to the Ethernet card in the computer that is dedicated to the LC system (typically Network Interface Card number 3).
8. Use the Xcalibur data system Instrument Configuration dialog box to assign contact closure control to the Agilent 1100 Series Autosampler:
  - a. Choose **Start > Programs > Xcalibur > Instrument Configuration** to open the Instrument Configuration dialog box.
  - b. Scroll through the Available Devices group box and double-click on the Agilent 1100 AS button. The Agilent 1100 AS button is copied to the Configured Devices group box and is displayed as a Configured Devices button.
  - c. Double-click on the Agilent 1100 AS button in the Configured Devices group box. Xcalibur opens the Agilent 1100 Autosampler Configuration dialog box.
  - d. Click on the General tab to open the General page. See Figure 6-2.







**Figure 6-2. Agilent Autosampler dialog box**

- e. Select the Contact Board Installed check box.

**Note.** The TCP/IP settings are shared by all Agilent 1100 LC modules in the stack. Changing the value of a setting for one module in the Instrument Configuration dialog box changes the value of that setting for all modules in the stack.

- f. In the Stack MAC address text box, enter the Media Access Control address for your Agilent LC stack. The stack MAC address is a unique identification for each network card. The manufacturer usually stamps it on the network card.
- g. In the Stack IP Address list box, enter the IP address for your Agilent 1100 LC stack. Contact your network administrator for the IP address.
- h. In the Sub-mask text box, enter the subnet mask (address mask). Leave the subnet mask set to its default value, or contact your network administrator for the subnet mask.
- i. In the Bootp Server text box, enter the IP address for the network card in your PC that is responsible for assigning the stack IP address for your Agilent 1100 LC system. Contact your network administrator for the BOOTP server IP address.
- j. Click on **OK** to save the settings and close the dialog box.

9. Use the Xcalibur data system Instrument Setup to select the Agilent 1100 Series Autosampler contact closure terminal and trigger type:



- a. Choose **Start > Programs > Xcalibur > Xcalibur** to open the Home Page. Then, click on the Instrument Setup button to open the Instrument Setup window.
- b. Click on the Agilent 1100 AS button in the Instrument Setup viewbar on the left side of the window to open the Instrument Setup view. Then, click on the Timed Events tab to open the Timed Events page. See Figure 6-3.
- c. Click on the Contact 1 text box to activate the list box. Then, select *Closed* in the list box.
- d. Ensure that all of the other Contact text boxes display *Open*.
- e. Select **File > Exit** to close the Instrument Setup window. Xcalibur prompts you with the Save As dialog box, the File Summary Information Dialog box, and the File Save – Audit Trail dialog box

		Timed Events				
		Time(min)	Contact 1	Contact 2	Contact 3	Contact 4
1		0.00	Closed	Open	Open	Open
*		1.00	Open	Open	Open	Open

**Figure 6-3.** Instrument Setup window, showing the Agilent 1100 Series Autosampler view with a portion of the Timed Events page displayed. The Timed Events page is for selecting the Agilent 1100 Series Autosampler contact closure terminal and contact closure trigger type.

10. Ensure that the Xcalibur Home Page is still open and power up the Agilent 1100 Series modules.
11. Verify that the correct firmware is installed in the Agilent 1100 Series modules. (Refer to 6-1.)

**Note.** The solvent tracking feature on the Agilent 1100 LC pumps is not supported by Xcalibur at this time. This feature must be turned off to prevent error messages from terminating the data acquisition.

12. Turn off the solvent tracking feature on the Agilent 1100 pump:
  - a. Close the Xcalibur Home Page.
  - b. Using the Agilent 1100 handheld control module, on the Analysis screen press the Settings button <F1>.
  - c. Press the number corresponding to the pump.

**Finnigan LTQ**

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- d. Press the Bottle Fillings button <F4>.
  - e. Set all of the solvent Total boxes to 0. The solvent Actual boxes are then automatically set to 0.
  - f. Clear the Error If Empty check box by using the right arrow to move the focus to this setting and then pressing **Enter**.
  - g. Press the Done button <F6>.
13. Choose **Start > Programs > Xcalibur > Xcalibur** to open the Home Page. The Agilent 1100 devices should reconnect and appropriately display their status.



# Chapter 7

## Upgrading the HP 1100 Series LC

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The Xcalibur data system allows control of the Hewlett-Packard® (HP) 1100 Series LC *only* if you upgrade the HP 1100 communication interface to an Ethernet interface.

Upgrade your HP 1100 Series LC as follows:

1. Order the appropriate upgrade parts from your local office for Thermo Electron San Jose products:
  - If the HP 1100 is **not** currently interfaced to a Finnigan mass spectrometer as an Xcalibur-controlled GPIB inlet device, order the kit listed below in Table 7-1.

**Table 7-1. Xcalibur Kit to upgrade the HP 1100 Series LC**

Part Number	Description of Kit
OPTON-30018	<b>JetDirect Ethernet Control Kit</b> Contact closure PCB External contact closure cable Ethernet 10 Base-T cable (2) 10/100 Autosensing 8-port Ethernet switch HP JetDirect 400N PCB

- If the HP 1100 is currently interfaced to a Finnigan mass spectrometer as an Xcalibur-controlled GPIB inlet device, order the parts listed below in Table 7-2.

**Table 7-2. Parts to upgrade an Xcalibur-controlled HP 1100 Series LC**

Part Number	Description of Part
00825-01140	HP JetDirect 400N PCB
00012-70008	Ethernet 10 Base-T cable (2)

**Note.** An HP 1100 LC system that is currently interfaced to a Finnigan mass spectrometer as an Xcalibur-controlled GPIB inlet device already should have installed the contact closure PCB and the external contact closure cable. Therefore, you need to order only the parts specified in Table 7-2.

2. Follow the instructions in **Chapter 6: Connecting the Agilent 1100 Series LC** to install the JetDirect 400N PCB.

**Note.** After the communication interface in the HP 1100 LC system is upgraded to an Ethernet interface, the system is the same as, and will be referred to as, an Agilent 1100 LC system.

3. Continue to follow the instructions in **Chapter 6: Connecting the Agilent 1100 Series LC** to connect the LTQ MS Detector to the system.

# Chapter 8

## Connecting the Waters LC

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The Xcalibur data system allows control of the Waters Alliance<sup>®</sup> and Alliance HT Separations Modules.

This chapter contains the following sections:

- Connecting to the Waters Alliance or the Alliance HT Separations Module
- Connecting to the Waters 2487 Dual  $\lambda$  Absorbance Detector

Table 8-1 lists the Xcalibur kits used with the Waters LC.

**Table 8-1. Xcalibur kits used with the Waters LC**

Part Number	Description of Kit
OPTON-21710	<b>Xcalibur Waters Interface Kit</b> Waters serial I/F cable 2-wire trigger cable (contact closure)
OPTON-21721	<b>Xcalibur SS420x Interface Kit</b> SS420x PCB serial cable 2-wire trigger cable (contact closure) power supply Xcalibur Additional 4-Port Serial Kit

## 8.1 Connecting to the Waters Alliance or the Alliance HT Separations Module

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Table 6-2 lists the Xcalibur supported firmware version for the Waters Alliance and Alliance HT Separations Modules.

**Table 8-2. Xcalibur supported firmware version for the Waters Alliance and Alliance HT Separations Modules**

Module	Model Number	Firmware Version*
Separations module	2690	1.22
Separations module	2695	2.02
High throughput separations module	2795	2.02

\*To obtain the firmware version for the Waters Separations Module, turn on the instrument and watch the front panel display as the instrument cycles through the system startup.

For additional information about the Waters Alliance or Alliance HT Separations Module, refer to the operator's guide that came with your Waters HPLC system.

To connect the LTQ MS Detector to a Waters Alliance or Alliance HT Separations Module, proceed as follows. See Figure 8-1.

1. Connect the serial cable (P/N 00012-51086) from the RS-232 connector (labeled *B*) located on the rear of the Waters Alliance or Alliance HT Separations Module to an available RS-232 connector located on the rear of the data system computer.
2. Connect the 2-wire trigger cable (in kit P/N OPTON-21710) from the LTQ MS Detector power entry module to the contact closure terminal (labeled *B*) located on the rear of the Waters Alliance or Alliance HT Separations Module following the wiring scheme shown in Table 8-3.



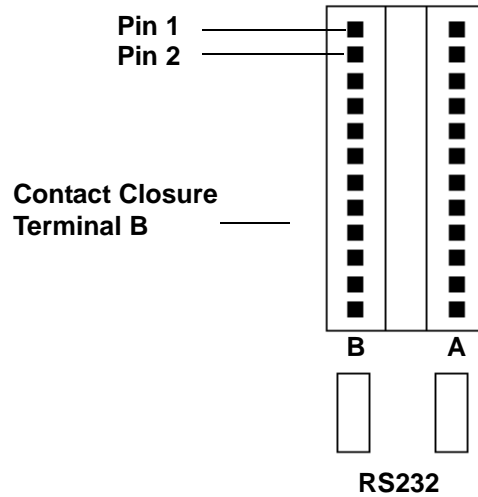
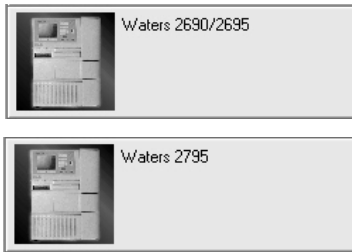


Figure 8-1. Waters Alliance or Alliance HT Separations Module rear panel contact closure terminals

