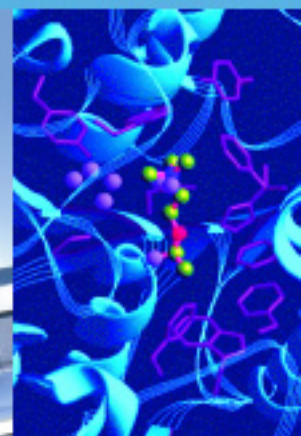
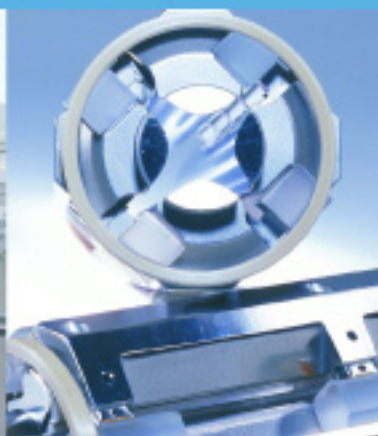


# Finnigan™ LXQ™

## Hardware Manual

97055-97043 Revision B

June 2006



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## Regulatory Compliance

Thermo Electron San Jose performs complete testing and evaluation of its products to ensure full compliance with applicable domestic and international regulations. When the system is delivered to you, it meets all pertinent electromagnetic compatibility (EMC) and safety standards as described below.

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

EMC compliance has been evaluated by U.L. Underwriter's Laboratory Inc.

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

### **Low Voltage Safety Compliance**

This device complies with Low Voltage Directive 73/23/EEC and harmonized standard EN 61010-1:2001.

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

## FCC Compliance Statement

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



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

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For your safety, and in compliance with international regulations, the physical handling of this Thermo Electron San Jose instrument *requires a team effort* for lifting and/or moving the instrument. This instrument is too heavy and/or bulky for one person alone to handle safely.

## **Notice on the Proper Use of Thermo Electron San Jose Instruments**

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.



## WEEE Compliance

This product is required to comply with the European Union's Waste Electrical & Electronic Equipment (WEEE) Directive 2002/96/EC. It is marked with the following symbol:



Thermo Electron has contracted with one or more recycling/disposal companies in each EU Member State, and this product should be disposed of or recycled through them. Further information on Thermo Electron's compliance with these Directives, the recyclers in your country, and information on Thermo Electron products which may assist the detection of substances subject to the RoHS Directive are available at [www.thermo.com/WEEERoHS](http://www.thermo.com/WEEERoHS).

## WEEE Konformität

Dieses Produkt muss die EU Waste Electrical & Electronic Equipment (WEEE) Richtlinie 2002/96/EC erfüllen. Das Produkt ist durch folgendes Symbol gekennzeichnet:



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## Conformité DEEE

Ce produit doit être conforme à la directive européenne (2002/96/EC) des Déchets d'Equipements Electriques et Electroniques (DEEE). Il est marqué par le symbole suivant:



Thermo Electron s'est associé avec une ou plusieurs compagnies de recyclage dans chaque état membre de l'union européenne et ce produit devrait être collecté ou recyclé par celles-ci. Davantage d'informations sur la conformité de Thermo Electron à ces directives, les recycleurs dans votre pays et les informations sur les produits Thermo Electron qui peuvent aider la détection des substances sujettes à la directive RoHS sont disponibles sur [www.thermo.com/WEERoHS](http://www.thermo.com/WEERoHS).

CAUTION Symbol	CAUTION	VORSICHT	ATTENTION	PRECAUCION	AVVERTENZA
	<b>Electric Shock:</b> High Voltages capable of causing personal injury are used in the instrument. The instrument must be shut down and disconnected from line power before service is performed. Do not operate the instrument with the top cover off. Do not remove protective covers from PCBs.	<b>Elektroschock:</b> In diesem Gerät werden Hochspannungen verwendet, die Verletzungen verursachen können. Vor Wartungsarbeiten muß das Gerät abgeschaltet und vom Netz getrennt werden. Betreiben Sie Wartungsarbeiten nicht mit abgenommenem Deckel. Nehmen Sie die Schutzabdeckung von Leiterplatten nicht ab.	<b>Choc électrique:</b> L'instrument utilise des tensions capables d'infliger des blessures corporelles. L'instrument doit être arrêté et débranché de la source de courant avant toute intervention. Ne pas utiliser l'instrument sans son couvercle. Ne pas enlever les étuis protecteurs des cartes de circuits imprimés.	<b>Descarga eléctrica:</b> Este instrumento utiliza altas tensiones, capaces de producir lesiones personales. Antes de dar servicio de mantenimiento al instrumento, éste deberá apagarse y desconectarse de la línea de alimentación eléctrica. No opere el instrumento sin sus cubiertas exteriores quitadas. No remueva las cubiertas protectoras de las tarjetas de circuito impreso.	<b>Shock da folgorazione.</b> L'apparecchio è alimentato da corrente ad alta tensione che può provocare lesioni fisiche. Prima di effettuare qualsiasi intervento di manutenzione occorre spegnere ed isolare l'apparecchio dalla linea elettrica. Non attivare lo strumento senza lo schermo superiore. Non togliere i coperchi a protezione dalle schede di circuito stampato (PCB).
	<b>Chemical:</b> Hazardous chemicals might be present in the instrument. Wear gloves when handling toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Use approved containers and procedures for disposing of waste oil.	<b>Chemikalien:</b> Dieses Gerät kann gefährliche Chemikalien enthalten. Tragen Sie Schutzhandschuhe beim Umgang mit toxischen, karzinogenen, mutagenen oder ätzenden/reizenden Chemikalien. Entsorgen Sie verbrauchtes Öl entsprechend den Vorschriften in den vorgeschriebenen Behältern.	<b>Chimique:</b> Des produits chimiques dangereux peuvent se trouver dans l'instrument. Portez des gants pour manipuler tous produits chimiques toxiques, cancérogènes, mutagènes, ou corrosifs/irritants. Utilisez des récipients et des procédures homologuées pour se débarrasser des déchets d'huile.	<b>Química:</b> El instrumento puede contener productos químicos peligrosos. Utilice guantes al manejar productos químicos tóxicos, carcinógenos, mutágenos o corrosivos/irritantes. Utilice recipientes y procedimientos aprobados para deshacerse del aceite usado.	<b>Prodotti chimici.</b> Possibile presenza di sostanze chimiche pericolose nell'apparecchio. Indossare dei guanti per maneggiare prodotti chimici tossici, cancerogeni, mutageni, o corrosivi/irritanti. Utilizzare contenitori aprovo e seguire la procedura indicata per lo smaltimento dei residui di olio.
	<b>Heat:</b> Allow heated components to cool before servicing them.	<b>Hitze:</b> Warten Sie erhitzte Komponenten erst nachdem diese sich abgekühlt haben.	<b>Haute Temperature:</b> Permettre aux composants chauffés de refroidir avant toute intervention.	<b>Altas temperaturas:</b> Permita que los componentes se enfríen, ante de efectuar servicio de mantenimiento.	<b>Calore.</b> Attendere che i componenti riscaldati si raffreddino prima di effettuare l'intervento di manutenzione.
	<b>Fire:</b> Use care when operating the system in the presence of flammable gases.	<b>Feuer:</b> Beachten Sie die einschlägigen Vorsichtsmaßnahmen, wenn Sie das System in Gegenwart von entzündbaren Gasen betreiben.	<b>Incendie:</b> Agir avec précaution lors de l'utilisation du système en présence de gaz inflammables.	<b>Fuego:</b> Tenga cuidado al operar el sistema en presencia de gases inflamables.	<b>Incendio.</b> Adottare le dovute precauzioni quando si usa il sistema in presenza di gas infiammabili.
	<b>Eye Hazard:</b> Eye damage could occur from splattered chemicals or flying particles. Wear safety glasses when handling chemicals or servicing the instrument.	<b>Verletzungsgefahr der Augen:</b> Verspritzte Chemikalien oder kleine Partikel können Augenverletzungen verursachen. Tragen Sie beim Umgang mit Chemikalien oder bei der Wartung des Gerätes eine Schutzbrille.	<b>Danger pour les yeux:</b> Des projections chimiques, liquides, ou solides peuvent être dangereuses pour les yeux. Porter des lunettes de protection lors de toute manipulation de produit chimique ou pour toute intervention sur l'instrument.	<b>Peligro par los ojos:</b> Las salicaduras de productos químicos o partículas que saltan bruscamente pueden causar lesiones en los ojos. Utilice anteojos protectores al manipular productos químicos o al darle servicio de mantenimiento al instrumento.	<b>Pericolo per la vista.</b> Gli schizzi di prodotti chimici o delle particelle presenti nell'aria potrebbero causare danni alla vista. Indossare occhiali protettivi quando si maneggiano prodotti chimici o si effettuano interventi di manutenzione sull'apparecchio.
	<b>General Hazard:</b> A hazard is present that is not included in the above categories. Also, this symbol is used on the instrument to refer the user to instructions in this manual.  When the safety of a procedure is in doubt, before you proceed, contact your local Technical Support Organization for Thermo Electron San Jose Products.	<b>Allgemeine Gefahr:</b> Es besteht eine weitere Gefahr, die nicht in den vorstehenden Kategorien beschrieben ist. Dieses Symbol wird im Handbuch außerdem dazu verwendet, um den Benutzer auf Anweisungen hinzuweisen.  Wenn Sie sich über die Sicherheit eines Verfahrens im unklaren sind, setzen Sie sich, bevor Sie fortfahren, mit Ihrer lokalen technischen Unterstützungsorganisation für Thermo Electron San Jose Produkte in Verbindung.	<b>Danger général:</b> Indique la présence d'un risque n'appartenant pas aux catégories citées plus haut. Ce symbole figure également sur l'instrument pour renvoyer l'utilisateur aux instructions du présent manuel.  Si la sûreté d'une procédure est incertaine, avant de continuer, contacter le plus proche Service Clientèle pour les produits de Thermo Electron San Jose.	<b>Peligro general:</b> Significa que existe un peligro no incluido en las categorías anteriores. Este símbolo también se utiliza en el instrumento para referir al usuario a las instrucciones contenidas en este manual.  Cuando la certidumbre acerca de un procedimiento sea dudosa, antes de proseguir, póngase en contacto con la Oficina de Asistencia Técnica local para los productos de Thermo Electron San Jose.	<b>Pericolo generico.</b> Pericolo non compreso tra le precedenti categorie. Questo simbolo è utilizzato inoltre sull'apparecchio per segnalare all'utente di consultare le istruzioni descritte nel presente manuale.  Quando è in dubbio la misura di sicurezza per una procedura, prima di continuare, si prega di mettersi in contatto con il Servizio di Assistenza Tecnica locale per i prodotti di Thermo Electron San Jose.

CAUTION Symbol	CAUTION	危險警告	危險警告
	<p><b>Electric Shock:</b> High Voltages capable of causing personal injury are used in the instrument. The instrument must be shut down and disconnected from line power before service is performed. Do not operate the instrument with the top cover off. Do not remove protective covers from PCBs.</p>	<p>電撃：この計測器は高電圧を使用し、人体に危害を与える可能性があります。保守・修理は、必ず操作を停止し、電源を切ってから実施して下さい。上部カバーを外したままでは計測器を使用しないで下さい。プリント配線板の保護カバーは外さないで下さい。</p>	<p>電撃：儀器設備使用會造成人身傷害的高伏電壓。在維修之前，必須先關儀器設備並切除電源。務必要在頂蓋蓋上的情況下操作儀器。請勿拆除PCB保護蓋。</p>
	<p><b>Chemical:</b> Hazardous chemicals might be present in the instrument. Wear gloves when handling toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Use approved containers and procedures for disposing of waste oil.</p>	<p>化学物質：危険な化学物質が計測器中に存在している可能性があります。毒性、発がん性、突然変異性、腐食・刺激性などのある薬品を取り扱う際は、手袋を着用して下さい。廃油の処分には、規定の容器と手順を使用して下さい。</p>	<p>化學品：儀器設備中可能存在有危險性的化學物品。接觸毒性致癌、誘變或腐蝕／刺激性化學品時，請配帶手套。處置廢油時，請使用經過許可的容器和程序。</p>
	<p><b>Heat:</b> Allow heated components to cool before servicing them.</p>	<p>熱：熱くなった部品は冷えるのを待ってから保守・修理を行って下さい。</p>	<p>高溫：請先等高溫零件冷卻之後再進行維修。</p>
	<p><b>Fire:</b> Use care when operating the system in the presence of flammable gases.</p>	<p>火災：可燃性のガスが存在する場所でシステムを操作する場合は、充分な注意を払って下さい。</p>	<p>火災：在有易燃氣體的場地操作該系統時，請務必小心謹慎。</p>
	<p><b>Eye Hazard:</b> Eye damage could occur from splattered chemicals or flying particles. Wear safety glasses when handling chemicals or servicing the instrument.</p>	<p>眼に対する危険：化学物質や微粒子が飛散して眼を傷つける危険性があります。化学物質の取り扱い、あるいは計測器の保守・修理に際しては防護眼鏡を着用して下さい。</p>	<p>眼睛傷害危險：飛濺的化學品或顆粒可能造成眼睛傷害。處理化學品或維儀器設備時請佩戴安全眼鏡。</p>
	<p><b>General Hazard:</b> A hazard is present that is not included in the above categories. Also, this symbol is used on the instrument to refer the user to instructions in this manual.</p> <p>When the safety of a procedure is in doubt, before you proceed, contact your local Technical Support Organization for Thermo Electron San Jose Products.</p>	<p>一般的な危険：この標識は上記以外のタイプの危険が存在することを示します。また、計測器にこの標識がついている場合は、本マニュアル中の指示を参照して下さい。</p> <p>安全を確保する手順がよくわからない時は、作業を一時中止し、お近くのサーモエレクトロンサンローゼプロダクトのテクニカルサポートセンターにご連絡ください。</p>	<p>一般性危險：說明未包括在上述類別中的其他危險。此外，儀器設備上使用這個標誌，以指示用戶本使用手冊中的說明。</p> <p>如對安全程序有疑問，請在操作之前與當地的菲尼根技術服務中心聯繫。</p>

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# Preface

## About This Guide

Welcome to the Thermo Electron, Finnigan™ LXQ™ system. The LXQ is a member of the Finnigan family of mass spectrometer (MS) detectors.

This guide describes the modes of operation and principal hardware components of your LXQ system. In addition, this manual provides step-by-step instructions for cleaning and maintaining your LXQ MS detector.

## Related Documentation

In addition to this guide, Thermo Electron provides the following documents for the LXQ as .PDF files:

- Preinstallation Guide
- Getting Started
- Getting Connected

Online Help available from within the software

## Safety and Special Notices

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

Safety and special notices include the following:



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

**IMPORTANT** Highlights information necessary to avoid damage to software, loss of data, invalid test results, or information critical for optimal performance of the system.

**Note** Highlights information of general interest.

**Tip** Helpful information that can make a task easier.

## Safety Precautions

Observe the following safety precautions when you operate or perform service on the MS detector:



**Do Not Perform Any Servicing Other Than That Contained in the LXQ Hardware Manual.** To avoid personal injury or damage to the instrument, do not perform any servicing other than that contained in the *LXQ Hardware Manual* or related manuals unless you are qualified to do so.