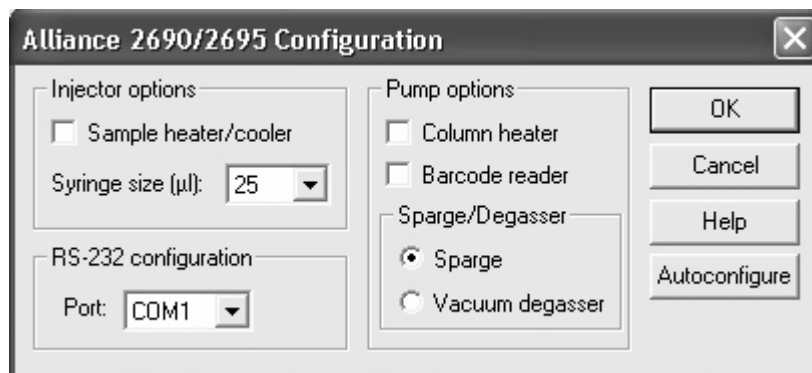
Table 8-3. Wiring the LTQ MS Detector and the Waters Alliance or Alliance HT Separations Module for contact closure

Waters Alliance or Alliance HT Separations Module Contact Closure Terminal B	LTQ MS Detector Power Entry Module
pin 1	Start In +
pin 2	Start In ground

3. Set the Waters Alliance or Alliance HT Separations Module RS-232 communication to ASCII:
  - a. From the Main page on the instrument display, press the <Config> key to open the Configuration page.
  - b. Use the <▶> key to select the Controlled via RS-232 option in the System group box. Then press the <Enter> key to open the list box.
  - c. Use the <▲> and <▼> keys to select Controlled by RS-232 (ASCII) in the list box. Then press the <Enter> key to save the change.
  - d. Press the <Exit> key to return to the Main page.
4. Use the Xcalibur data system Instrument Configuration dialog box to assign the RS-232 connection from the Waters Alliance or Alliance HT Separations Module to the port selected in step 1, such as COM1 (port A), of the data system computer:
  - a. Choose **Start > Programs > Xcalibur > Instrument Configuration** to open the Instrument Configuration dialog box.



- b. Scroll through the Available Devices group box and double-click on the appropriate button for your device (Waters 2690/2695 or Waters 2795). The button is copied to the Configured Devices group box and is displayed as a Configured Devices button.
- c. In the Configured Devices group box, double-click on the button for your device.
  - If you double-click on the Waters 2690/2695 button, Xcalibur opens the Alliance 2690/2695 Configuration dialog box. See Figure 8-2.
  - If you double-click on the Waters 2795 button, Xcalibur opens the Alliance 2795 Configuration dialog box. See Figure 8-3.
- d. Confirm that the Port list box in the RS-232 Configuration group box is set to the port that you selected in step 1.
  - If you have a Waters Alliance 2690 or Alliance 2695 Separations Module, skip to step 4.f.
  - If you have a Waters Alliance HT 2795 Separations Module, continue with the next step.
- e. In the Carrier Plate group boxes, specify the tray type that you are using and the sequential reference counting order for each plate.
- f. Click on **Autoconfigure**, then click on **OK** to save the settings and close the dialog box.



**Figure 8-2. Alliance 2690/2695 Configuration dialog box**

**Alliance 2795 Configuration**

Injector options

Sample heater/cooler

Syringe size (µl): 100

RS-232 configuration

Port: COM1

Pump options

Column heater

Barcode reader

Sparge/Degasser

Sparge

Vacuum degasser

OK

Cancel

Help

Autoconfigure

Carrier Plate Position 1

Plate Type: 24 uCfuge tube 1.5 mL

Sequential Ref: Discontinuous (horizont)

Carrier Plate Position 2

Plate Type: 24 uCfuge tube 1.5 mL

Sequential Ref: Discontinuous (horizont)

Carrier Plate Position 3

Plate Type: 24 uCfuge tube 1.5 mL

Sequential Ref: Discontinuous (horizont)

Carrier Plate Position 4

Plate Type: 24 uCfuge tube 1.5 mL

Sequential Ref: Discontinuous (horizont)

Figure 8-3. Alliance 2795 Configuration dialog box

## 8.2 Connecting to the Waters 2487 Dual $\lambda$ Absorbance Detector

If your Waters LC system is equipped with a Waters 2487 Dual  $\lambda$  Absorbance Detector and you want to record analog output from the detector, you need to connect the SS420x to the data system computer.

**Note.** Xcalibur 1.4 supports the Waters 2487 Dual  $\lambda$  Absorbance Detector only when it is used in conjunction with the Waters Alliance 2690 or 2695 Separations Module.

For instructions on how to install and configure the SS420x refer to **Chapter 9: Connecting the SS420x Analog-to-Digital Interface Kit.**

Connect the Waters 2487 Dual  $\lambda$  Absorbance Detector to the SS420x as follows:

Connect the 2-wire signal cable (in kit P/N OPTON-21710) from the terminal (labeled *B*) located on the rear of the Waters 2487 Dual  $\lambda$  Absorbance Detector to the bus terminal located on the SS420x terminal panel interface. Follow the wiring scheme shown in 8-4.

**Table 8-4. Wiring connection for the Waters 2487 Dual  $\lambda$  Absorbance Detector and the SS420x terminal panel**

Waters 2487 Dual $\lambda$ Absorbance Detector Terminal B	SS420x Terminal Panel (use any channel 1 to 4)
Pin 1	CH +
Pin 3	CH -

**Note.** Confirm that the Waters 2487 Dual  $\lambda$  Absorbance Detector is connected to the Waters Alliance 2690 or 2695 Separations Module with the GPIB cable that was supplied with your LC system. Turn on the detector before you turn on the Waters Alliance 2690 or 2695 Separations Module.

# Chapter 9

## Connecting the SS420x Analog-to-Digital Interface Kit

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The SS420x offers four independent (20-bit resolution) analog-to-digital (A/D) converters for data acquisition from devices that are not currently controlled by Xcalibur. Additionally, there are four inputs and eight outputs that provide contact closure control for devices that are not currently controlled by Xcalibur. For this chapter, contact closure refers to open collector, TTL logic, or relay closure.

Xcalibur can support up to four SS420x units; however, only one unit can be used at a time.

This chapter contains the following sections:

- Connecting and configuring the SS420x
- Configuring the SS420x for data acquisition and control of external devices

Table 9-1 lists the Xcalibur kit used with the SS420x.

**Table 9-1. Xcalibur Kit used with the SS420x**

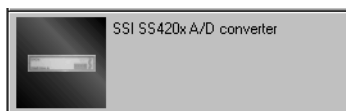
Part Number	Description of Kit
OPTON-21721	<b>Xcalibur SS420x Interface Kit</b> SS420x serial cable 2-wire trigger cable (contact closure) power supply Xcalibur Additional 4-Port Serial Kit

## 9.1 Connecting and Configuring the SS420x

---

Connect the SS420x to the data system computer and configure it for the Xcalibur data system as follows:

1. Turn off the data system computer.
2. Connect the serial cable to the RS-232 port on the rear of the SS420x.
3. Connect the other end of the serial cable to the RS-232 port located on the rear of the data system computer. Be sure to use only ports 1 through 4 to connect the SS420x.
4. Connect the power cable from the 9 V dc power supply included with the SS420x to the POWER inlet located on the rear of the SS420x.
5. Restart the data system computer.
6. Verify that the SS420x is configured for Xcalibur data system control:
  - a. Choose **Start > Programs > Xcalibur > Instrument Configuration** to open the Instrument Configuration dialog box.
  - b. Scroll through the Available Devices group box and double-click on the SSI SS420x A/D Converter button. The SSI SS420x A/D Converter button is copied to the Configured Devices group box and is displayed as a Configured Devices button.
  - c. Double-click on the SSI SS420x A/D Converter button in the Configured Devices group box. Xcalibur opens the SS420x Configuration dialog box.
  - d. Select the COM port to which the device is attached.
  - e. Click on **OK** to save the changes and close the SS420x Configuration dialog box.
  - f. Click on **Done** to close the Instrument Configuration dialog box.



## 9.2 Configuring the SS420x for Data Acquisition and Control of External Events

---

The SS420x has two functions as described in the following topics:

- Data acquisition from analog devices
- Control of external events

### Data Acquisition from Analog Devices

---

The SS420x has four channels on the analog-to-digital converter (Channel A to Channel D) that allow for data input from analog devices not currently controlled by Xcalibur.

**Note.** The following procedure is a general procedure for connecting up to four analog devices to the SS420x. Your particular application might require a different procedure or a different configuration of devices.

To acquire data from an analog device, the following connections are required:

- A 2-wire **signal** cable from each analog device to the SS420x
- A 2-wire **trigger** cable from the analog device(s) to the LC autosampler
- A 2-wire **trigger** cable (contact closure) from the LC autosampler to the SS420x
- A 2-wire **trigger** cable (contact closure) from the LC autosampler to the LTQ MS detector