**Shut Down the MS Detector and Disconnect It From Line Power Before You Service It.** High voltages capable of causing personal injury are used in the instrument. Some maintenance procedures require that the MS detector be shut down and disconnected from line power before service is performed. Do not operate the MS detector with the top or side covers off. Do not remove protective covers from PCBs.



**Respect Heated Zones.** Treat heated zones with respect. The ion transfer capillary and the APCI vaporizer might be very hot and might cause severe burns if touched. Allow heated components to cool before you service them.



**Place the MS Detector in Standby (or Off) Before You Open the Atmospheric Pressure Ionization (API) Source.** The presence of atmospheric oxygen in the API source when the MS detector is On could be unsafe. (LXQ automatically turns the MS detector Off when you open the API source; however, it is best to take this added precaution.)



**Make Sure You Have Sufficient Nitrogen For Your API Source.** Before you begin normal operation each day, make sure that you have sufficient nitrogen for your API source. The presence of atmospheric oxygen in the API source when the MS detector is On could be unsafe. (LXQ automatically turns the MS detector Off when you run out of nitrogen, however, it is best to take this added precaution.)



**Provide an Adequate Fume Exhaust System and Contain Waste Streams.** You must provide an adequate fume exhaust system. Samples and solvents that are introduced into the LXQ are eventually exhausted from the forepump. Therefore, connect the forepump to a fume exhaust system. Consult local regulations for the proper method of exhausting the fumes from your system. The API source can accommodate high flow rates.



Therefore, you must make provisions to collect the waste solvent. The API source is fitted with a 6 mm (0.25 in.) ID connector for solvent drainage. A 6 mm (0.25 in.) PVC drain tube, which is provided with the system, should be connected between the API source and an appropriate collection container. (The waste container can be something as simple as an old solvent bottle with a modified cap.)

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 forepump. The analyzer optics become contaminated if the API source drain tube and the (blue) forepump exhaust tubing are connected to the same fume exhaust system.

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



**Use Care When Changing Vacuum Pump Oil.** Treat drained vacuum pump oil and pump oil reservoirs with care. Hazardous compounds introduced into the system might have become dissolved in the pump oil. Always use approved containers and procedures for disposing of waste oil. Whenever a pump that has been operating on a system used for the analysis of toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals, you must decontaminate the pump and certify that it is free of contamination before repairs or adjustments are made by a Thermo Electron San Jose Customer Support Engineer or before it is sent back to the factory for service.

## Solvent and Gas Purity Requirements

Use the highest purity solvents available. The LXQ MS detector is extremely sensitive to solvent impurities. Some solvent impurities are transparent to UV/Visible detectors, but are easily detected by the LXQ MS detector. Liquid chromatography grade is the minimum acceptable purity. Higher grade solvents are preferred. Distilled water is recommended. Deionized water contains chemicals and should not be used.

The following is a list of international sources that can supply high quality solvents:

Solvent Source	Telephone Number
Mallinckrodt/Baker, Inc.	Tel: (800) 582-2537 Fax: (908) 859-9370
Burdick & Jackson, Inc.	Tel: (800) 368-0050 Fax: (616) 725-6216
E. M. Science, Inc.	Tel: (800) 222-0342 Fax: (800) 336-4422

The LXQ MS detector uses helium as a collision gas. The helium should be high purity (99.995%). The required gas pressure is  $135 \pm 70$  kPa ( $20 \pm 10$  psig). Thermo Electron does not recommend particulate filters because they are often contaminated.

The LXQ MS detector uses nitrogen as a sheath gas and auxiliary gas. The nitrogen should be high purity (99%). The required gas pressure is  $759 \pm 69$  kPa ( $110 \pm 10$  PSI).

## Contacting Us

There are several ways to contact Thermo Electron Corporation.

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In the US and Canada for ordering information:  
Phone: 1-800-532-4752  
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- Fill out a reader survey online at [www.thermo.com/lcms-techpubs](http://www.thermo.com/lcms-techpubs)
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# Chapter 1 Introduction

This chapter provides an overview of the LXQ. Specific topics covered are as follows:

- Ion Polarity Modes
- Ionization Techniques
- Scan Power and Scan Modes
- Scan Types
- Data Types
- Experiment Types

The LXQ™ is a member of the Finnigan™ family of mass spectrometer (MS) detectors. The Finnigan LXQ (Figure 1) is an advanced analytical instrument that includes a syringe pump, a divert/inject valve, an MS detector, and the Xcalibur® data system. In a typical analysis, a sample can be introduced in any of the following ways:

- Using the syringe pump (direct infusion)
- Using the divert/inject valve fitted with a sample loop and LC (flow injection analysis)
- Using the divert/inject valve and HPLC fitted with a column (LC/MS)

In analysis by LC/MS, a sample is injected onto an LC column. The sample is then separated into its various components. The components elute from the LC column and pass into the MS detector where they are analyzed. Analysis by direct infusion or flow injection provides no chromatographic separation of components in the sample before it passes into the MS detector. The data from the MS detector are then stored and processed by the data system.



**Figure 1.** Finnigan LXQ system

The LXQ MS detector consists of an atmospheric pressure ionization (API) source, ion optics, mass analyzer, and ion detection system. The ion optics, mass analyzer, ion detection system, and part of the API source are enclosed in a vacuum manifold. Ionization of the sample takes place in the API source. The specific method used to ionize the sample is referred to as the *ionization technique*. The ions produced in the API source are transmitted by the ion optics into the mass analyzer, where they are trapped in stable orbits by a time-varying electric field. The polarity of the potentials applied to the API source and ion optics determines whether positively charged ions or negatively charged ions are transmitted to the mass analyzer. You can configure the LXQ to analyze positively or negatively charged ions (called the positive or negative *ion polarity mode*).

The lenses in the API source and ion optics act as a gate to start and stop the transmission of ions from the API source to the mass analyzer. The function of these lenses is controlled by an automatic gain control (AGC) that sets them to transmit the optimum number of ions to the mass analyzer.

The mass-to-charge ratios of the ions produced in the API source are measured by the mass analyzer. Selected ions are ejected from the mass analyzer and reach the ion detection system where they produce a signal. The signal produced is then amplified by the detection system electronics.

The ion detection system signal is analyzed by the LXQ data system. The data system serves as the user interface to the MS detector, autosampler, LC, and syringe pump. Refer to the online Help for more information on the LXQ data processing and instrument control software.

Each sequence of loading the mass analyzer with ions followed by mass analysis of the ions is called a *scan*. The LXQ uses several different *scan modes* and different *scan types* to load, fragment, and eject ions from the mass analyzer. The ability to vary the scan mode and scan type, as well as the ionization and ion polarity modes, affords the user great flexibility in the instrumentation for solving complex analytical problems.

## Ion Polarity Modes

You can operate the LXQ in either of two *ion polarity modes*: positive or negative. The LXQ can control whether positive ions or negative ions are transmitted to the mass analyzer for mass analysis by changing the polarity of the potentials applied to the API source and ion optics. The ion optics are located between the API source and the mass analyzer.

The information obtained from a positive-ion mass spectrum is different from and complementary to that obtained from a negative-ion spectrum. Thus, the ability to obtain both positive-ion and negative-ion mass spectra aids you in the qualitative analysis of your sample. You can choose the ion polarity mode and ionization technique to obtain maximum sensitivity for the particular analysis of interest.



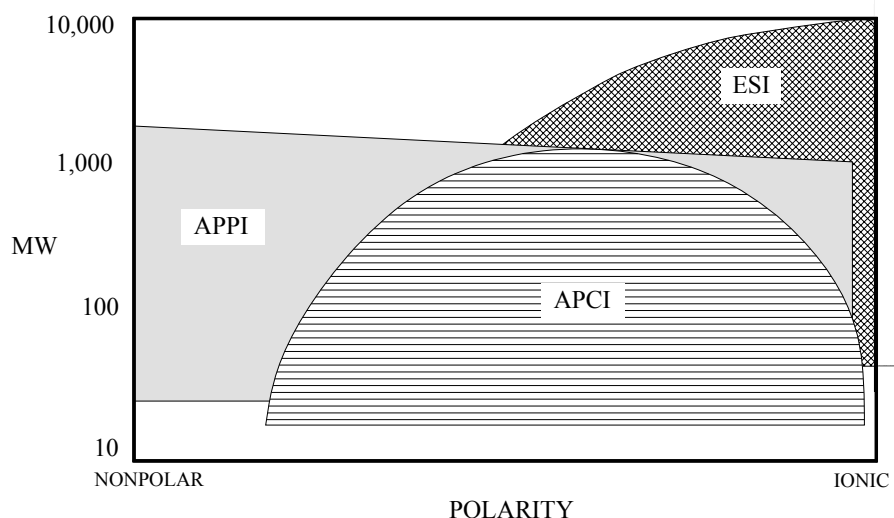
## Ionization Techniques

You can operate the LXQ using any of four ionization techniques, as follows:

- [Electrospray Ionization \(ESI\)](#)
- [Atmospheric Pressure Chemical Ionization \(APCI\)](#)
- [Atmospheric Pressure Photoionization \(APPI\)](#)
- [Nanospray Ionization \(NSI\)](#)

**Note** Because the APCI, ESI, APPI, and NSI techniques use the same ion source interface (that is, the portion of the API source that is under vacuum), you can switch between these four ionization techniques in just a few minutes. Switching ionization techniques merely involves switching the probes and does not break vacuum.

Figure 2 shows the ranges of applicability (molecular weight as a function of polarity) of three of the ionization techniques being discussed: atmospheric pressure photoionization (APPI), atmospheric pressure chemical ionization (APCI) and electrospray ionization (ESI).



**Figure 2.** Ranges of applicability of APPI, APCI, and ESI

## Electrospray Ionization

The electrospray ionization (ESI) technique transforms ions in solution into ions in the gas phase<sup>1</sup>. Many samples that previously were not suitable for mass analysis (for example, heat-labile compounds or high molecular weight compounds) can be analyzed by the use of ESI. ESI can be used to analyze

any polar compound that makes a preformed ion in solution. The term *preformed ion* can include adduct ions. For example, polyethylene glycols can be analyzed from a solution containing ammonium acetate, because of adduct formation between the  $\text{NH}_4^+$  ions in the solution and oxygen atoms in the polymer. With ESI, the range of molecular weights that can be analyzed by the LXQ is greater than 100,000 u, due to multiple charging. ESI is especially useful for the mass analysis of polar compounds, which include: biological polymers (for example, proteins, peptides, glycoproteins, and nucleotides); pharmaceuticals and their metabolites; and industrial polymers (for example, polyethylene glycols).

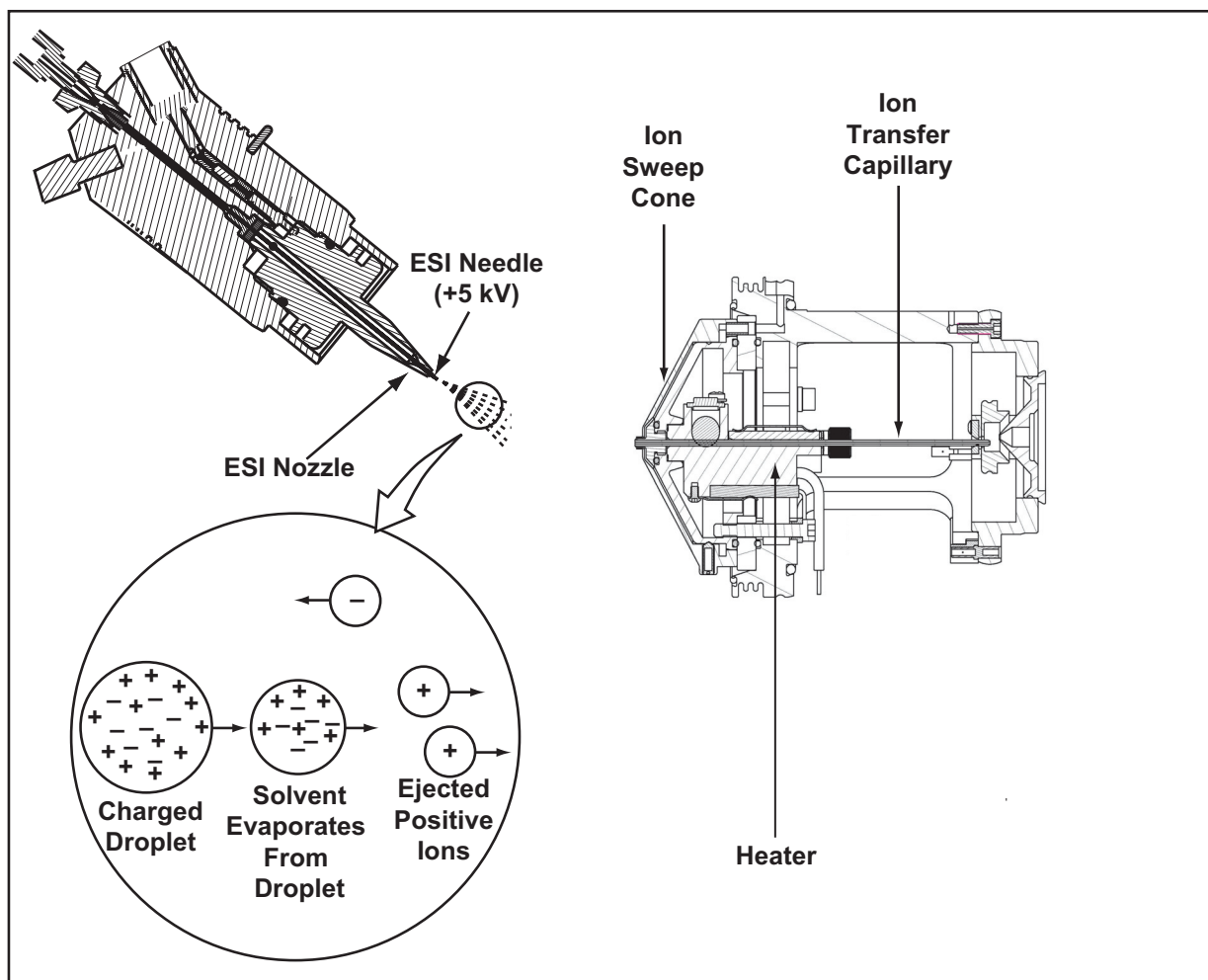
In ESI, ions are produced and analyzed as follows:

1. The sample solution enters the ESI needle, to which a high voltage is applied.
2. The ESI needle sprays the sample solution into a fine mist of droplets that are electrically charged at their surface.
3. The electrical charge density at the surface of the droplets increases as solvent evaporates from the droplets.
4. The electrical charge density at the surface of the droplets increases to a critical point, known as the Rayleigh stability limit. At this critical point, the droplets divide into smaller droplets because the electrostatic repulsion is greater than the surface tension. The process is repeated many times to form very small droplets.
5. From the very small, highly-charged droplets, sample ions are ejected into the gas phase by electrostatic repulsion.
6. The sample ions pass through an ion transfer capillary, enter the MS detector and are analyzed.

In the LXQ, the ESI needle is 60 degrees to the axis of the ion transfer capillary that carries ions to the MS detector. This geometry keeps the ion transfer capillary clean. The ion sweep cone serves as a mechanical barrier that keeps large droplets and particulates from entering the ion transfer capillary. [Figure 3](#) shows the steps in the formation of ions from highly-charged droplets, and the relationship between the ESI probe and the ion transfer capillary.

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<sup>1</sup> Refer to the following papers for more information on the electrospray ionization process: Fenn, J. B.; Mann, M.; Meng, C. K.; Wong, S. F.; Whitehouse, C. M. *Mass Spectrom. Reviews* **1990**, 9, 37; Smith, R. D.; Loo, J. A.; Edmonds, C. G.; Barinaga, C. J.; Udseth, H. R. *Anal. Chem.* **1990**, 62, 882; Ikononou, M. G.; Blades, A. T.; Kebarle, P. *Anal. Chem.* **1991**, 63, 1989.



**Figure 3.** ESI process in the positive ion polarity mode

You can use the ESI probe in either positive or negative ion polarity mode. The ion polarity mode of choice is determined by the polarity of the preformed ions in solution; that is, acidic molecules form negative ions in solution, and basic molecules form positive ions. The ejection of sample ions from droplets is facilitated if the ionic charge and surface charge of the droplet are of the same polarity. Thus, a positively charged needle is used to analyze positive ions and a negatively charged needle is used to analyze negative ions.

Sample ions can carry a single charge or multiple charges. The number of charges carried by the sample ions depends on the structure of the analyte of interest and the carrier solvent. (In ESI, the buffer and the buffer strength both have a noticeable effect on sensitivity. Therefore, it is important to

choose these variables correctly.) With higher molecular weight proteins or peptides, the resulting mass spectrum consists typically of a series of peaks corresponding to a distribution of multiply charged analyte ions.

The ESI process is affected by droplet size, surface charge, liquid surface tension, solvent volatility, and ion solvation strength. Large droplets with high surface tension, low volatility, strong ion solvation, low surface charge, and high conductivity prevent good electrospray.

Organic solvents such as methanol, acetonitrile, and isopropyl alcohol are superior to water for ESI. Volatile acids such as acetic acid (1% vol/vol) and formic acid (0.1% vol/vol) and volatile bases such as ammonium hydroxide and triethanolamine are also good for ESI. Use volatile salts such as ammonium acetate or ammonium formate at concentrations below 10 mM. Strong acids and bases, mineral acids, and nonvolatile salts (such as those containing potassium or sodium) are detrimental.

To ensure a good electrospray:

- Keep salts out of the solvent system.
- Use the lowest possible HPLC flow rates.
- Use organic/aqueous solvent systems and volatile acids and bases.
- Optimize the pH of the solvent system.

## **Atmospheric Pressure Chemical Ionization**

Atmospheric pressure chemical ionization (APCI) is a soft ionization technique. APCI is used to analyze nonpolar compounds and compounds of medium polarity that are relatively low in molecular weight and have some volatility.

In APCI, ions are produced and analyzed as follows:

1. The APCI nozzle sprays the sample solution into a fine mist of droplets.
2. The droplets are vaporized in a high temperature tube (the vaporizer).
3. A high voltage is applied to a needle located near the exit end of the tube. The high voltage creates a corona discharge that forms reagent ions through a series of chemical reactions with solvent molecules and nitrogen sheath gas.
4. The reagent ions react with sample molecules to form sample ions.

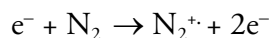
5. The sample ions pass through an ion transfer capillary, enter the MS detector, and are analyzed.

In the LXQ, the sample tube in the APCI nozzle is 60 degrees to the axis of the ion transfer capillary that carries ions to the MS detector. This geometry keeps the ion transfer capillary clean. The ion sweep cone serves as a mechanical barrier that keeps large droplets and particulates from entering the ion transfer capillary.

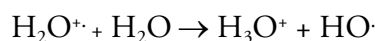
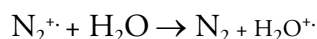
APCI is a gas phase ionization technique. Therefore, the gas phase acidities and basicities of the analyte and solvent vapor play an important role in the APCI process.

In the positive-ion mode, sample ionization occurs in a series of reactions that start with the electron-initiated cation formation. Typical examples of primary, secondary, and adduct ion formation include:

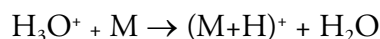
Primary ion formation



Secondary ion formation



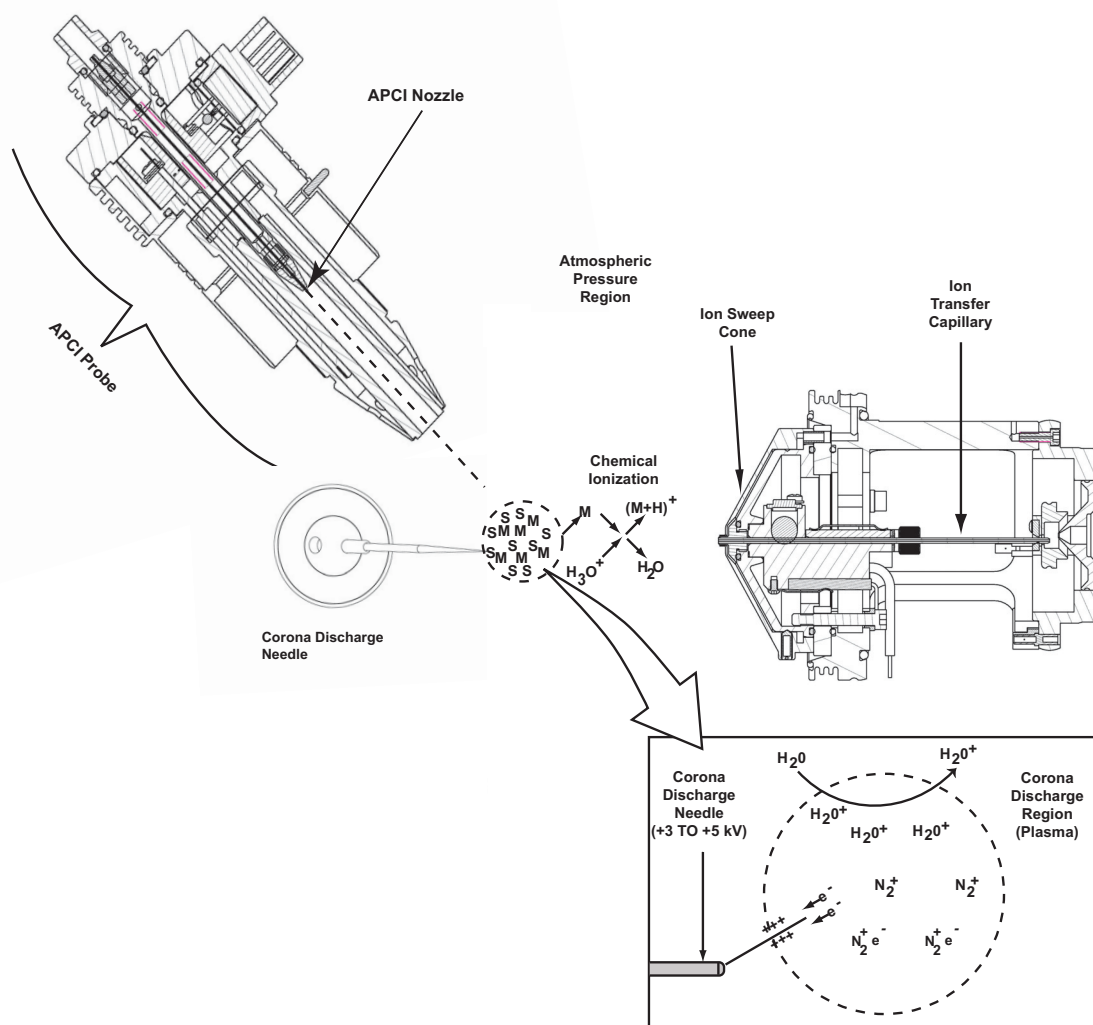
Proton transfer



In negative-ion mode,  $(M-H)^{-}$  is typically formed by the abstraction of a proton by  $OH^{-}$ .

APCI is used to analyze small molecules with molecular weights up to 2000 u. APCI is not affected by minor changes in most variables such as changes in buffer or buffer strength.

Figure 4 shows the APCI process in the positive-ion polarity mode.



**Figure 4.** APCI process in the positive ion polarity mode

You can use APCI in positive-ion or negative-ion polarity mode. For most molecules, the positive-ion mode produces a stronger ion current. This is especially true for molecules with one or more basic nitrogen (or other basic) atoms. Exceptions to this general rule are molecules with acidic sites such as carboxylic acids and acid alcohols, which produce more negative ions than positive ions.

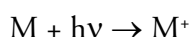
While, in general, fewer negative ions are produced than positive ions, negative ion polarity is sometimes the mode of choice. This is because the negative ion polarity mode sometimes generates less chemical noise than does the positive mode. Thus, selectivity might be better in the negative ion mode than in the positive ion mode.

## Atmospheric Pressure Photoionization

Atmospheric pressure photoionization (APPI) is also a soft ionization technique. In APPI, an ion is generated from a molecule when it interacts with a photon from the light source. APPI generates molecular ions for molecules that have an ionization potential below the photon energy of the light being emitted by the light source.

In APPI, ions are produced and analyzed as follows:

1. The nozzle sprays the sample solution into a fine mist of droplets.
2. The droplets are vaporized in a high temperature tube (the vaporizer).
3. The analyte molecule interacts with the light from the PhotoMate light source. The analyte molecule M is ionized to a molecular ion  $M^+$  if the ionization potential of the analyte is less than the photon energy  $h\nu$ :

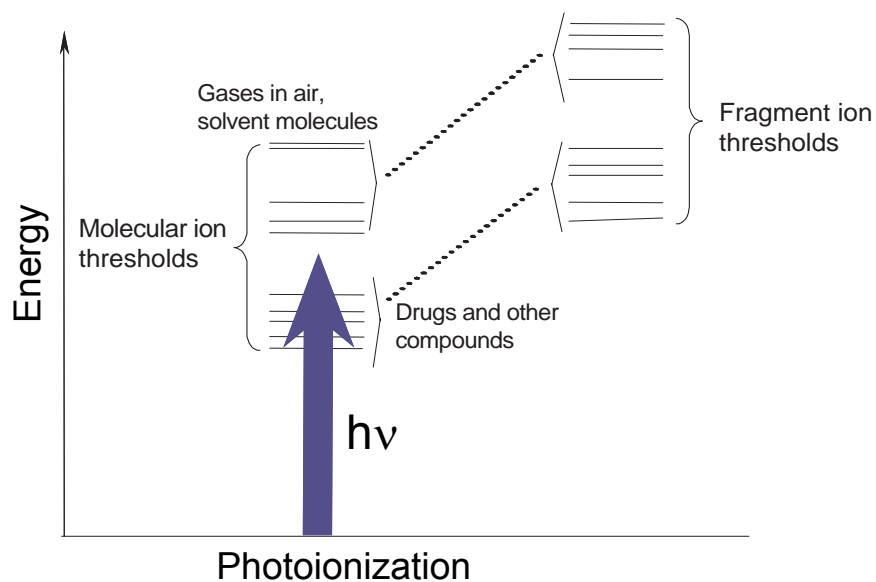


4. In the presence of protic solvents, the analyte ion may extract a hydrogen to form an  $MH^+$  ion:

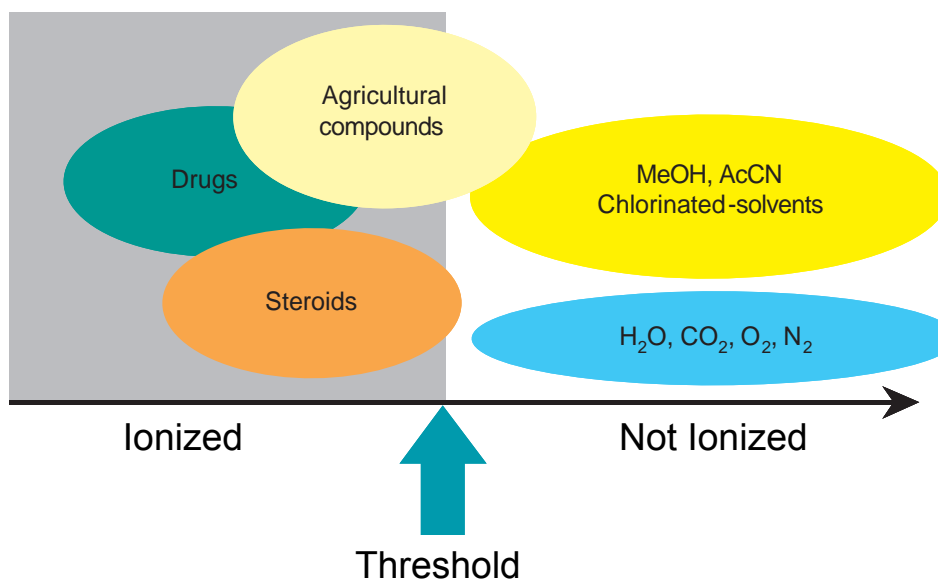


5. The analyte ions pass through the ion transfer capillary, enter the MS detector, and are analyzed.

Molecules including steroids, basic-drug entities, and pesticides have ionization potentials below the threshold and protonated molecules are generated in the LC/MS experiment. APPI reduces fragmentation because only a small amount of energy is deposited in the molecule. Molecules such as nitrogen in the sheath, sweep, and auxiliary gas, and the simple solvents used for LC/MS, are not ionized because their ionization potentials are greater than the photon energy. The result is selective ionization of analyte versus background. See [Figure 5](#) and [Figure 6](#).



**Figure 5.** Energetics of photoionization



**Figure 6.** Selective photoionization



The light source is a krypton lamp which emits photons with energies of 10.0 and 10.6 eV. Molecules with ionization potentials less than 10 eV ionize to form  $MH^+$  while those with greater ionization potentials do not. Figure 7 shows ionization potentials of typical compounds and solvents.

**Krypton 10.0 eV, 10.6 eV**

<u>Ionization Potentials (IP)</u>		<u>Solvent Ionization Potentials (IP)</u>	
<b>Anthracene</b>	<b>7.4 eV</b>	<b>Toluene</b>	<b>8.82 eV</b>
<b>Fluoranthene</b>	<b>7.8 eV</b>	<b>Acetone</b>	<b>9.70 eV</b>
<b>Caffeine</b>	<b>8.0 eV</b>		
<b>4-Nitrotoluene</b>	<b>9.5 eV</b>		
<b>10. eV</b> .....			
		<b>Methanol</b>	<b>10.85 eV</b>
		<b>Acetonitrile</b>	<b>12.19 eV</b>
		<b>Water</b>	<b>12.61 eV</b>

**Figure 7.** Ionization potentials of typical compounds and solvents

## Nanospray Ionization

Nanospray ionization (NSI) is a technique for performing electrospray ionization on amounts of liquid as small as 1  $\mu$ L for time periods of greater than 30 min. Stable mass spectra can be obtained for very small amounts of biomolecules such as proteins, peptides, oligonucleotides, and oligosaccharides.