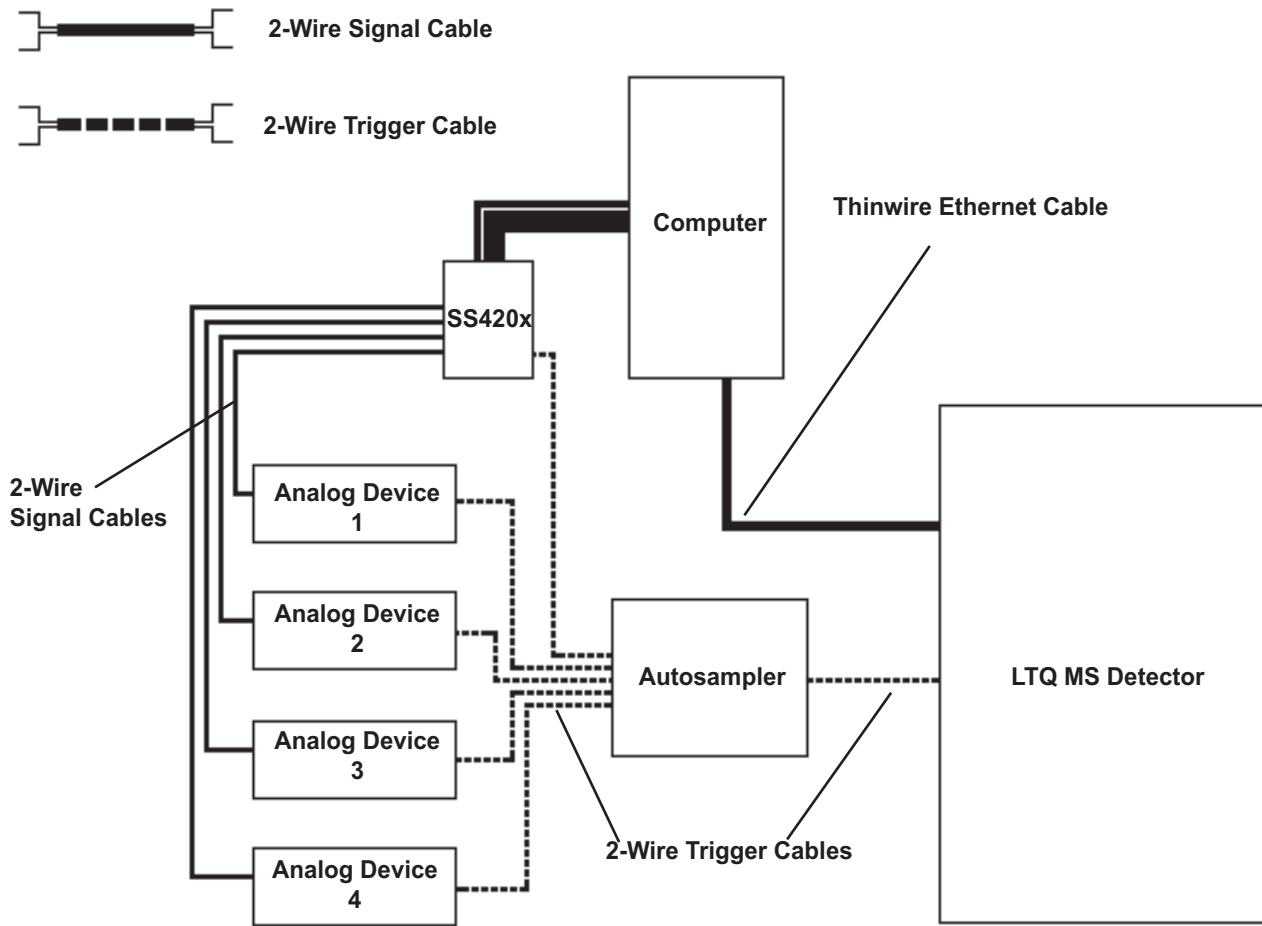
Connect the cables and configure the SS420x as follows. See Figure 9-1.

**Note.** Figure 9-1 shows how to connect the maximum of four analog devices to the SS420x. Your particular application might require a different configuration of devices or a different wiring scheme.

1. Connect the 2-wire **signal** cable from the SS420x to the analog device. Follow the wiring scheme shown in Table 9-2. If you want to connect more than one analog device to the SS420x, use a separate channel (Channel A to Channel D) for each device.

**Table 9-2. Wiring an analog device and the SS420x for A/D data acquisition**

SS420x Analog Inputs	Analog Device (0 to 1 V or 0 to 10 V Output)
CH1 +	Signal output pin
CH1 -	Ground pin



**Figure 9-1. Wiring diagram showing four analog devices connected to the SS420x and autosampler. Each analog device is connected with a 2-wire signal cable and 2-wire trigger cable (contact closure).**



2. Connect a 2-wire **trigger** cable from the analog device to the LC autosampler. Follow the wiring scheme shown in Table 9-3.

**Table 9-3. Wiring the LC autosampler and the analog device for contact closure**

Analog Device	LC autosampler
Start in pin	Inject out pin
Ground pin	Ground pin

3. Connect a 2-wire **trigger** cable from the LC autosampler to the SS420x. Follow the wiring scheme shown in Table 9-4.

**Table 9-4. Wiring the LC autosampler and the SS420x for contact closure**

LC autosampler	SS420x (START1 to START4)
Inject out pin	START1 +
Ground pin	GND1 –

4. Connect a 2-wire **trigger** cable from the LC autosampler to the LTQ MS detector. Follow the wiring scheme shown in Table 9-5.

**Table 9-5. Wiring the LC autosampler and the LTQ MS detector for contact closure**

LC autosampler	LTQ MS detector Inputs
Inject out pin	START IN +
Ground pin	START IN ground pin

5. Configure the SS420x for data acquisition:
  - a. Choose **Start > Programs > Xcalibur > Xcalibur** to open the Xcalibur data system Home Page. Then, click on the Instrument Setup button to open the Instrument Setup window.
  - b. Click on the SSI SS420x A/D Converter button to open the SS420x Instrument Setup view with the Acquisition page displayed. See Figure 9-2.
  - c. Select *1* in the Number of Channels In Use spin box. (If more than one channel is to be used, select the appropriate number of channels.)
  - d. Select the data acquisition rate in the Frequency list box.

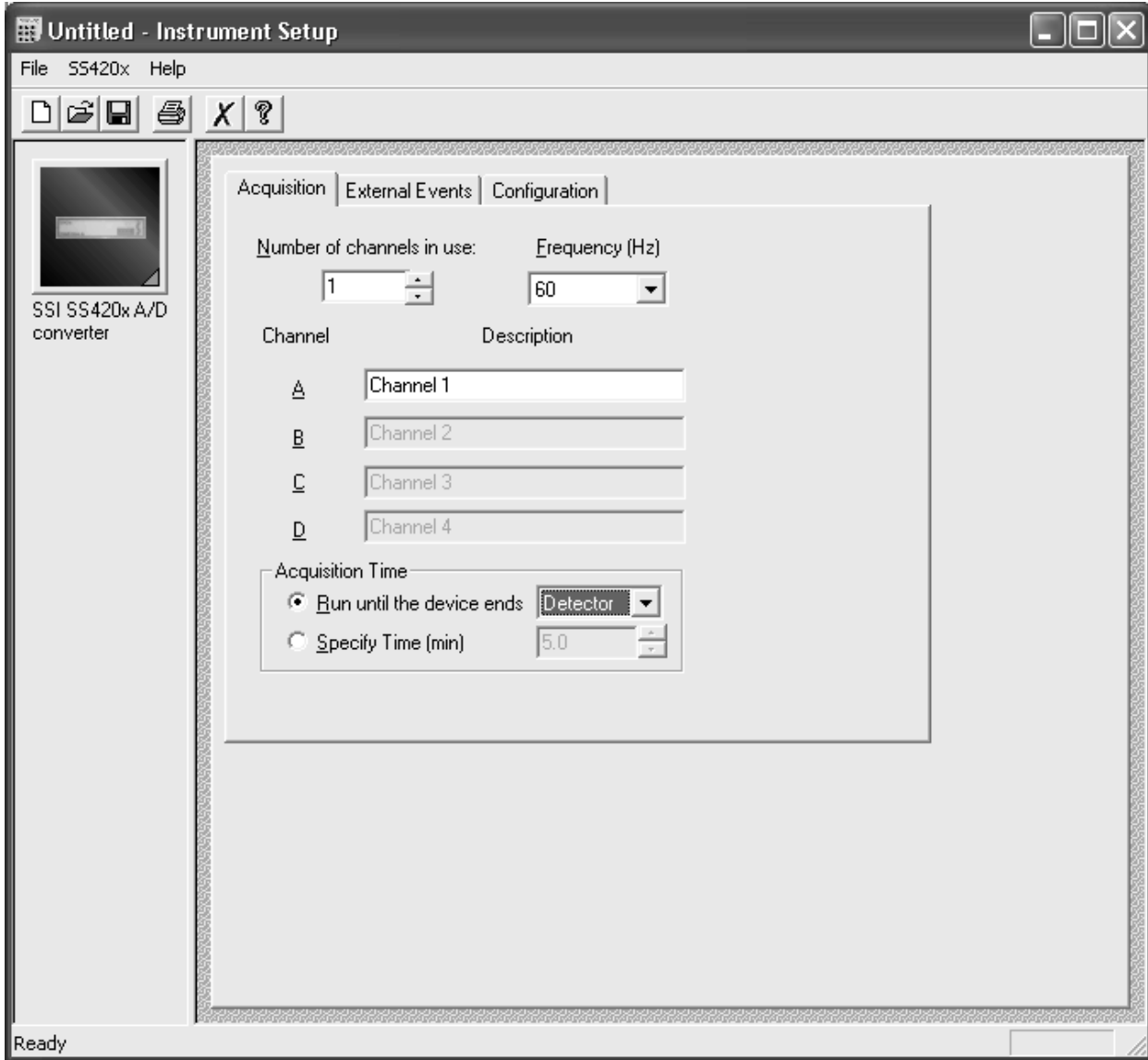
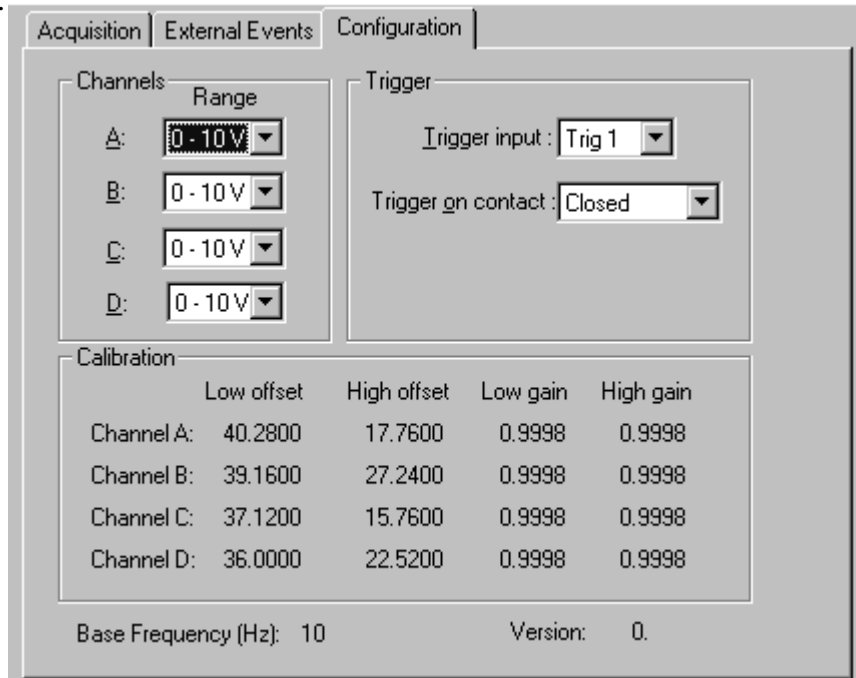