For more information on NSI, refer to the manual that came with your NSI source.

## Scan Power and Scan Modes

Ions produced in the ion source are often referred to as *parent ions*. These parent ions can be mass analyzed to produce a mass spectrum. Alternatively, by varying the RF voltages of the mass analyzer, LXQ can first eject all ions except for several selected parent ions, and then collide these ions with helium that is present in the mass analyzer. This helium is known as buffer gas. The collisions of the selected precursor ions with the helium can cause them to fragment into *product ions*. The product ions can be mass analyzed.

The number of stages of mass analysis is represented as  $MS^n$  where  $n$  is the *scan power*. (Each stage of mass analysis includes an ion selection step.) LXQ supports scan powers of  $n = 1$  to  $n = 10$ . The higher the scan power, the more structural information is obtained about the analyte.

The scan powers supported by LXQ in its standard configuration are as follows:

- MS scan mode ( $n = 1$ )
- MS/MS scan mode ( $n = 2$ )
- $MS^n$  scan mode ( $n = 3$  to  $10$ )

### MS Scan Mode

The mass spectrometry (MS) scan mode corresponds to a single stage of mass analysis (that is, a scan power of  $n = 1$ ). The MS scan mode only involves parent ions, and no fragmentation of the parent ions occurs. The MS scan mode can be a full scan experiment or a selected ion monitoring (SIM) experiment (see [“Selected Ion Monitoring”](#) on page 16).

### MS/MS Scan Mode

The *MS/MS scan* corresponds to two stages of mass analysis ( $n = 2$  scan power). In an MS/MS scan, parent ions are fragmented into product ions. An MS/MS scan can be a full scan experiment or a selected reaction monitoring (SRM) experiment (see [“Selected Reaction Monitoring”](#) on page 17).

### $MS^n$ Scan Mode

An  *$MS^n$  scan* involves three to ten stages of mass analysis ( $n = 3$  to  $n = 10$  scan power). [However, the term can also be applied to one stage of mass analysis (with  $n = 1$ ) or to two stages of mass analysis (with  $n = 2$ ).] An  $MS^n$  scan can be either a full scan experiment or a consecutive reaction monitoring (CRM) experiment (see [“Consecutive Reaction Monitoring”](#) on page 17).

## Scan Types

You can operate the LXQ in the following scan types:

- Full Scan
- Selected Ion Monitoring (SIM)
- Selected Reaction Monitoring (SRM)
- Consecutive Reaction Monitoring (CRM)
- ZoomScan

### Full Scan

A full scan scan provides a full mass spectrum of each analyte or parent ion. With full scan, in the last step of mass analysis (ion scan-out) the mass analyzer is scanned from the first mass to the last mass without interruption.

A full scan scan provides more information about an analyte than does selected ion monitoring (SIM) or selected reaction monitoring (SRM). A full scan does not provide the sensitivity that can be achieved by the other scan types.

The full scan scan type includes the following:

- Single-stage full scan
- Two-stage full scan

### Single-Stage Full Scan

The single-stage full scan has one stage of mass analysis (where  $n = 1$  scan power). With single-stage full scan, the ions formed in the ion source are stored in the mass analyzer. These ions are then sequentially scanned out of the mass analyzer to produce a full mass spectrum.

Use single-stage full scan experiments to determine the molecular weight of unknown compounds or the molecular weight of each component in a mixture of unknown compounds. For example, you need a full scan to determine the molecular weight of each component of a mixture of unknown compounds, because you do not know what masses to expect from the mixture.

To use the SIM or SRM scan type, you need to know what ions you are looking for before you can perform an experiment. Thus, for SIM or SRM you can use a full scan to determine the identity of an analyte and obtain its mass spectrum. Then, you can use SIM or SRM for routine quantitative analysis of the compound.

## Two-Stage Full Scan

The two-stage full scan has two stages of mass analysis (where  $n = 2$  scan power). In the first stage of mass analysis, the ions formed in the ion source are stored in the mass analyzer. Then, ions of one mass-to-charge ratio (the parent ions) are selected and all other ions are ejected from the mass analyzer. The parent ions are excited and collide with background gas that is present in the mass analyzer. The collisions of the parent ions cause them to fragment to produce one or more product ions.

In the second stage of mass analysis, the product ions are stored in the mass analyzer. Then, they are sequentially scanned out of the mass analyzer to produce a full product ion mass spectrum.

The two-stage full scan gives you more information about a sample than does SRM but does not yield the speed that can be achieved by SRM. With a two-stage full scan, you spend more time monitoring the product ions than you do with SRM. Thus, the two-stage full scan provides greater information but at lower speed than SRM does.

To use the SRM scan you need to know which parent and product reaction ions you need to observe. To obtain this information you could use a one-stage full scan to determine the parent mass spectrum and a two-stage full scan to determine the product mass spectrum for the parent ions of interest. For subsequent routine quantitative analysis you would use an SRM scan type based on the one-stage and two-stage full scan results.

## Selected Ion Monitoring

*Selected ion monitoring* (SIM) is a single-stage (where  $n = 1$  scan power) technique in which a particular ion or set of ions is monitored. In the SIM scan ions formed in the ion source are stored in the mass analyzer. Ions of one or more mass-to-charge ratios are then selected and all other ions are ejected from the mass analyzer. The selected ions are then sequentially scanned out of the mass analyzer to produce a SIM mass spectrum.

Use SIM experiments to detect small quantities of a target compound in a complex mixture when the mass spectrum of the target compound is known. SIM is useful in trace analysis and in the rapid screening of a large number of samples for a target compound.

Because only a few ions are monitored, SIM provides lower detection limits and greater speed than a single-stage full scan analysis. SIM achieves lower detection limits because more time is spent monitoring significant ions that are known to occur in the mass spectrum of the target sample. SIM achieves greater speed because only a few ions of interest are monitored; regions of the spectrum that are empty or have no ions of interest are not monitored.

SIM can improve the detection limit and decrease analysis time, but it can also reduce *target compound* specificity. This is because SIM analysis only monitors particular *ions*. Thus, *any compound* that produces the ion or ions being monitored would *appear* to be the target compound. It is recommended to verify that the ions being monitored with SIM are from the target compound and nothing else. False positive results could be obtained if this verification is not carried out.

## Selected Reaction Monitoring

*Selected reaction monitoring* (SRM) is a two-stage ( $n = 2$  scan power) technique in which parent ion and product ion *pairs* are monitored.

In the first stage of mass analysis, the ions formed in the ion source are stored in the mass analyzer. Ions of one mass-to-charge ratio (the parent ions) are selected and all other ions are ejected from the mass analyzer. Then, the parent ions are excited so that they collide with background gas that is present in the mass analyzer. The collisions of the parent ions cause them to fragment to produce one or more product ions.

In the second stage of mass analysis, the product ions are stored in the mass analyzer. Ions of one or more mass-to-charge ratios are selected and all other ions are ejected from the mass analyzer. Then, the selected ions are sequentially scanned out of the mass analyzer to produce an SRM product ion mass spectrum.

Like SIM, SRM allows for very rapid analysis of trace components in complex mixtures. However, because you are monitoring pairs of ions (one product ion for each parent ion), the specificity obtained in SRM can be much greater than that obtained in SIM. Thus, you are very unlikely to get a false positive result with SRM. To get a false positive result, the interfering compound must do the following: First, it must form a parent ion of the same mass-to-charge ratio as the selected parent ion from the target compound. Second, it must also fragment to form a product ion of the same mass-to-charge ratio as the selected product ion from the target compound.

## Consecutive Reaction Monitoring

*Consecutive reaction monitoring* (CRM) is the multi-stage ( $n = 3$  to  $n = 10$  scan power) analog of SIM ( $n = 1$ ) and SRM ( $n = 2$ ), in which a multistep reaction path is monitored. In the first stage of mass analysis, the ions formed in the ion source are stored in the mass analyzer. Ions of one mass-to-charge ratio (the parent ions) are selected and all other ions are ejected from the mass analyzer. The parent ions are excited so that they collide with background gas that is present in the mass analyzer. The collisions of the parent ions cause them to fragment to produce one or more product ions.

In the second stage of mass analysis, the product ions are stored in the mass analyzer. Product ions of one mass-to-charge ratio are then selected and all other ions are ejected from the mass analyzer. The selected product ions now become the new parent ions for the next stage of mass analysis. The new parent ions are excited so that they collide with background gas. The collisions of the new parent ions cause them to fragment producing one or more new product ions.

In the third stage of mass analysis, the new product ions are stored in the mass analyzer. This process is repeated up to seven more times until the final product ions of interest are produced.

In the  $n$ th stage of mass analysis, the final product ions are stored in the mass analyzer. Ions of one or more mass-to-charge ratios are selected and all other ions are ejected from the mass analyzer. The selected ions are then sequentially scanned out of the mass analyzer to produce a CRM final product ion mass spectrum.

In CRM, the specificity increases as the number of consecutive reactions that you monitor increases. However, the sensitivity decreases as the number of consecutive reactions that you monitor increases—especially if there are many fragmentation pathways available to the ion.

## **ZoomScan**

The determination of the mass of an ion from its mass-to-charge ratio may be complicated by the fact that the charge state of the ion may be unknown. *ZoomScan* is a high resolution MS scan in which the LXQ performs a high resolution scan to determine the charge state and molecular weight of an ion. LXQ conducts a high resolution scan of 10 u width and evaluates the  $^{12}\text{C}/^{13}\text{C}$  isotopic separation of a specified ion or ions. If the isotopic peaks are 1 u apart, the ion has a charge state of  $\pm 1$ . If the isotopic peaks are 0.5 u apart, the ion has a charge state of  $\pm 2$ . If the isotopic peaks are 0.33 u apart, the ion has a charge state of  $\pm 3$ , and so on. You can then determine the molecular weight of the ion from a knowledge of the charge state and mass-to-charge ratio of the ion. You can conduct a ZoomScan analysis of up to ten ions by specifying the mass-to-charge ratios of the ions that you want to examine.

## Data Types

You can acquire and display mass spectral data (intensity versus mass-to-charge ratio) with the LXQ in one of two data types:

- Profile data type
- Centroid data type

### Profile Data

With *profile data*, you can see the shape of the peaks in the mass spectrum. Each atomic mass unit is divided into approximately 15 sampling intervals. The intensity of the ion current is determined at each of the sampling intervals. The intensity at each sampling interval is displayed with the intensities connected by a continuous line. In general, the profile scan data type is used when you tune and calibrate the MS detector so that you can easily see and measure mass resolution.

### Centroid Data

With *centroid data*, the mass spectrum is displayed as a bar graph. In this scan data type, the intensities of each set of 11 sampling intervals are summed. This sum is displayed versus the integral center of mass of the 11 sampling intervals. The disk space requirements for centroid data are about one-tenth of what is required for profile data. Consequently, data processing for centroid data is faster than that for profile data.

## Experiment Types

This topic describes several types of experiments that you can perform with the LXQ. The experiments can be grouped into the following categories:

- General MS or MS<sup>n</sup>
- Data-Dependent™
- Ion Mapping™
- Ion Tree

You can specify which type of experiment you want to perform in the Instrument Setup window, and then save it in an Instrument Method (.meth) file.

**Note** Procedures for these experiments are beyond the scope of this manual. If you need more information, refer to the online Help.

### General MS or MS<sup>n</sup> Experiments

A General MS or MS<sup>n</sup> experiment is best used for the quantitative analysis of known compounds. However, you can also use a General experiment to collect qualitative data for structural analysis. Xcalibur includes an Instrument Method template in Instrument Setup so you can get started with a General MS or MS<sup>n</sup> experiment.

In a General *MS* quantitation experiment, you need to specify the mass range of your analyte(s) of interest. In a General *MS/MS* quantitation experiment, you need to specify a parent (precursor ion) that fragments into distinctive product ions. In a General *MS<sup>n</sup>* quantitation experiment, you need to specify the mass-to-charge ratios of *all* the parent ions of interest. The LXQ can then collect data on the ions in the range or on the product ions of the parent ion(s) that you specify.

If you use a General experiment to collect data for qualitative (structural) analysis, you specify the scan mode (MS through MS<sup>n</sup>) for which you want data in the Scan Event Settings group box. If you specify MS/MS or MS<sup>n</sup>, you select the parent ion(s) for which you want data in the Set Parent List dialog box. The LXQ then collects distinct qualitative information for structural analysis or for spectral reference.

The LXQ can generate reproducible, product-specific spectra, even from laboratory to laboratory. Consequently, reference spectra that are generated with the LXQ can be used to confirm structures of compounds generated with other LXQ systems.



## Data-Dependent Experiments

A Data-Dependent experiment is best used for the qualitative analysis of unknown compounds for structure elucidation or confirmation. The LXQ uses the information in a Data-Dependent experiment to make decisions about the next step of the experiment automatically — without input from a user. Instrument Setup contains the Instrument Method templates that you need to get started with Data-Dependent experiments.

A Data-Dependent experiment produces a great deal of data from a single sample analysis. You can run a Data-Dependent experiment even if you know very little about your sample, and even if you are unfamiliar with the variables of mass spectroscopy. In a Data-Dependent experiment, you can specify parent ions for fragmentation or you can let the LXQ automatically select the ions for fragmentation. The LXQ can collect the structural information for every parent ion in the sample automatically, even if the sample is a mixture of compounds.

A Data-Dependent experiment requires minimal input from a user about how the experiment should best proceed. The user specifies that one or more scan events of an experiment segment are to be run as Data-Dependent. Then, the LXQ collects MS/MS or MS<sup>n</sup> data and makes decisions about what the next step in the experiment should be to collect even more data. For example, in a Data-Dependent Triple Play experiment for a mixture of compounds, the LXQ can decide which parent ion to isolate, the charge state of the parent ion, and the molecular weight of the compound.

Ion Mapping experiments can be Data-Dependent (The Total Ion Map, Neutral Loss Ion Map, and Parent Ion Map experiments are *not* Data-Dependent). The Data-Dependent Zoom Map experiment collects ZoomScan data on every scan interval in a specified mass range.

Ion Tree experiments are types of Data-Dependent experiments that provide methods for automatically interpreting MS<sup>n</sup> data and arranging the data in easy-to-manipulate formats.

You can approach the setup of Data-Dependent experiments in either of two ways:

- If you have some idea of the parent ion, or if you expect a certain kind of parent, you set up a list of possible parent ions. Then, when one of the parent ions you specified is detected, you can acquire product spectra and analyze the information. Conversely, you can also set up a list of ions that you do not want to be selected for fragmentation.

- If you have little information about your compound, you can set up the parameters of a Data-Dependent experiment so that if the intensity of the ion signal is above a specified threshold, the LXQ generates product spectra. Later, you decide if the information is useful. Parameters might include threshold values for the intensity of the MS or MS<sup>n</sup> ion signal. Whatever threshold values you choose should isolate your parent ions of interest.