Figure 9-2. Instrument Setup window, showing the SS420x view with the Acquisition page displayed

- e. In the Channel A text box enter the name of the analog device. (If more than one channel is to be used, enter the name of each device in the appropriate channel text box.)
  - f. The acquisition of data through the SS420x can be stopped by either an Xcalibur-controlled device or after a specified time:
    - In the Acquisition Time group box, select the Run Until The Device Ends option button if you want a device to stop the SS420x data acquisition. In the Run Until The Device Ends list box, select the device that will signal the stop of data acquisition.or
    - In the Acquisition Time group box, select the Specify Time option button if you want the SS420x to stop data acquisition after a specified time. In the Specify Time spin box, enter the acquisition time.
6. Click on the Configuration tab to open the Configuration page. See Figure 9-3. Then, setup the SS420x:
- a. Confirm that the appropriate Channel (Channel A to Channel D) Range is selected from the range list box:
    - $0 - 1\text{ V}$ , if the output signal from the analog device is between  $-1$  and  $+1\text{ V}$
    - $0 - 10\text{ V}$ , if the output signal from the analog device is between  $-10$  and  $+10\text{ V}$
  - b. Select *Trig 1* in the Trigger Input list box. If you want to use a device other than the LC autosampler to start data acquisition, select the appropriate trigger line that is connected to the device.

**Note.** The analog device can be triggered by either a closed contact or open contact signal. Refer to the reference manual that is supplied with your device to determine its trigger type.

- c. Select *Closed Contact* in the Trigger On Contact list box or refer to the analog device reference manual to determine the trigger type setting.



**Figure 9-3. Instrument Setup window, showing the SS420x view with the Configuration page displayed**

**Note.** In the Configuration dialog box, the values that appear in the Calibration group box are set by the manufacturer to ensure proper performance of the A/D converter.

**Note.** After you have set up your sequence and loaded the autosampler with your samples, open the Run Sequence dialog box and verify that no instrument is selected as a Start Instrument. Start the run and watch the Home Page - Status View (choose **View > Status View**) until both the SS420x and LTQ MS detector display *Wait for Contact Closure*. Then, manually start the autosampler.

## Control of External Events

The SS420x has eight digital outputs (labeled *RLY1* to *RLY8*) that can be used to control devices that are not currently controlled by Xcalibur.

**Note.** External devices can be triggered by either a closed contact or open contact signal. Refer to the reference manual that is supplied with your external device to determine its trigger type.

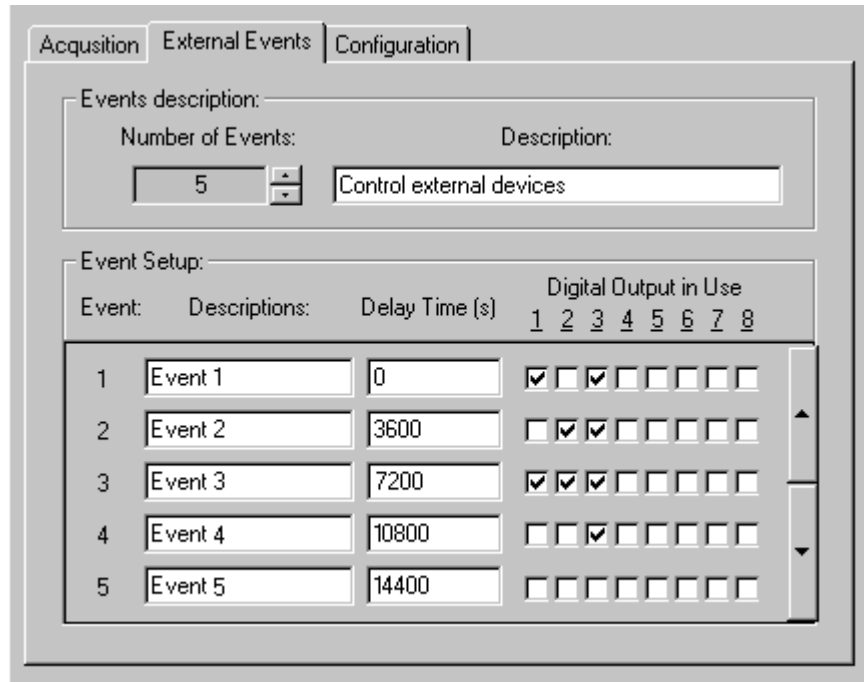
To connect an external device to the SS420x and to configure the SS420x, proceed as follows:

1. Connect a 2-wire trigger cable from input terminals of the external device to the SS420x. Follow the wiring scheme shown in Table 9-6.

**Table 9-6. Wiring an external device and the SS420x for contact closure**

External Device	SS420x (RLY1 to RLY8)
Input pin	RLY A
Ground pin	RLY B

2. Configure the SS420x to control an external device:
  - a. Choose **Start > Programs > Xcalibur > Xcalibur** to open the Xcalibur data system Home Page. Then, click on the Instrument Setup button to open the Instrument Setup window.
  - b. Click on the SSI SS420x A/D Converter button to open the SS420x view with the Acquisition page displayed. See Figure 9-2. Then, click on the External Events tab to open the External Events page. See Figure 9-4.



**Figure 9-4. Instrument Setup window, showing the SS420x view with the External Events page displayed. In this example the SS420x controls three devices. The three devices are Trigger Type - Closed Contact**

- c. In the Events Description group box select the number of events you want to control in the Number of Events spin box. You can control up to 50 events.
- d. In the Description text box, enter a description of the multi-event procedure you want to run.
- e. Set up an event in the Event Setup group box:
  - i. In the Event 1 row, enter a description of the first event in the Descriptions text box.
  - ii. Enter a delay time for the event in the Delay Time text box. The delay time determines when an event occurs. The delay time equals zero when the SS420x starts acquisition or the LTQ MS detector sends a contact closure signal.

- iii. Select the digital output terminal that you want to trigger:
  - For a Trigger Type - Closed Contact device:  
When the Digital Output In Use check box is selected, the external device receives a closed contact signal at the specified delay time. When the Digital Output In Use check box is not selected, the external device receives an open contact signal at the specified delay time.

or

  - For a Trigger Type - Open Contact device:  
When the Digital Output In Use check box is selected, the external device receives an open contact signal at the specified delay time. When the Digital Output In Use check box is not selected, the external device receives a closed contact signal at the specified delay time.
- iv. Repeat steps i-iii for the next event.

Figure 9-4 shows an example of the SS420x controlling three external devices with five events over a period of 4 hours (14400 seconds). For this example all devices are Trigger Type - Closed Contact. When a closed contact event occurs, the external device turns on and performs its function. When the open contact event occurs, the external device turns off and ceases its function.





# Chapter 10

## Connecting the 4-Port Serial PCB

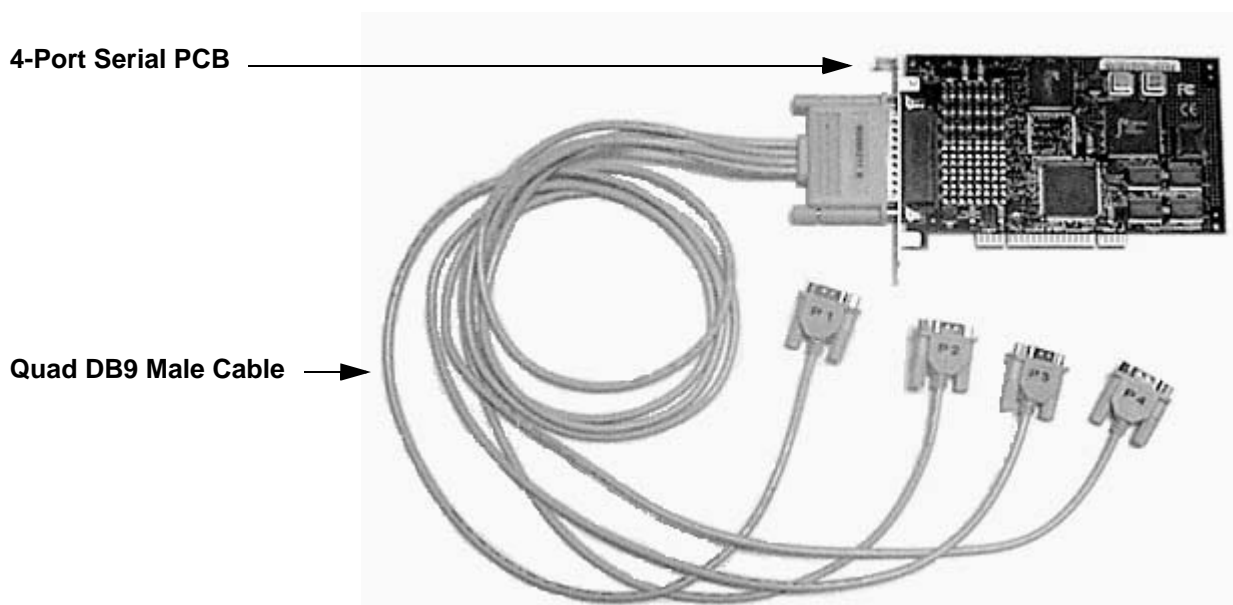
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The 4-Port Serial PCB and Quad DB9 male cable (P/N OPTON-21709) provide four additional communication ports for the data system computer. See Figure 10-1.