You can find useful structural information about your compound automatically with the simplest Data-Dependent experiment, Data-Dependent MS/MS. You specify the MS scan range, and you do not need to specify a parent ion. The LXQ then collects full scan MS data, picks the most intense parent ion in the spectrum, and fragments the ion to generate product ions.

A Data-Dependent Triple-Play experiment is the same as Data-Dependent MS/MS, but includes the identification of the charge state of the parent with the LXQ ZoomScan feature. A Data-Dependent Triple-Play experiment collects full scan MS data, and then uses ZoomScan to determine the charge state of the parent ion and calculate the molecular weight. The parent ion is then fragmented into product ions (MS/MS). For example, if the LXQ determines a charge state equal to 2, and if the mass-to-charge ratio of the parent ion is  $m/z$  500, then the mass-to-charge ratios of the product ions can be up to  $m/z$  1000 (or  $2 \times 500$ ).

Use a Data-Dependent experiment (from templates in Instrument Setup) to do the following:

- Identify low-level impurities in high-purity compounds (Data-Dependent MS/MS)
- Identify metabolites in a complex mixture (Chromatographic Separation with Data-Dependent MS/MS)
- Build a custom library of composite MS<sup>n</sup> spectra (Ion Tree)

Use a Data-Dependent MS<sup>n</sup> experiment to identify process impurities. In the quality assurance process for aspirin, for example, the LXQ can identify impurities of 0.1%.

A Data-Dependent MS/MS experiment of a complex mixture of drug metabolites can provide highly specific structural information. Characteristic masses along the metabolic pathways of a drug, for example, can produce MS/MS spectra that are specific to the structure of the drug. These spectra are essential to metabolite identification.

A Data-Dependent experiment can produce a composite spectrum of, for example,  $MS^2$ ,  $MS^3$ , and  $MS^4$  data. The LXQ can store the  $MS^n$  fingerprint data in a custom  $MS^n$  library spectrum. The data is valuable for use in process control, quality assurance, or research.

## **Ion Mapping Experiments**

Use an Ion Mapping experiment to get full structural characterization of unknown molecules in complex mixtures. In an Ion Mapping experiment, you can get product ion scans on every parent ion over a specified mass range. An Ion Mapping experiment can help to identify automatically which parent ions were fragmented to yield a specified product ion. The experiment “maps” one or more parent ions by using the information from product ion scans.

The LXQ includes Ion Mapping templates in Instrument Setup. Use one of the following templates to start with an Ion Mapping experiment:

- Total (or full scan) Ion Map
- Neutral Loss Ion Map
- Parent Ion Map

These experiments, in general, require that sample solution enter the MS Detector at a composition that is constant throughout. Therefore, use infusion to introduce your sample for these experiments.

In a Total (or full scan) Ion Mapping experiment, product ion scans are produced for each parent ion, so you can determine which parent ions lost a particular fragment to yield a particular product ion. Furthermore, determine which parent ions are related to specific product ions. For example, you can map the spectral peaks in a mass range from  $m/z$  400 to  $m/z$  2000 and specify to scan for MS/MS product ions in incremental steps of every mass-to-charge ratio, every fifth mass-to-charge ratio, or every tenth mass-to-charge ratio.

A Neutral Loss Ion Mapping experiment collects scans for masses that have lost neutral fragments. As with full scan Ion Mapping, you can get product ion scans on every parent ion. However, a Neutral Loss Ion Map identifies which parent ions lost a neutral fragment of a particular mass. For example, you can specify a neutral loss of 80 u (as in the case of a phosphorylated peptide in a tryptic digest). A Neutral Loss Ion Mapping experiment can step through each product mass in the mixture. The experiment searches for evidence of the loss of a neutral moiety of mass 80 u.

A Parent Ion Mapping experiment identifies all the ions that produce a particular molecular ion that you specify. For example, if you specify a product ion mass of  $m/z$  50, a Parent Ion Map includes all the parent ions that yielded the specified product ion,  $m/z$  50.

A Data-Dependent Zoom Map is an Ion Mapping experiment that collects ZoomScan data on every scan interval in a mass range that you specify, as well as Data-Dependent MS/MS product spectra on every mass above an intensity threshold.

The results of any of the Ion Mapping experiments can be viewed in the Xcalibur Qual Browser window.

## Ion Tree Experiments

In an Ion Tree experiment, the LXQ can collect  $MS^n$  data automatically. You can specify a particular parent ion for fragmentation or let the LXQ find the parent ions automatically and fragment them to any level between  $MS^2$  and  $MS^{10}$ . The LXQ automates the collection of data by deciding what actions need to occur next for the experiment to progress.

In an Ion Tree experiment, you can specify either of two options that prioritize how the LXQ gathers information: *Depth Focus* and *Breadth Focus*.

- Depth Focus characterizes an ion by performing a series of  $MS^n$ -level fragmentations (for example,  $MS/MS$ ,  $MS^3$ ,  $MS^4$ , etc.) before characterizing the next most intense ion in the  $MS^n$  series.
- Breadth Focus characterizes all ions to the same  $MS^n$  level before advancing to the next  $MS^n$  level.

For example, if you specify a *Maximum Depth* of 3 and a *Maximum Breadth* of 2 in an Ion Tree experiment, the following occurs:

1. With either Depth or Breadth Focus, the LXQ scans for parent ions ( $MS$ ) over the specified mass range. The most intense ion of the  $MS$  spectrum is selected for fragmentation ( $MS/MS$ ).
2. If you chose the Depth Focus, after the most intense ion of the  $MS$  spectrum is fragmented — producing an  $MS/MS$  spectrum — the LXQ selects and fragments the most intense ion of the  $MS/MS$  spectrum. This results in an  $MS^3$  spectrum, the level specified as the maximum depth for this example. The LXQ then backs up one level and fragments the second most intense ion of the  $MS/MS$  spectrum, creating more product ions on the level of  $MS^3$  from this parent ion. This process is then repeated for the second most intense ion in the  $MS$  spectrum.

3. If you chose the Breadth Focus, after the most intense ion of the MS spectrum is fragmented — producing an MS/MS spectrum — the LXQ selects and fragments the second most intense ion of the *same* MS spectrum. The fragmentation of parent ions continues to the *Max Breadth* level that you specified (in this example, 2). After the two most intense peaks on the MS level are fragmented, the LXQ scans the first *MS/MS* spectrum to select and fragment the two most intense ions. This results in product ions on the level of  $MS^3$ , the level specified as the maximum depth for this example. This process is then repeated for the second most intense ion in the *MS* spectrum.

The results of a Data-Dependent Ion Tree experiment can be viewed in the Xcalibur Qual Browser window. The results are displayed as a structure tree that originates from a particular parent ion.



## Chapter 2 Functional Description

This chapter describes the principal components of the LXQ system and their respective functions. The principal components of the LXQ system are as follows:

- Autosampler (optional)
- Liquid Chromatograph (optional)
- Syringe Pump
- Divert/Inject Valve
- Mass Spectrometer (MS) Detector
- Data System

A functional block diagram of the LXQ system is shown in [Figure 8](#). A sample transfer line connects the LC to the MS detector. The autosampler and LC are usually installed on the left of the MS detector. The syringe pump and divert/inject valve are integrated into the MS detector cabinet.

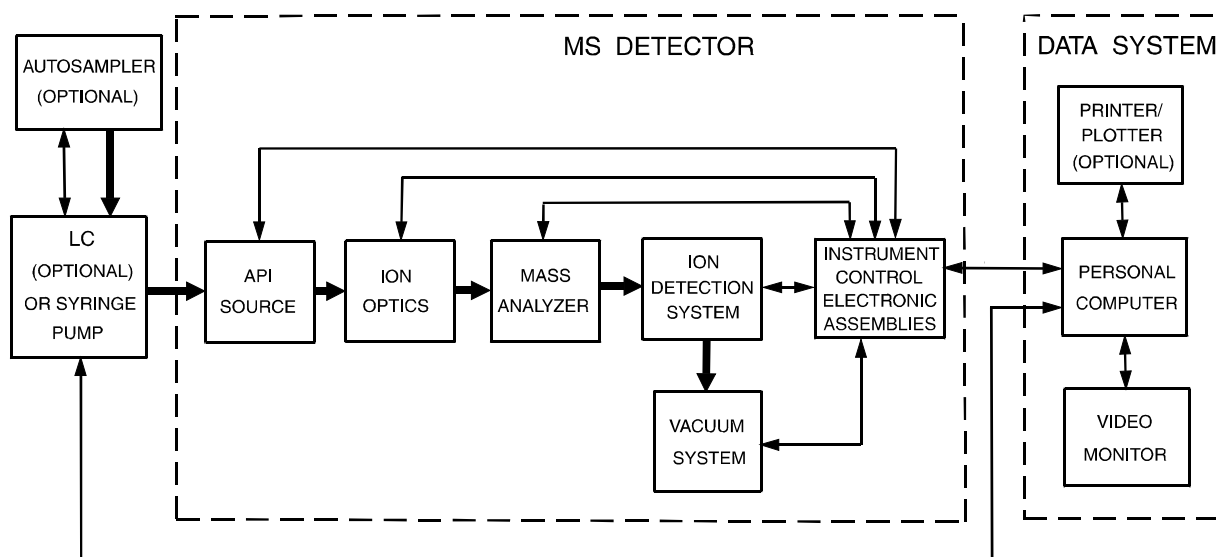
In a typical analysis, a sample can be introduced by any of the following ways:

- Using the syringe pump (direct infusion)
- Using the divert/inject valve fitted with a loop and an LC (flow injection analysis)
- Using a divert/inject valve and LC fitted with a column (LC/MS)

In analysis by LC/MS, a sample is injected onto an LC column. The sample is then separated into its various components. The components elute from the LC column and pass into the MS detector where they are analyzed.

Upon entering the atmospheric ionization (API) source, sample molecules are ionized by electrospray ionization (ESI), atmospheric pressure chemical ionization (APCI), atmospheric pressure photoionization (APPI), or nanospray ionization (NSI). The ion optics focus and accelerate the resulting sample ions into the mass analyzer, where they are analyzed according to their mass-to-charge ratios. The sample ions are then detected by an ion detection system that produces a current proportional to the

number of ions detected. The current from the ion detection system is received and amplified by the LXQ electronics, it is then passed on to the data system for further processing, storage, and display. The data system provides the primary LXQ user interface.



**Figure 8.** The LXQ system (functional block diagram). The broad, single-headed arrows represent the flow of sample molecules through the instrument. The narrow, double-headed arrows represent electrical connections.



## Autosampler

The *autosampler* is used to inject samples automatically into the LC inlet. You control the Thermo Electron (Finnigan Surveyor, AS3000, and AS3500), Waters (2690, 2695, and 2795), and Agilent (1100) autosamplers directly from the LXQ data system computer. With an autosampler, you can automate your LC/MS analyses.

**Note** For other autosamplers, LXQ provides contact closure Start/Stop signals. Refer to *Finnigan LXQ Getting Connected* for information on connecting an autosampler to the LXQ by contact closure Start/Stop signals.

Configure the Xcalibur data system for your autosampler from the data system computer. Specify the model name and model number by selecting the appropriate instrument button in the Instrument Configuration window, which is available by choosing **Start > Programs > Xcalibur > Instrument Configuration**. Refer to the Xcalibur online Help for a description of Instrument Configuration.

You also set up, monitor, and control the autosampler from the data system computer from the Instrument Setup window, which is available by choosing **Start > Programs > Xcalibur > Xcalibur** and then clicking **Instrument Setup**. Refer to the Xcalibur online Help for a description of Instrument Setup.

Front-panel (or keypad) operation of the autosampler and maintenance procedures for the autosampler are described in the documentation provided with your autosampler.

# Liquid Chromatograph

The high performance *liquid chromatograph* (LC) separates a sample mixture into its chemical components by liquid chromatography. In liquid chromatography, the sample mixture partitions between a solid stationary phase of large surface area and a liquid mobile phase that percolates over the stationary phase. The molecular structure of each component of the mixture determines when each component elutes from the LC and enters the MS detector.

You control the Thermo Electron (Finnigan Surveyor MS, Surveyor LC, TSP P2000, TSP P4000), and Agilent (1100) LCs (and the corresponding UV detectors) directly from the LXQ data system computer. Refer to *Finnigan LXQ Getting Connected* for information on connecting an LC to the LXQ.

You configure the Xcalibur data system for your LC and UV detector from the data system computer. Specify the model name and model number by selecting the appropriate instrument button in the Instrument Configuration window. Refer to the Xcalibur Online Help for a description of Instrument Configuration.

You also set up, monitor, and control the LC and UV detector from the data system computer from the Instrument Setup window. Refer to the Xcalibur online Help for a description of Instrument Setup.

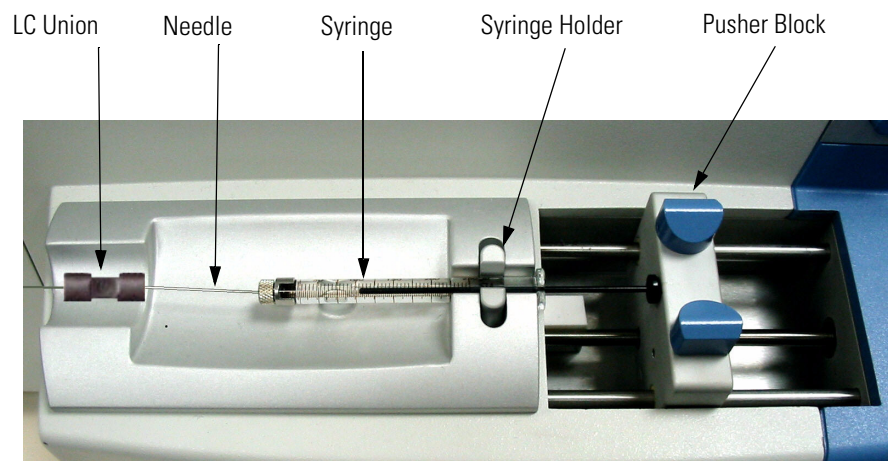
Front-panel (or keypad) operation of the LC and maintenance procedures for the LC are described in the documentation provided with the LC.

## Syringe Pump

The LXQ includes an electronically-controlled, integrated, syringe pump. The *syringe pump* delivers sample solution from the syringe into the API source. See [Figure 9](#). When the syringe pump is operating, a motor drives a *pusher block* that depresses the plunger of the syringe at a rate (volume per minute) that is user adjustable. Liquid flows out of the syringe needle and into the sample transfer line as the plunger is depressed. The syringe is held in place by a *syringe holder*. Refer to *Finnigan LXQ Getting Started* for instructions on setting up the syringe pump.

You can start and stop the syringe pump from the Syringe Pump dialog box, which can be reached from the Tune Plus window (or by choosing **Start > Programs > Xcalibur > LXQ Tune**). You can also specify the Purge mode, in which the flow rate is 5% of the syringe volume per minute. Refer to the Xcalibur Online Help for instructions on operating the syringe pump from the data system.

The *syringe pump light emitting diode (LED)* is green whenever the syringe pump is pumping. The LED is off if the syringe pump is at the end of its travel.



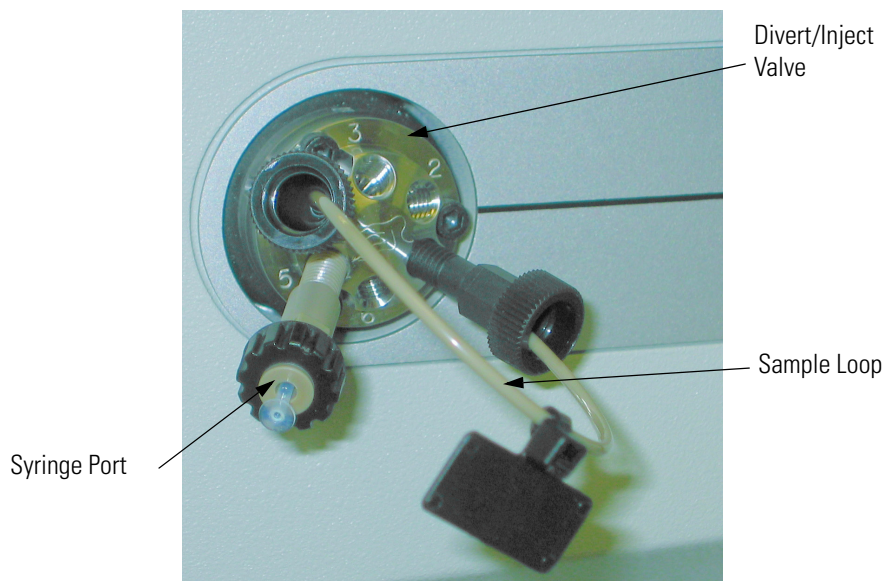
**Figure 9.** Syringe pump

## Divert/Inject Valve

The divert/inject valve is located on the front of the LXQ to the left of the API source. See [Figure 10](#). You can configure (plumb) the divert/inject valve as a loop injector (for flow injection analysis) or as a divert valve. Procedures for plumbing the valve in the loop injector or divert valve configuration are given in **Finnigan LXQ Getting Connected**.

You can control the divert/inject valve from the data system. You specify the parameters of the divert/inject valve in the Divert/Inject Valve dialog box, which can be reached from the Tune Plus window, or the Divert Valve page, which can be reached from the Instrument Setup window. Refer to the online Help for instructions on operating the divert/inject valve from the data system.

You can also use the divert/inject valve button to divert the LC flow between the MS detector and waste when the valve is in the divert valve configuration, or switch between load and inject modes when the valve is in the loop injector configuration.



**Figure 10.** Divert/inject valve

## Mass Spectrometer (MS) Detector

The *MS detector* provides sample ionization and mass analysis of injected samples or samples eluted from a liquid chromatograph. The LXQ MS detector uses a linear ion trap mass analyzer with an ion source external to the mass analyzer. Several important features of the LXQ MS detector includes:

- Universal, selective, and specific detector
- High sensitivity
- Multiple mass ranges
- ESI, APCI, APPI, and NSI ionization techniques
- Positive and negative ion polarity modes
- MS, MS/MS, and MS<sup>n</sup> scan modes
- Full scan, SIM, SRM and CRM scan types
- Data-Dependent, Ion Mapping, and Ion Tree experiments

The MS detector includes the following components:

- Controls and indicators
- API source
- Ion optics
- Mass analyzer
- Ion detection system
- Vacuum system and inlet gasses hardware
- Cooling fans
- Electronic assemblies

### Controls and Indicators

Five LEDs are located at the upper right side of the front panel of the MS detector. See [Figure 11](#).

The Power LED is green whenever power is supplied to the vacuum system and electronic assemblies of the MS detector. It is off when power is not being supplied to the LXQ.

The Vacuum LED is green whenever the vacuum protection circuitry indicates that the vacuum is OK. The vacuum LED is yellow when a vacuum sensor detects a fault and power is being applied to the LXQ components. If the vacuum LED is not illuminated, high voltage is not being applied to the LXQ components.

The Communication LED is illuminated yellow when the MS detector and the data system are trying to establish a communication link. The Communication LED is illuminated green when the communication link between the MS detector and the data system has been made.

The System LED is illuminated yellow whenever the API interlock is open (that is, high voltage is not supplied to the API source, mass analyzer, and ion detection system, but the MS detector power is on). The System LED is illuminated green whenever the MS detector is On (that is, high voltage is supplied to the API source, mass analyzer, and ion detection system).

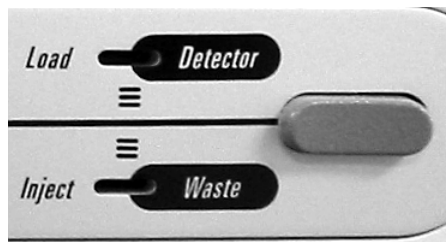
The Scanning LED flashes blue whenever the MS detector is On and scanning ions.



**Figure 11.** Front panel LEDs of the MS detector

Two additional LEDs and a push-button switch are located on the front panel above the divert/inject valve. See [Figure 12](#). When the divert/inject valve is set up for loop injections, the divert/inject valve button toggles the valve between load and inject modes and the labels *Load* and *Inject* apply.

When the divert/inject valve is set up for divert valve operation, the divert/inject valve button toggles the LC flow between the MS detector and the waste container and the labels *Detector* and *Waste* apply.



**Figure 12.** Divert/inject valve button and LEDs

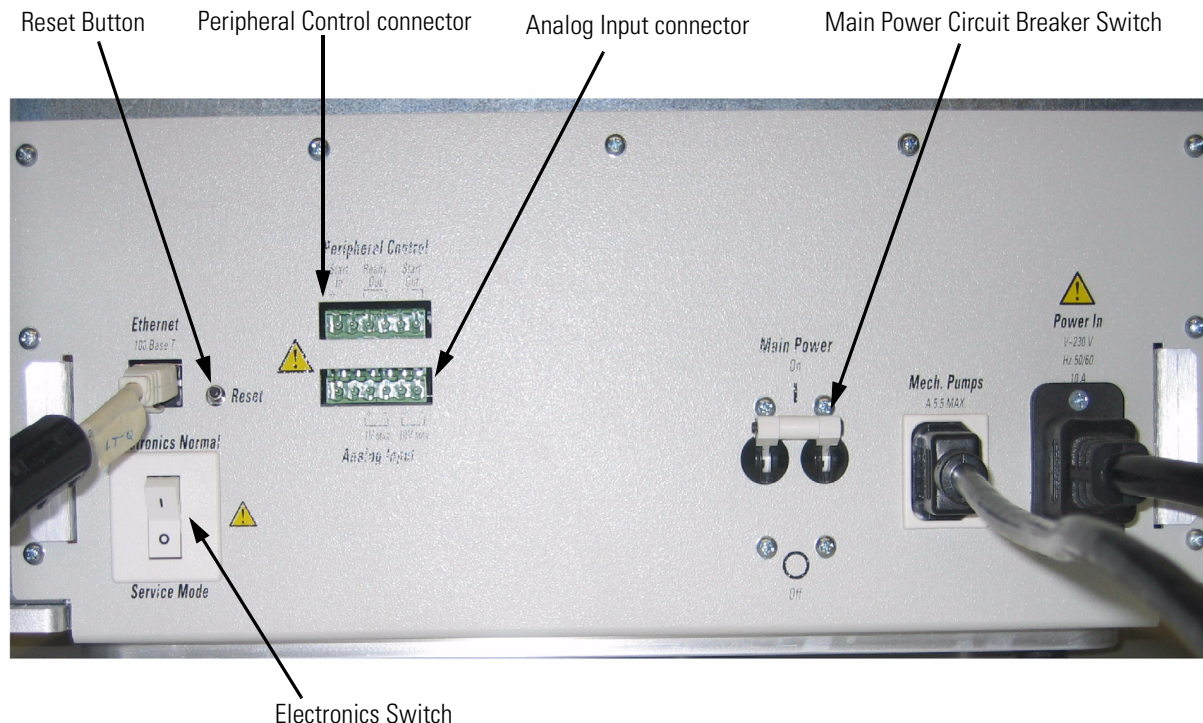
The *main power circuit breaker switch* (labeled *Main Power*) is located on the power panel, which is located at the lower right corner of the right side panel of the MS detector. See [Figure 13](#). In the Off (O) position, the circuit breaker removes all power to the MS detector, including the vacuum pumps. In the On (I) position, power is supplied to the MS detector. In the standard operational mode, the circuit breaker is kept in the On (I) position.

The *electronics service switch* is located on the power panel, see [Figure 13](#). In the Service position the switch removes power to all components of the MS detector other than the vacuum system. In the Electronics Normal position power is supplied to all components of the MS detector.



**CAUTION** To shut off all power to the MS detector in an emergency, place the main power circuit breaker switch (labeled *Main Power*) in the Off (O) position. Do not use the electronics service switch .





**Figure 13.** Power panel

The *reset button* is also located on the power panel. When you briefly press the reset button LXQ software is reloaded from the data system. Refer to the topic “[Resetting the MS Detector](#)” on [page 136](#) in [Chapter 5](#) of this Manual for information on resetting the MS detector.

## API Source

The *atmospheric pressure ionization (API) source* forms gas phase sample ions from sample molecules that are contained in solution. The API source also serves as the interface between the LC and the MS detector. You can operate the API source using either the electrospray ionization (ESI), atmospheric pressure chemical ionization (APCI), atmospheric pressure photoionization (APPI), or nanospray ionization (NSI) technique.

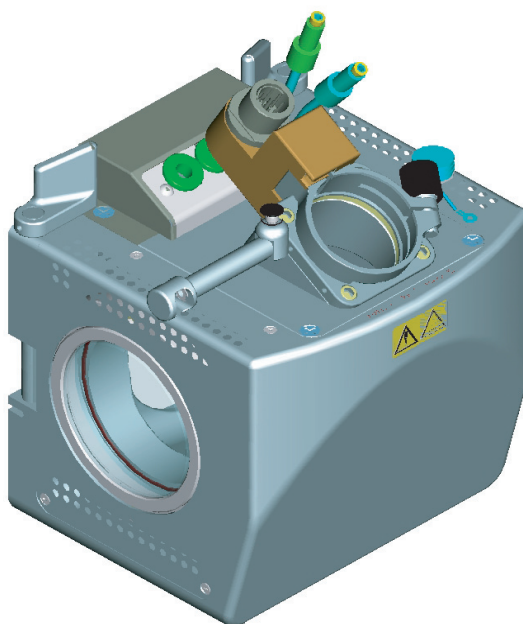
The API source consists of:

- Ion Max<sup>™</sup> or Ion Max-S<sup>™</sup> ion source
- Ion source interface



### **Ion Max Ion Source**

The Ion Max-S™ ion source (see [Figure 14](#)) is the part of the API source that is at atmospheric pressure. The Ion Max-S™ ion source can be configured to operate in any of several API modes, including: electrospray ionization (ESI), atmospheric pressure chemical ionization (APCI) and atmospheric pressure photoionization (APPI). The ions produced in the API source are transmitted by the ion optics into the mass analyzer, where they are separated according to their mass-to-charge ratio.



**Figure 14.** Ion Max-S ion source

The Ion Max ion source housing enables you to quickly switch between ionization modes without the need for specialized tools. Ventilating the ion source housing keeps the housing cool and easy to handle. The ion source is kept at atmospheric pressure. This reduces the chemical noise that could occur if the ionized sample was in a higher pressure environment due to an improperly vented ion source. The probe mounting angle is fixed at the optimum angle for signal intensity and ion source robustness. The probe position in the Z dimension is adjustable to allow for further optimization of signal intensity. A view port is placed at the side of the ion source housing. This enables visual control of probe positioning and monitoring during operation, and facilitates the easy addition of accessories.

Ion source lifetime is excellent due to several special features. The drain size and angle prevents ion source corrosion by allowing eluants to flow directly from the probe into the drain when auxiliary gases are off. For liquids that do not enter the drain directly, the floor of the ion source interior is sloped to enable maximum drainage of collected eluants. Additionally, the zero dead volume LC grounding union that connects the LC flow to the ESI sample inlet is offset from the ion source to prevent LC leaks from dripping directly on the ion source housing.

The Ion Max ion source has a universal mounting platform and interface for use with ESI, APCI, NSI, and APPI ionization sources. For more information on the analysis of ions produced by the Ion Max ion source, refer to the *Finnigan Ion Max API Source Manual*.

### **Ion Source Interface**

The *ion source interface* consists of the components of the API source that are held under vacuum (except for the atmospheric pressure side of the ion sweep cone). The ion source interface includes an ion sweep cone, vent prevent ball, ion transfer capillary, two cartridge heaters, heater block, platinum probe sensor, tube lens, and skimmer. Refer to [Figure 15](#) and [Figure 16](#) to better understand the following description of the ion source interface.

The *ion sweep cone* is a metallic cone over the ion transfer capillary. The ion sweep cone acts as a physical barrier that protects the entrance of the capillary. The *ion transfer capillary* assists in desolvating ions that are produced by ESI, APCI, NSI, or APPI. This capillary is a 4-in. long cylindrical tube made of metal. The *vent prevent ball* falls into the space occupied by the ion transfer capillary when the capillary is removed, thus preventing air from entering the vacuum manifold. The vent prevent ball allows you to remove the ion transfer capillary for cleaning without venting the system. Two *heater cartridges* are embedded in the heater block. The *heater block* surrounds the ion transfer capillary and heats it to temperatures up to 400 °C. A *platinum probe sensor* measures the temperature of the heater block. Typical temperatures of the ion transfer capillary are 270 °C for ESI and 250 °C for APCI. Ions are drawn into the ion transfer capillary in the atmospheric pressure region and transported to the capillary-skimmer region of the vacuum manifold by a decreasing pressure gradient. A potential of typically 0 to  $\pm 10$  V (positive for positive ions and negative for negative ions) assists in repelling ions from the ion transfer capillary to the skimmer.