Table 10-1 lists the Xcalibur kit used with the 4-Port Serial PCB.

**Table 10-1. Xcalibur Kit used with the 4-Port Serial PCB**

Part number	Description of kit
OPTON-21709	<b>Xcalibur Additional 4-Port Serial Kit</b> 4-Port Serial PCB (PCI) and software Quad DB (male adapter)



**Figure 10-1. 4-Port Serial PCB and Quad DB9 male cable**

To install the 4-Port Serial PCB in the data system computer, proceed as follows:

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 damaging 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 connector faces the rear 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. Use the screw from the slot cover plate to secure the 4-Port Serial PCB in place.
8. Replace the computer cover.
9. Connect the Quad DB9 male cable to the connector located on the 4-Port Serial PCB. Connect the other end of the cable to the appropriate inlet device.
10. Restart the data system computer.

The 4-Port Serial PCB is a Plug and Play device. When Windows<sup>®</sup> XP starts, it automatically detects and configures the new 4-Port Serial PCB and then loads the appropriate drivers.

# Chapter 11

## Making Plumbing Connections to Run Samples on the LTQ MS detector

---

This chapter describes how to make plumbing connections to run samples on the LTQ MS detector.

The following topics are discussed in this chapter:

- Plumbing connections for ESI/MS
- Plumbing connections for APCI/MS










Table 11-1 summarizes the sample introduction and analytical techniques for ESI/MS and APCI/MS.

**Table 11-1. Sample introduction and analytical techniques for ESI/MS and APCI/MS**

Sample Introduction to LTQ Mass Spectrometer	ESI Analytical Technique	APCI Analytical Technique
Syringe pump ESI/MS (Figure 11-1, page 11-6)	Analysis of a pure analyte Automatic calibration and tuning	
Syringe pump injection into LC solvent flow ESI/MS (Figure 11-2, page 11-7) APCI/MS (Figure 11-6, page 11-12)	Analysis of a pure analyte	Analysis of a pure analyte
Loop injection into LC solvent flow ESI/MS (Figure 11-3, page 11-8) ESI/MS (Figure 11-5, page 11-10) APCI/MS (Figure 11-7, page 11-13)	Analysis of a pure analyte Automatic optimization of tuning using an analyte	Analysis of a pure analyte Automatic optimization of tuning using an analyte
Autosampler without chromatographic separation ESI/MS (Figure 11-4, page 11-9) APCI/MS (Figure 11-8, page 11-14)	Analysis of one or more pure analytes	Analysis of one or more pure analytes
Autosampler with chromatographic separation ESI/MS (Figure 11-4, page 11-9) APCI/MS (Figure 11-8, page 11-14)	Analysis of a mixture	Analysis of a mixture







Table 11-2 lists the frequently used parts for making plumbing connections for ESI/MS and APCI/MS.

**Table 11-2. Frequently used parts for making plumbing connections for ESI/MS and APCI/MS**

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 x 0.4 mm OD (infusion line)	00106-10504
	Tubing, fused-silica, 0.1 mm ID x 0.190 mm OD (fused-silica sample tube and fused-silica capillary tube)	00106-10499
	Tubing, PEEK, 0.005 in. ID x 1/16 in. OD (red)	00301-22912
	Tube, Teflon, 0.03 in. ID x 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
	Fitting, Adapter, Kel-F, Upchurch Scientific (connects directly to ESI probe inlet)	00101-18080
	Fitting, Fingertight, Upchurch Scientific (brown) (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
	Ferrule, 0.016 in. ID, PEEK, Upchurch Scientific (brown) (for use with fused-silica infusion line)	00101-18120
	Ferrule, LC, 1/16 in., stainless steel, Valco (used to connect the (red) PEEK tubing and the sample loop to the divert/inject valve)	00101-18122
	Fitting, grounding union, 1/16 in. orifice, stainless steel	00101-18182
	Fitting, Fingertight, Upchurch Scientific (red) (used with (red) PEEK tubing)	00101-18195
	Ferrule, Fingertight 2, Upchurch Scientific (brown) (used with the Teflon tubing and (red) PEEK tubing)	00101-18196

**Finnigan LTQ**

**Table 11-2. Frequently used parts for making plumbing connections for ESI/MS and APCI/MS**

Part	Part Description	Part Number
	Fitting, LC union, 0.010 in. orifice, PEEK (black)	00101-18202
	Fitting, LC TEE union, 0.020 in. orifice, PEEK (black)	00101-18204
	Fitting, adapter union, PEEK, Upchurch Scientific (brown) (used with blunt-tip 32 or 34-gauge stainless steel needle, included in Metal Needle Kit)	00101-18206
	Nut, LC 1/16 in. stainless steel, Rheodyne	2522-0066
	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
	20 µL sample loop, stainless steel, Rheodyne	00110-22028
	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

## 11.1 Plumbing Connections for ESI/MS

---

You can fit the ESI probe with either a fused-silica sample tube or an optional blunt-tip, 32- or 34-gauge stainless steel needle. The 0.100 mm ID × 0.190 mm OD fused-silica sample tube (P/N 00106-10499) is supplied in the standard Accessory Kit (P/N 97055-62003). The blunt-tip, 32-gauge stainless steel needle (P/N 97055-20217) is supplied in the optional Metal Needle Kit (P/N OPTON-20014). The blunt-tip, 34-gauge stainless steel needle (P/N 97055-20220) is supplied in the optional Metal Needle Kit (P/N OPTON-20015).

There are several operating conditions in which you might choose to use the stainless steel needle rather than the fused-silica sample tube.

These include the following:

- When you are analyzing compounds with polar functional groups, some of the compounds might show improved ionization efficiency, especially acidic compounds in negative ion electrospray mode.
- Operation at very low flow rates in pure electrospray mode (i.e., with sheath and auxiliary gases turned off). Using a smaller internal diameter needle or fused-silica capillary produces smaller droplets, which might improve signal and stability at flow rates from 3  $\mu\text{L}/\text{min}$  to 200 nL/min.
- Operation with acetonitrile in the mobile phase. Acetonitrile can cause elongation of the polyimide coating on the fused-silica capillary, which can degrade signal and signal stability over time. The stainless steel needle is not affected by acetonitrile.

The procedures for installing the blunt-tip stainless steel needles and for connecting the fused-silica capillary tube, with safety sleeve, to the ESI probe are described in the **Finnigan Ion Max API Source Hardware Manual**.

## **Plumbing Connection Diagrams for ESI/MS**

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The following ESI/MS plumbing diagrams are shown on pages 11-6 to 11-10.

The following ESI/MS plumbing diagrams are shown in this topic:

- Figure 11-1. Plumbing diagram showing ESI/MS sample introduction from the syringe pump
- Figure 11-2. Plumbing diagram showing ESI/MS sample introduction from the syringe pump connected via an LC TEE union into the solvent flow from an LC
- Figure 11-3. Plumbing diagram showing ESI/MS sample introduction by loop injection into the solvent flow from an LC
- Figure 11-4. Plumbing diagram showing ESI/MS sample introduction from an LC autosampler with or without chromatographic separation
- Figure 11-5. Plumbing diagram showing ESI/MS sample introduction by loop injection into the solvent flow from an LC

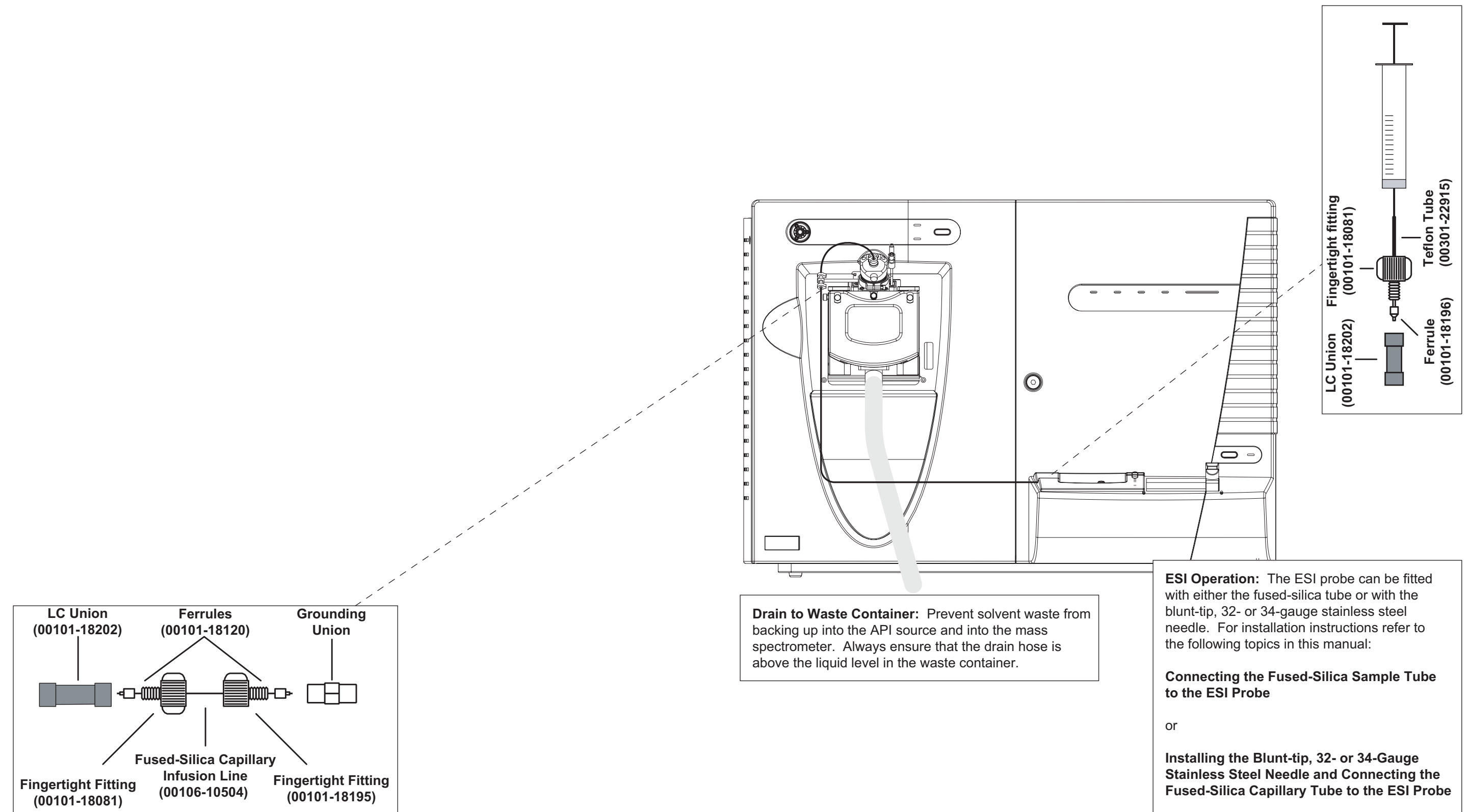


Figure 11-1. Plumbing diagram showing ESI/MS sample introduction from the syringe pump



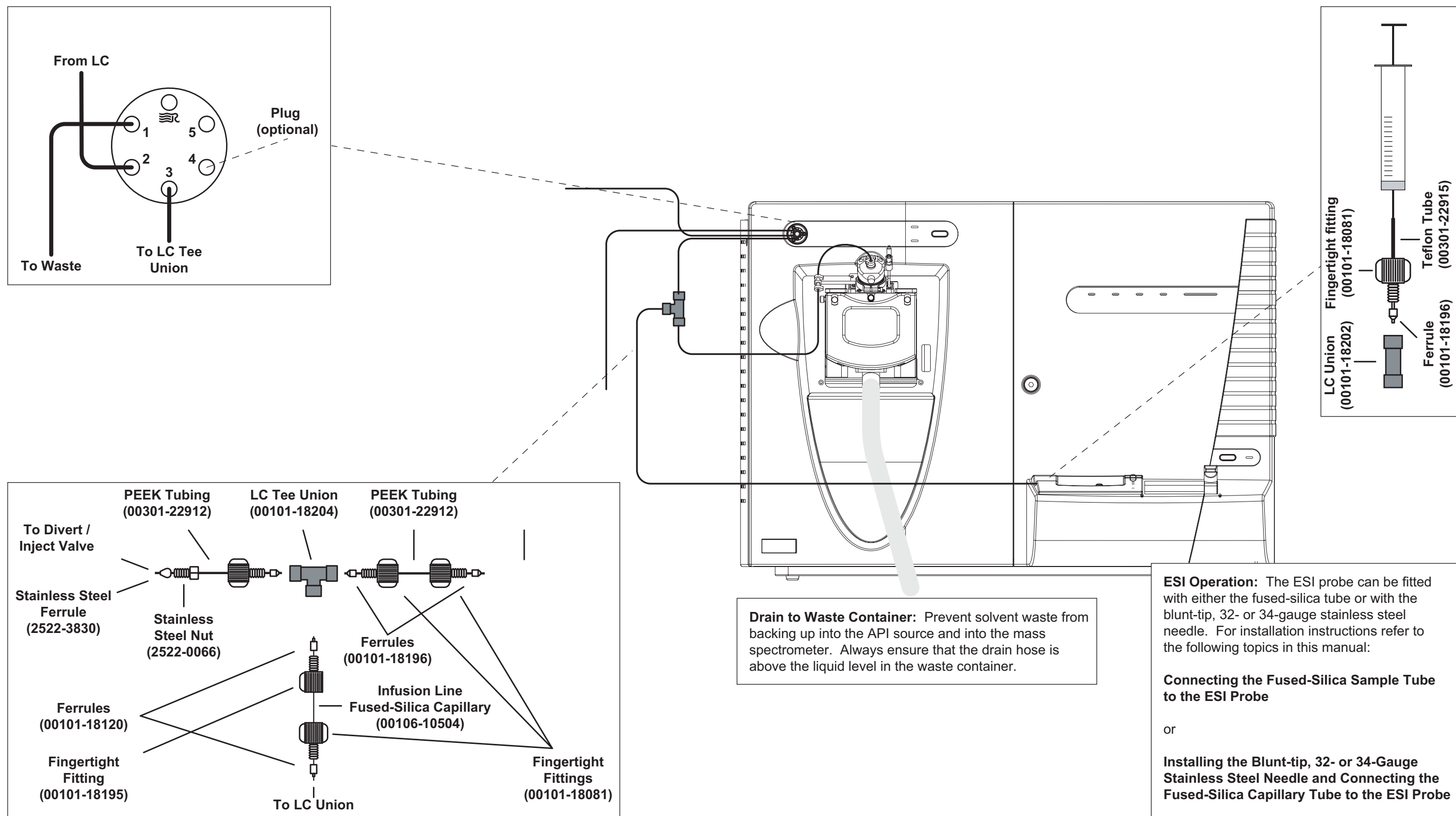


Figure 11-2. Plumbing diagram showing ESI/MS sample introduction from the syringe pump connected via an LC TEE union into the solvent flow from an LC

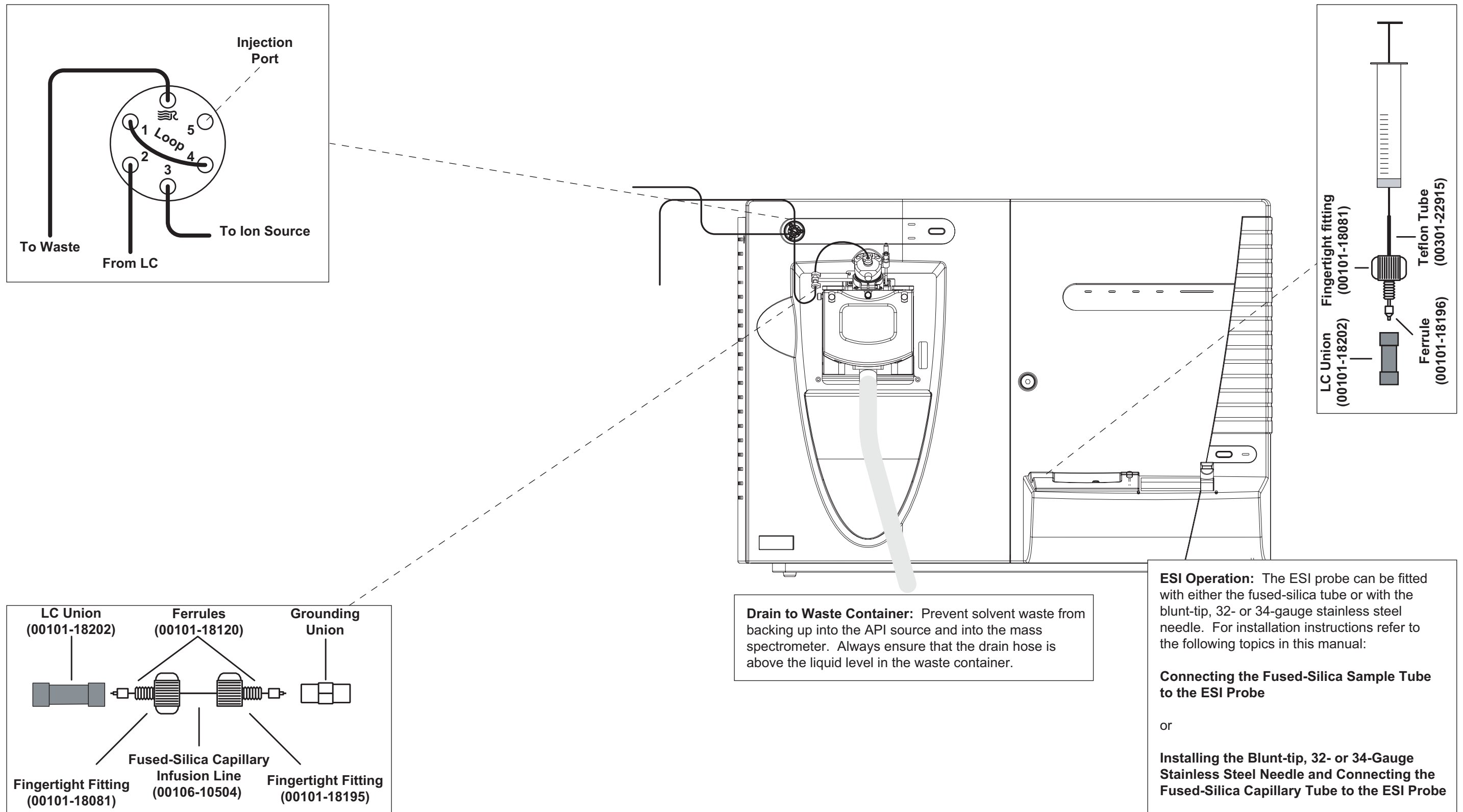


Figure 11-3. Plumbing diagram showing ESI/MS sample introduction by loop injection into the solvent flow from an LC