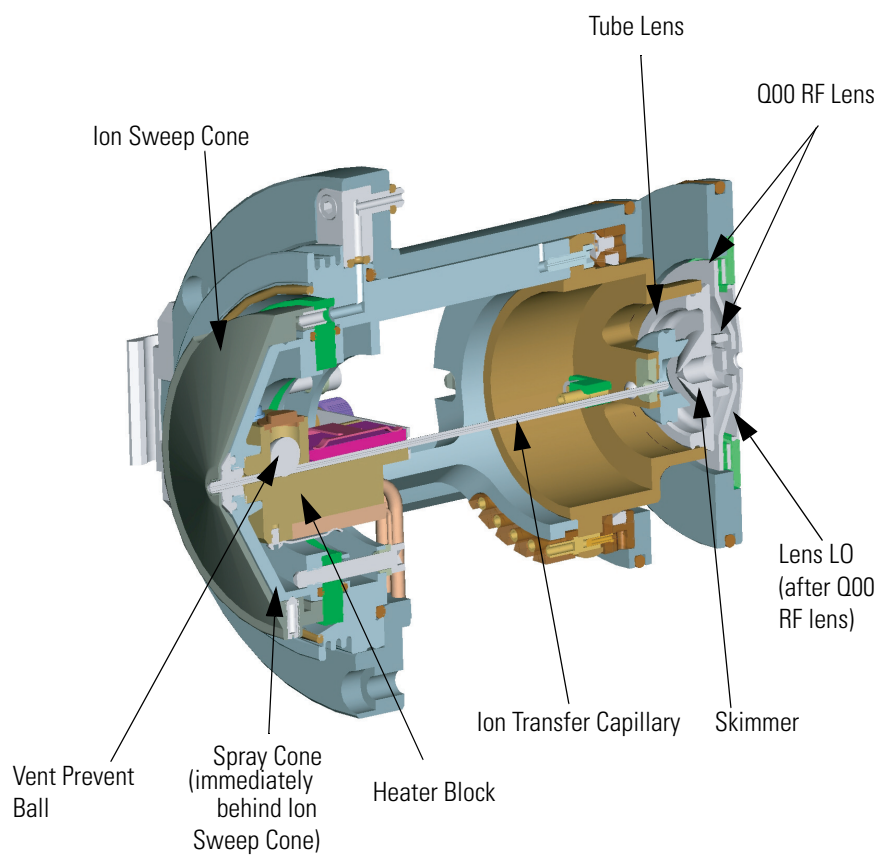
The system electronics includes a voltage monitor circuit and a over-temperature/under-temperature circuit to protect the heaters. The voltage monitoring circuit detects shorting failures. The over-temperature circuit operates as a thermal limit switch to prevent the heater from going

above a preset maximum temperature. The under-temperature feature protects against false low temperature readings. These could occur due to faults in the platinum probe temperature sensor that prevent it from sensing the preset maximum temperature. Such false low temperature readings could cause the heater to run at its maximum setting causing damage to the capillary.

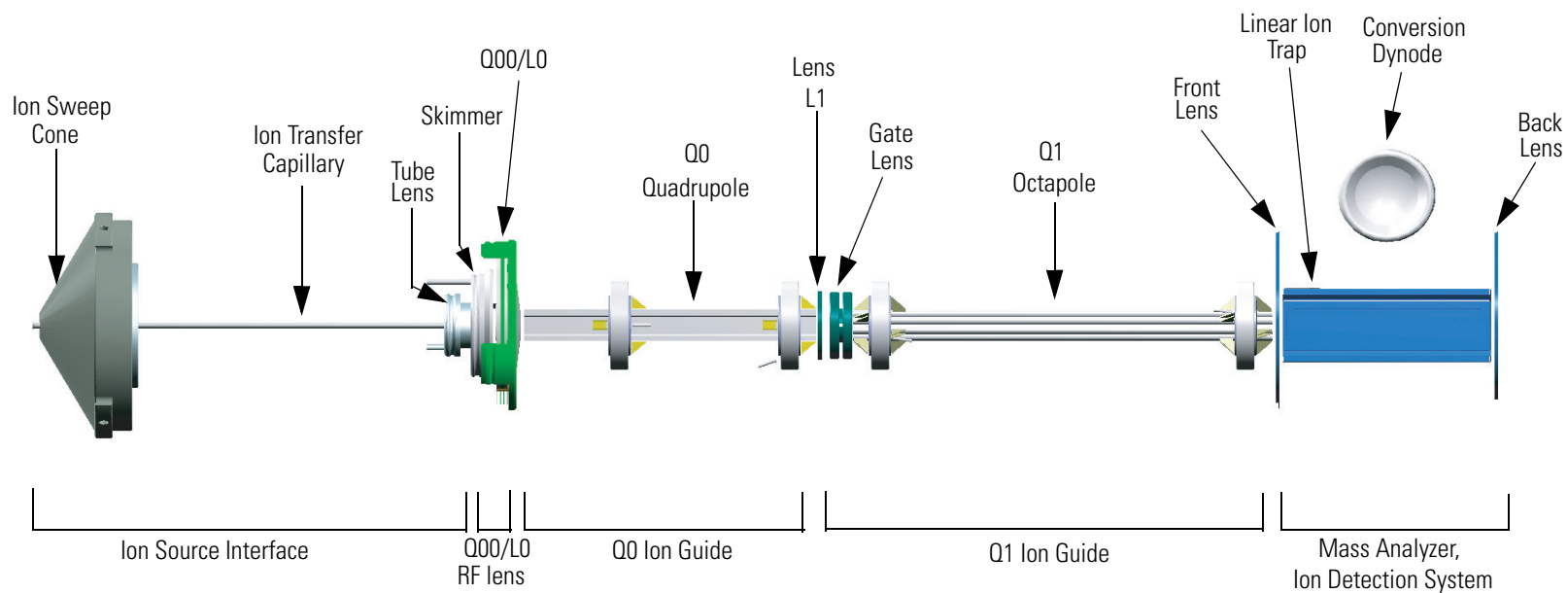
Ions from the ion transfer capillary enter the *tube lens*. The tube lens has a mass dependent potential applied to it that focuses the ions towards the opening of the skimmer. When you tune the LXQ, you adjust the tube lens offset voltage to maximize sensitivity by balancing desolvation with fragmentation.

Ions from the tube lens pass through the skimmer and move toward the Q00 RF lens. The *skimmer* acts as a vacuum baffle between the higher pressure ion source interface region and the lower pressure Q00 region of the vacuum manifold.

The ion source interface is enclosed in a vacuum chamber that is evacuated by the rotary-vane pump.



**Figure 15.** Cross sectional view of the ion source interface and Q00/L0 RF Lens



**Figure 16.** Internal (under vacuum) components of the MS detector

## **Ion Optics**

The *ion optics* focus the ions produced in the API source and transmit them to the mass analyzer. The ion optics consists of an RF lens and two ion guides:

- Q00/L0 RF lens
- Q0 ion guide
- Q1 ion guide

### **Q00/L0 RF Lens**

The *Q00/L0 RF lens* is located closest to the API source. The Q00/L0 RF lens includes the Q00 RF lens and L0 lens. See [Figure 15](#) and [Figure 16](#).

The *Q00 RF lens* is a square array of square-profile segments that acts as an ion focusing device. Any RF voltage that is applied to the optics produces an electric field that focuses the ions along the axis of the Q00 RF lens. A dc voltage offset from ground applied to the Q00 RF lens—called the *Q00 offset voltage*—increases the translational kinetic energy of ions emerging from the skimmer. During ion transmission, the offset voltage is negative for positive ions and positive for negative ions. Increasing the offset voltage will increase the translational kinetic energy of the ions. Typical values of the Q00 offset voltage are  $-4\text{ V}$  to  $+4\text{ V}$ .

The *lens L0* is a metal disk with a circular hole in the center through which the ion beam can pass. An electrical potential of between 0 and  $\pm 5\text{ V}$  (negative for positive ions and positive for negative ions) is applied to lens L0 to aid in ion transmission. Lens L0 also acts as a vacuum baffle between the Q00 RF lens and the Q0 ion guide. The Q00 RF lens chamber of the vacuum manifold is evacuated by the third inlet in the molecular drag section of the turbomolecular pump.

### **Q0 Ion Guide**

The *Q0 ion guide* transmits ions from the Q00 RF lens to the Q1 ion guide. The Q0 ion guide includes the Q0 quadrupole and lens L1. See [Figure 16](#).

The *Q0 quadrupole* is a square array of square-profile rods that acts as an ion transmission device similar to the Q00 RF lens. An RF voltage that is applied to the rods produces an electric field that guides the ions along the axis of the quadrupole. The *Q0 offset voltage* increases the translational kinetic energy of ions emerging from the Q00 RF lens. Q0 must be at a lower potential than the Q00 RF lens.

The *lens L1* is a metal disk with a circular hole in the center through which the ion beam can pass. An electrical potential can be applied to the lens to accelerate (or decelerate) ions as they approach the lens and to focus the ion beam as it passes through the lens. The value ranges between 0 and  $\pm 125\text{ V}$ .

Lens L1 also acts as a vacuum baffle between the Q0 ion guide chamber and the mass analyzer chamber. The Q0 ion guide chamber is evacuated by the interstage inlet of the turbomolecular pump.

### **Q1 Ion Guide**

The *Q1 ion guide* transmits ions from the Q0 ion guide to the mass analyzer. The Q1 ion guide includes the Q1 octapole and the gate lens. See [Figure 16](#).

The *Q1 octapole* is an octagonal array of round-profile rods that acts as an ion transmission device similar to the Q00 RF lens and Q0. An RF voltage that is applied to the rods produces an electric field that guides the ions along the axis of the octapole. The *Q1 offset voltage* increases the translational kinetic energy of ions emerging from Q0.

The *gate lens* is used to start and stop the injection of ions into the mass analyzer.

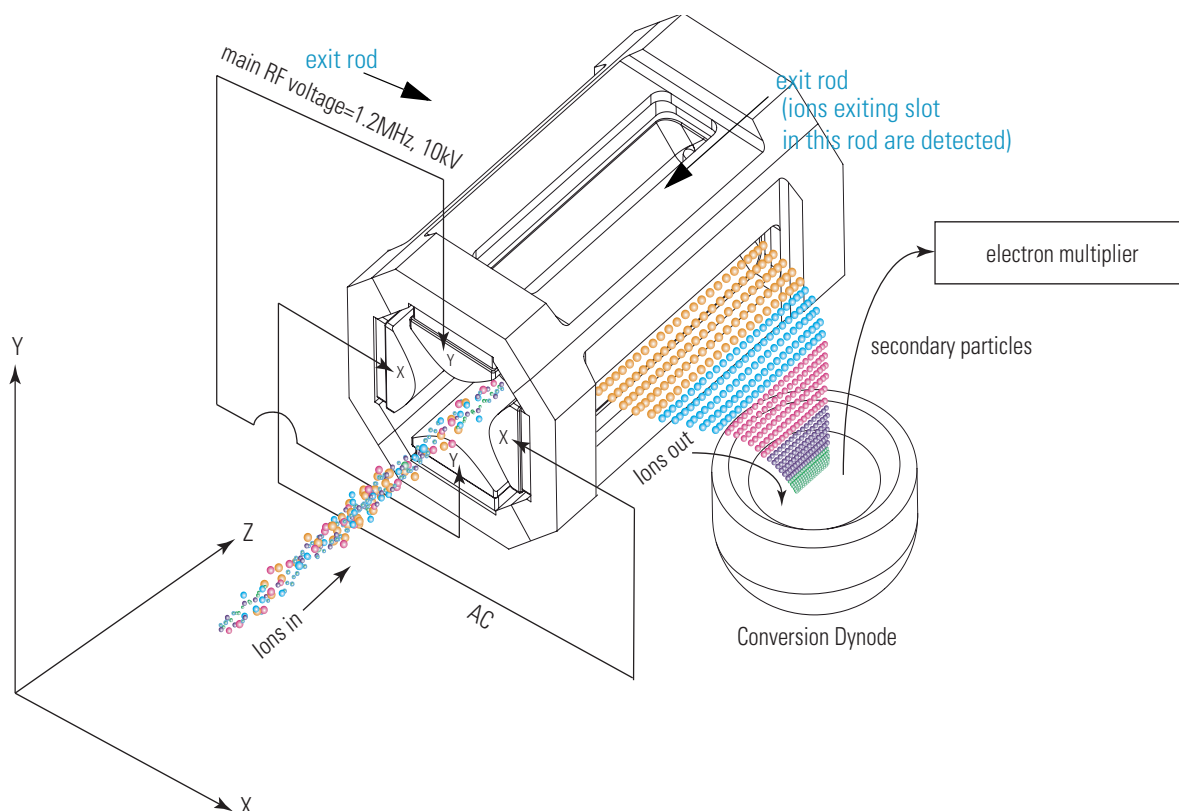
## **Mass Analyzer**

The *mass analyzer* is the site of mass analysis (that is, ion storage, ion isolation, collision induced dissociation, and ion scan out). This section describes the components of the mass analyzer, the voltages applied to the mass analyzer electrodes, the presence of helium damping gas in the mass analyzer cavity, and the operation of the mass analyzer during mass analysis.

### **Components of the Mass Analyzer**

The mass analyzer consists of a front lens, linear ion trap, and back lens ([Figure 16](#)). The *front* and *back lenses* are metal disks with a circular holes in their centers through which the ion beam can pass. The purpose of the front and back lenses is to provide conductance limits. During ion injection the back lens is +12 V relative to the trap and the front lens potential relative to the trap is adjustable by the user. During scan out both lenses are +200 V relative to the trap for positive ions and -200 V relative to the trap for negative ions.

The *linear ion trap* is a square array of precision-machined and precision-aligned hyperbolic rods. The basic design of the linear ion trap is shown in [Figure 17](#). Two of the rods, called *exit rods*, have a slot through which the ions are ejected during scan out. Ions coming out of only one of the slots are detected. Quartz spacers act as electrical insulators between adjacent rods. Rods opposite each other in the array are connected electrically. Thus, the four rods can be considered to be two pairs of two rods each.



**Figure 17.** Linear ion trap quadrupole rod assembly

### DC Axial Trapping Voltages

The mass analyzer of the LXQ is divided into three components. The components are: 1) the Front Lens (Figure 16), 2) the ion trap rods (labelled as x and y in Figure 17, or the linear ion trap in Figure 16), and 3) the Back Lens (Figure 16). The LXQ uses three *dc axial trapping voltages*, one for each component of the mass analyzer. These dc axial trapping voltages allow the mass analyzer to perform its storage and scan out functions. For the case of positively charged ions the following dc axial trapping potentials are applied to the components for either ion storage or scan out:

analyzer component	ion storage voltages	scan out voltages
Front Lens	adjustable	+100V
ion trap rods	-12V	-100V
Back Lens	0V	+100V

The signs of these voltages are reversed for negative ions.



## Main RF Voltage

Rods opposite each other in the array are connected electrically. RF voltages are applied to the rods and these voltages are ramped during the scan.

The RF voltage is applied only to the y rods (Figure 17) and is of constant frequency (1.2 MHz) and of variable amplitude (0 to 10,000 V zero-to-peak). Because the frequency of this RF voltage is in the radio frequency (RF) range, it is referred to as the *main RF voltage*. The application of the main RF voltage to the y rods produces a two-dimensional quadrupole field within the mass analyzer cavity. This time-varying field drives ionic motion in the radial (X,Y) directions. Ionic motion must be stable in the radial direction for an ion to remain trapped. (A stable trajectory is an oscillatory trajectory that is confined within the mass analyzer). During ion scan out, the system produces a mass-dependent instability to eject ions from the mass analyzer in the X direction. The ions are ejected from a slot in the side of one of the X rods and go to the dynode (Figure 17). The ions strike the dynode and release particles. These secondary particles are captured and amplified by an electron multiplier. The electron multiplier produces the signal that the instrument associates with the ions that are responding to the mass-dependent instability.