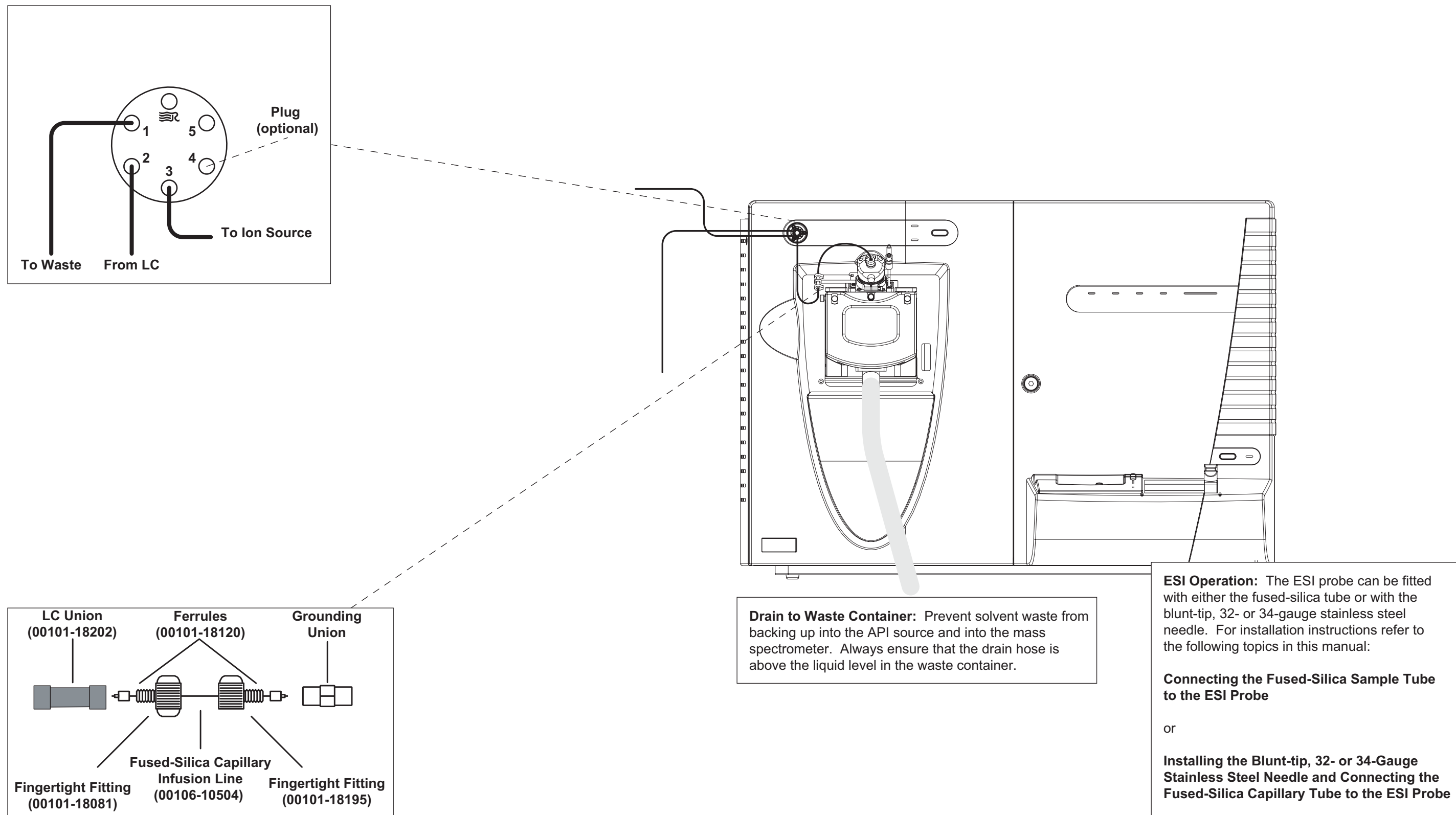


Figure 11-4. Plumbing diagram showing ESI/MS sample introduction from an LC autosampler with or without chromatographic separation

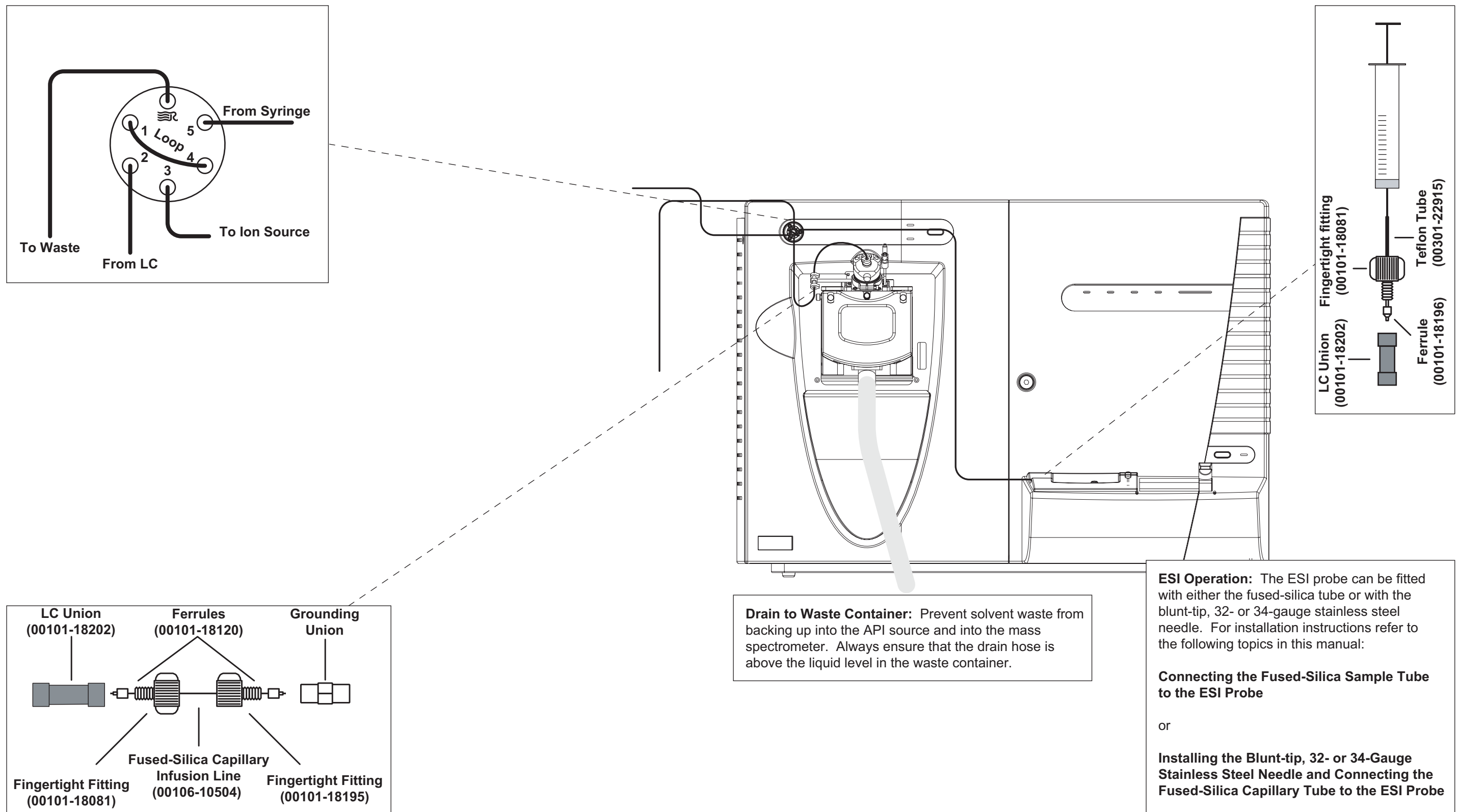


Figure 11-5. Plumbing diagram showing ESI/MS sample introduction by loop injection into the solvent flow from an LC

## 11.2 Plumbing Connections for APCI/MS

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If you need to install or replace the APCI source probe components, refer to the instructions in the **Finnigan Ion Max API Source Hardware Manual**.

The following APCI/MS plumbing diagrams are shown on pages 11-12 to 11-14:

- Figure 11-6. Plumbing diagram showing APCI/MS sample introduction from the syringe pump connected via an LC TEE into the solvent flow from an LC
- Figure 11-7. Plumbing diagram showing APCI/MS sample introduction by loop injection into the solvent flow from an LC
- Figure 11-8. Plumbing diagram showing APCI/MS sample introduction from an LC autosampler with or without chromatographic separation

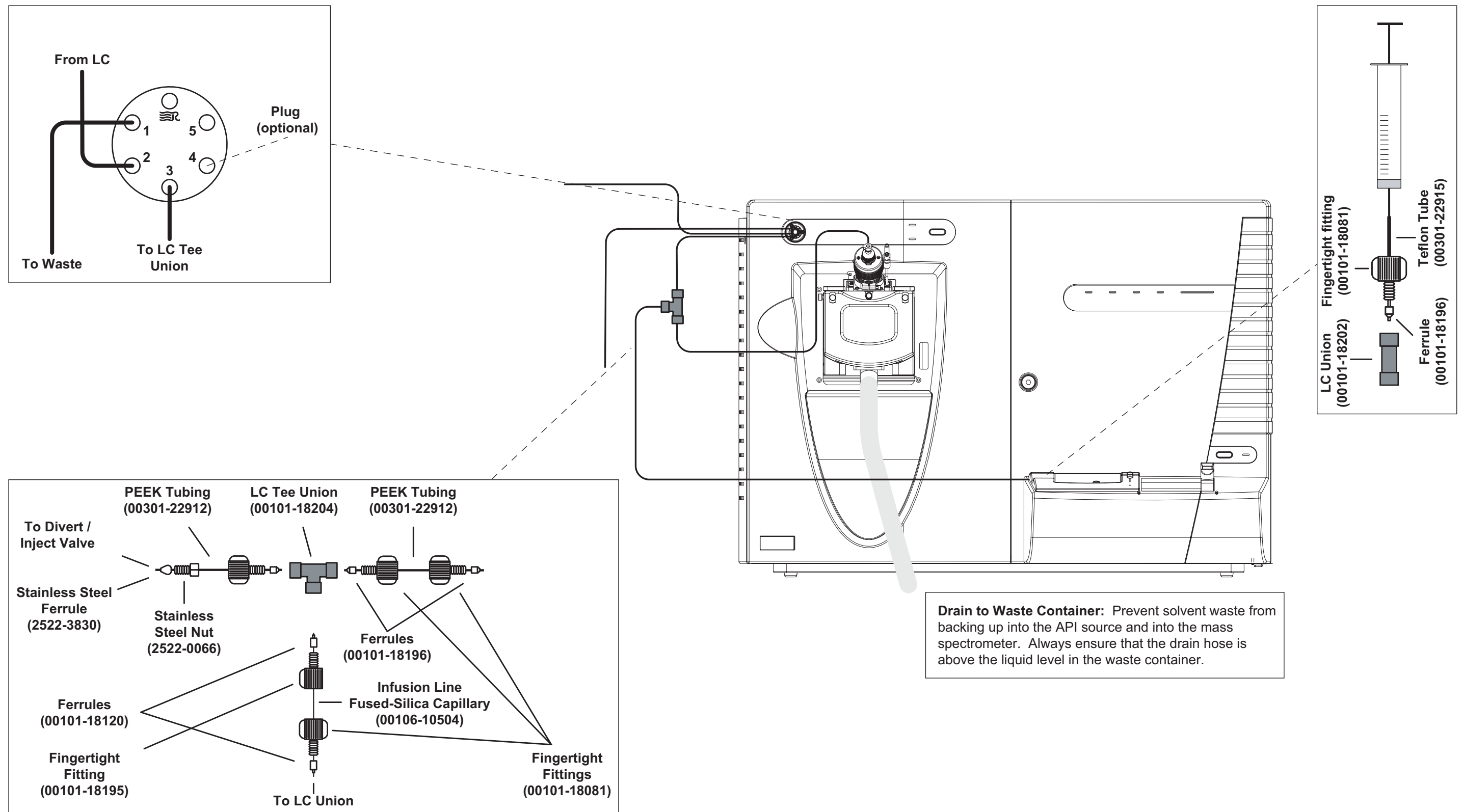


Figure 11-6. Plumbing diagram showing APCI/MS sample introduction from the syringe pump connected via an LC TEE into the solvent flow from an LC

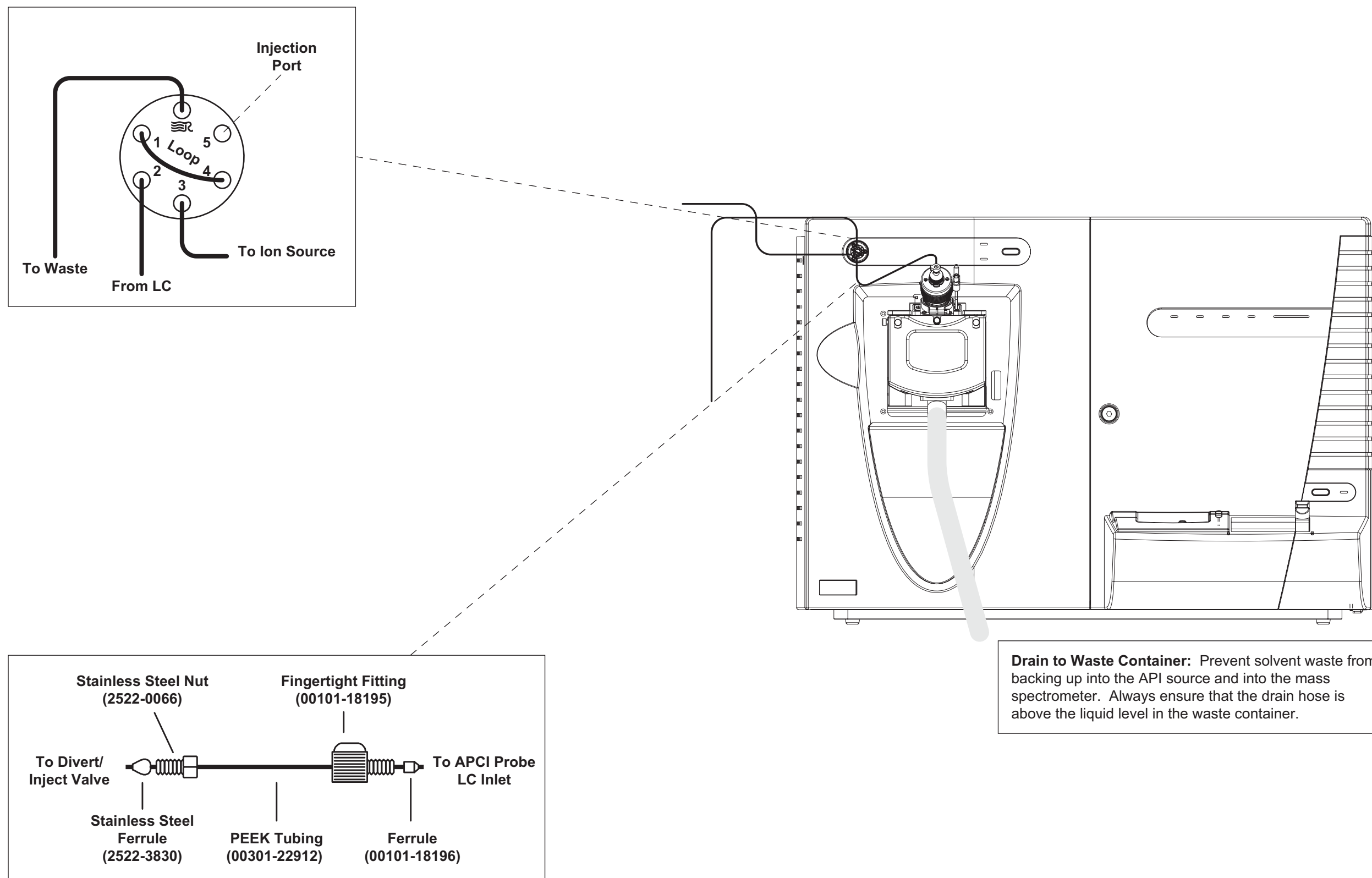


Figure 11-7. Plumbing diagram showing APCI/MS sample introduction by loop injection into the solvent flow from an LC

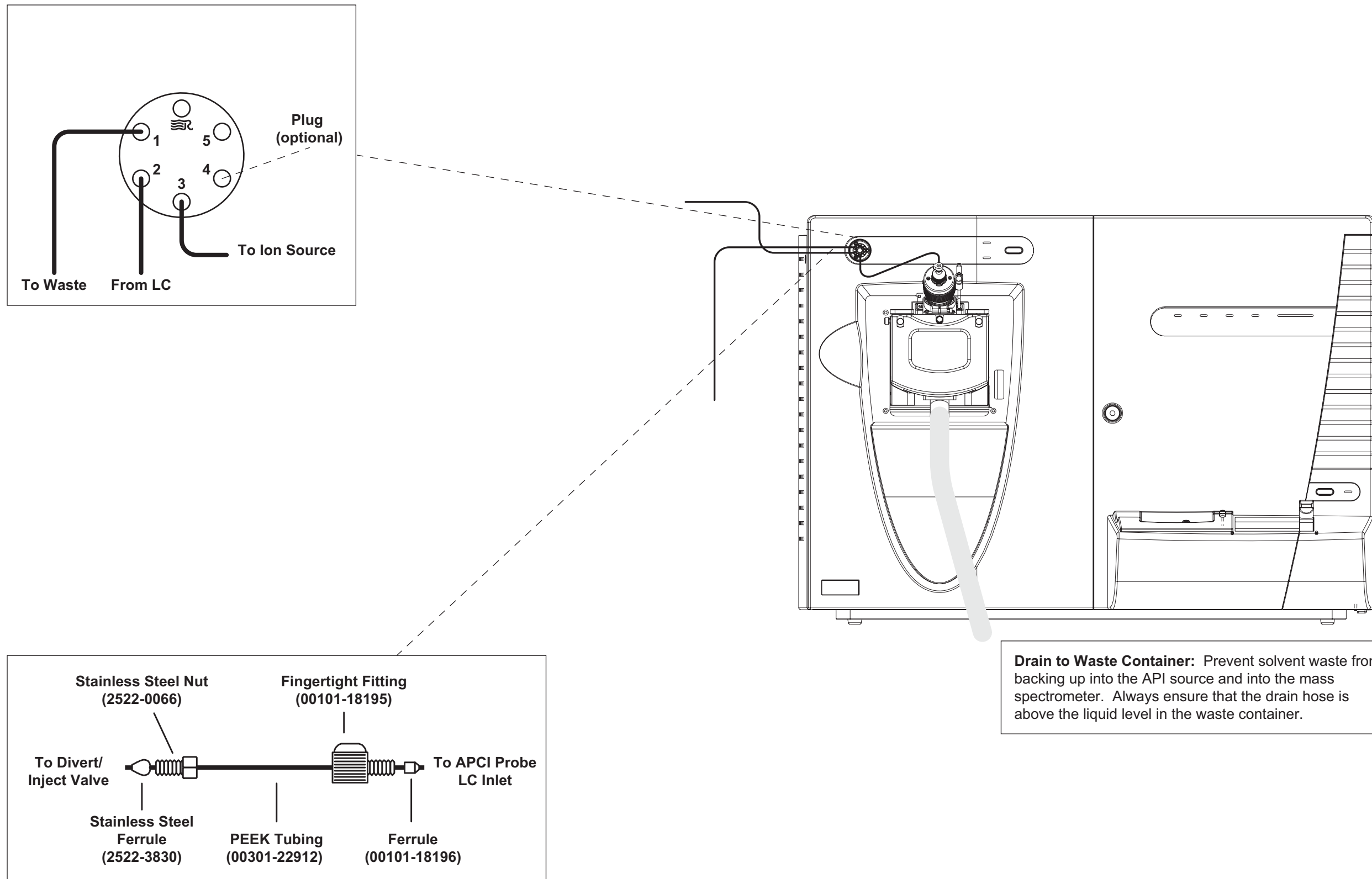


Figure 11-8. Plumbing diagram showing APCI/MS sample introduction from an LC autosampler with or without chromatographic separation



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