When the amplitude of the main RF voltage is low, all ions above a minimum mass-to-charge ratio are trapped. This RF voltage is referred to as the *storage voltage*, and the minimum mass-to-charge ratio is usually chosen to be greater than the mass-to-charge ratios associated with air, water, and solvent ions. During ion scan out, the main RF voltage is ramped at a constant rate corresponding to approximately 16,600 u/s (for unit resolution). As the main RF voltage increases, ions of increasing mass-to-charge ratio become successively unstable in the X direction and are ejected from the mass analyzer. The voltage at which an ion is ejected from the mass analyzer is defined as its *resonance voltage*. The ejection of ions of each mass-to-charge ratio occurs over a very short time. Many of these ions are detected by the ion detection system.

## Ion Isolation Waveform Voltage, Resonance Excitation AC Voltage, and Resonance Ejection AC Voltage Applied to the Exit Rods

The ion isolation waveform voltage, resonance excitation AC voltage, and resonance ejection AC voltage are AC voltages that are applied to the x rods (Figure 17) to stimulate motion of the ions in the direction of the ion detection system. The voltages applied to the x rods are equal in amplitude but are 180° out of phase to one another. When the AC frequency applied to the x rods equals the resonance frequency of a trapped ion (which depends on its mass) the ion gains kinetic energy. If the magnitude of the applied voltage is large enough or the ion is given sufficient time, the ion is ejected from the mass analyzer in the direction of the ion detection system (through the slot in one of the x rods as shown in Figure 17). The ion detection system consists of the conversion dynode and electron multiplier (Figure 16 and Figure 17).

The *ion isolation waveform voltage* consists of a distribution of frequencies between 5 and 600 kHz containing all resonance frequencies except for those corresponding to the ions to be trapped. The ion isolation waveform voltage acts during the ion isolation step of SIM, SRM, CRM, or MS<sup>n</sup> ( $n > 1$ ) full scan applications. The ion isolation waveform voltage, in combination with the main RF voltage, ejects all ions except those of a selected mass-to-charge ratio or narrow ranges of mass-to-charge ratios. The ion isolation waveform voltage is calculated by the LXQ and automatically applied at the correct time.

During the collision induced dissociation step of SRM, CRM, or MS<sup>n</sup> ( $n > 1$ ) full scan applications, the *resonance excitation AC voltage* is applied to the exit rods to fragment parent ions into product ions. The resonance excitation AC voltage is not strong enough to eject an ion from the mass analyzer. However, ion motion in the radial direction is enhanced and the ion gains kinetic energy. After many collisions with the helium damping gas, which is present in the mass analyzer, the ion gains enough internal energy to cause it to dissociate into product ions. The product ions are then mass analyzed.

During ion scan out, the *resonance ejection AC voltage* facilitates the ejection of ions from the mass analyzer and thus improves mass resolution. The resonance ejection AC voltage is applied at a fixed frequency and increasing amplitude during the ramp of the main RF voltage. Only when an ion is about to be ejected from the mass analyzer cavity by the main RF voltage is it in resonance with the resonance ejection AC voltage. When an ion approaches resonance, it moves farther away from the center of the mass analyzer, where the field generated by the main RF voltage is zero (and space-charge effects are strong), into a region where the field produced by the main RF voltage is strong (and space-charge effects are small). As a result, the ejection of the ion is facilitated, and mass resolution is significantly improved.

### **Helium Damping Gas in the Mass Analyzer Cavity**

The mass analyzer cavity contains helium that is used as a damping gas and a collision activation partner. The helium damping gas enters the mass analyzer cavity through a gap between the ion trap rods. The flow of gas (~1 mL/min) into the mass analyzer cavity is regulated by a pressure regulator and a capillary restrictor. The flow of gas out of the mass analyzer cavity (and into the turbomolecular pump) is restricted by the openings in the mass analyzer. The flows into and out of the cavity are matched so that the partial pressure of helium in the mass analyzer cavity is maintained at the proper pressure.

The collisions of the ions entering the mass analyzer with the helium slow the ions so that they can be trapped by the RF field in the mass analyzer.

The presence of helium in the mass analyzer cavity significantly enhances sensitivity and mass spectral resolution. Before their ejection from the mass analyzer cavity, sample ions collide with helium atoms. These collisions reduce the kinetic energy of the ions, thereby damping the amplitude of their oscillations. As a result, the ions are focused to the axis of the cavity rather than being allowed to spread throughout the cavity.

Helium in the mass analyzer cavity also serves as a collision activation partner. During the collision induced dissociation step of an SRM, CRM, or MS<sup>n</sup> (n > 1) full scan analysis, the resonance excitation AC voltage applied to the x rods drives parent ions into the helium atoms. After gaining sufficient internal energy from the resulting collisions, the parent ion dissociates into one or more product ions.

### **Summary of Mass Analyzer Operation**

The processes that occur in the mass analyzer can be broken down into four steps:

- Ion storage
- Ion isolation (SIM, SRM, CRM, or MS<sup>n</sup> (n > 1) full scan only)
- Collision induced dissociation (SRM, CRM, or MS<sup>n</sup> (n > 1) full scan only)
- Ion scan out (the ion detection step)

For SRM and MS/MS full scan applications the ion isolation and collision induced dissociation steps are performed once. For CRM and MS<sup>n</sup> (n > 1) full scan applications the ion isolation and collision induced dissociation steps are performed n-1 times.

Before ion storage, the following conditions are established:

- Helium is present in the mass analyzer cavity.
- Main RF voltage is set to the storage voltage.
- DC axial trapping voltages are set to the storage voltages.
- Ion isolation waveform voltage, resonance excitation AC voltage, and resonance ejection AC voltage on the exit rods are off.

With these conditions achieved, sample ions formed in the API source are trapped in the mass analyzer if the ions have mass-to-charge ratios greater than the minimum storage mass-to-charge ratio.

Next, for SIM, SRM, CRM, or  $MS^n$  ( $n > 1$ ) full scan, the ion isolation waveform voltage is applied to the exit rods, in combination with a ramp of the main RF voltage to a new storage voltage, to eject all ions except those of the selected mass-to-charge ratio.

Then, for SRM, CRM, or  $MS^n$  ( $n > 1$ ) full scan analyses, the resonance excitation AC voltage is applied to the exit rods to cause collision induced dissociation. Product ions with mass-to-charge ratio greater than the minimum storage mass-to-charge ratio are stored. (The minimum storage mass during collision induced dissociation is typically set to one quarter of the parent ion mass-to-charge ratio.)

For SRM and MS/MS full scan applications the ion isolation and collision induced dissociation steps are performed once. For CRM and  $MS^n$  ( $n > 1$ ) full scan applications the ion isolation and collision induced dissociation steps are performed  $n-1$  times.

Finally, the sample ions or product ions are scanned out: The main RF voltage is ramped from low voltage to high voltage, and simultaneously the resonance ejection AC voltage is applied to the exit rods to facilitate ejection. As the main RF voltage is increased, ions of greater and greater mass-to-charge ratios become unstable and are ejected through the slots in the exit rods. Many of these ions are focused toward the ion detection system where they are detected.

## **Ion Detection Systems**

The LXQ is equipped with one high sensitivity, off-axis *ion detection system* that produces a high signal-to-noise ratio and allows for voltage polarity switching between positive ion and negative ion modes of operation. The ion detection system includes a 15-kV conversion dynode and a channel electron multiplier. The ion detection system is located on one side of the mass analyzer (Figure 16, Figure 17).

The details of the ion detection system are shown in Figure 18. The *conversion dynode* is a concave metal surface that is located at a right angle to the ion beam. A potential of +15 kV for negative ion detection, or -15 kV for positive ion detection, is applied to the conversion dynode. When an ion strikes the surface of the conversion dynode, one or more secondary particles are produced. These secondary particles can include positive ions, negative ions, electrons, and neutrals. When positive ions strike a negatively charged conversion dynode, the secondary particles of interest are negative ions and electrons. When negative ions strike a positively charged conversion dynode, the secondary particles of interest are positive ions. These secondary particles are focused by the curved surface of the conversion dynode and are accelerated by a voltage gradient into the

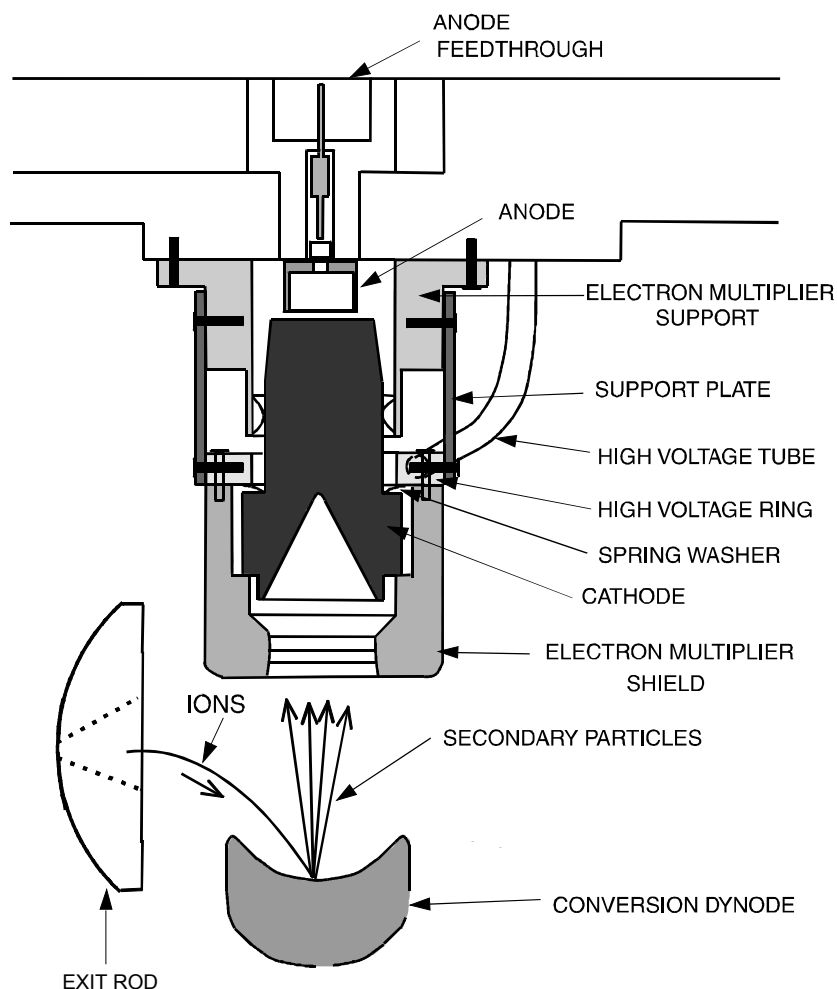
electron multiplier. The *conversion dynode shield* and *disk* shield the vacuum manifold from the electric field produced by the conversion dynode.

The electron multiplier is mounted on the top cover plate of the vacuum manifold next to the mass analyzer. See [Figure 18](#) and [Figure 23](#). The *electron multiplier* includes a cathode and an anode. The *cathode* of the electron multiplier is a lead-oxide, funnel-like resistor. A potential of up to -2.5 kV is applied to the cathode by the *high voltage ring*. The exit end of the cathode (at the anode) is near ground potential. The cathode is held in place by the high voltage ring, two *support plates*, the *electron multiplier support*, and the *electron multiplier shield*. A spring washer applies a force to the cathode to hold it in contact with the electron multiplier shield. The electron multiplier support is attached to the top cover plate of the vacuum manifold by two screws.

The *anode* of the electron multiplier is a small cup located at the exit end of the cathode. The anode collects the electrons produced by the cathode. The anode screws into the anode feedthrough in the top cover plate.

Secondary particles from the conversion dynode strike the inner walls of the electron multiplier cathode with sufficient energy to eject electrons. The ejected electrons are accelerated farther into the cathode, drawn by the increasingly positive potential gradient. Due to the funnel shape of the cathode, the ejected electrons do not travel far before they again strike the inner surface of the cathode, thereby causing the emission of more electrons. Thus, a cascade of electrons is created that finally results in a measurable current at the end of the cathode where the electrons are collected by the anode. The current collected by the anode is proportional to the number of secondary particles striking the cathode.

Typically, the electron multiplier is set to a gain of about  $1 \times 10^5$  (i.e., for each ion or electron that enters,  $1 \times 10^5$  electrons exit). The current that leaves the electron multiplier via the anode is converted to a voltage by the electrometer circuit and recorded by the data system. Refer to the topic “[Ion Detection System Electronic Assemblies](#)” on [page 66](#).



**Figure 18.** Cross sectional view of the ion detection system, showing the electron multiplier and the conversion dynode

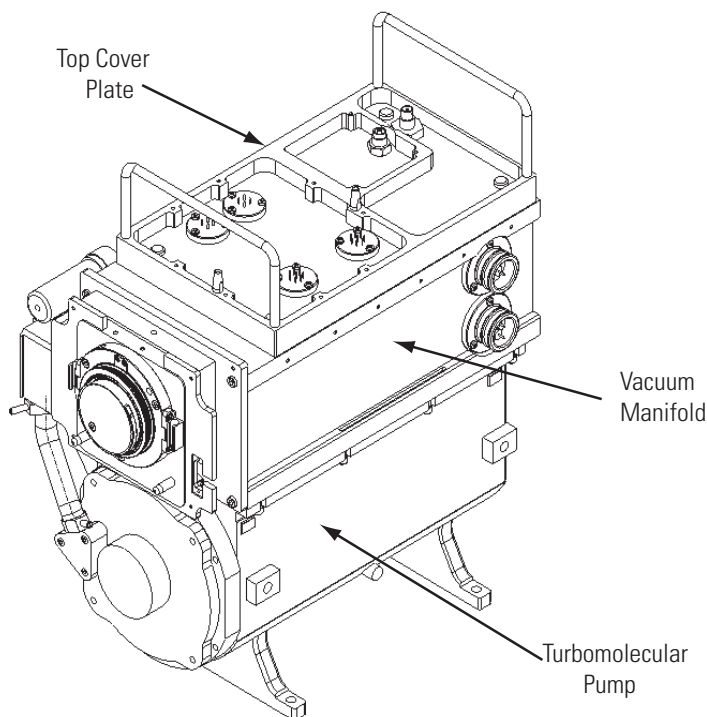
The ion detection system of the LXQ increases signal and decreases noise. The high voltage applied to the conversion dynode results in a high conversion efficiency and increased signal. That is, for each ion striking the conversion dynode, many secondary particles are produced. The increase in conversion efficiency is more pronounced for more massive ions than for less massive ions.

Because of the off-axis orientation of the ion detection system relative to the mass analyzer, neutral molecules from the mass analyzer tend not to strike the conversion dynode or electron multiplier. As a result, the noise from neutral molecules is reduced.

## Vacuum System and Inlet Gasses Hardware

The *vacuum system* evacuates the region around the API stack, ion optics, mass analyzer, and ion detection system. The vacuum system includes the following components illustrated in [Figure 19](#):

- Vacuum manifold
- Turbomolecular pump
- Forepump
- Convectron® gauge
- Ion gauge



**Figure 19.** Vacuum manifold with top cover plate and turbomolecular pump

The *inlet gasses hardware* controls the flow of damping gas, sheath gas, auxiliary gas, sweep gas, and air (during venting) into the MS detector. The inlet gasses hardware includes the following components:

- Vent gas valve
- Damping gas inlet assembly
- Sheath gas valve

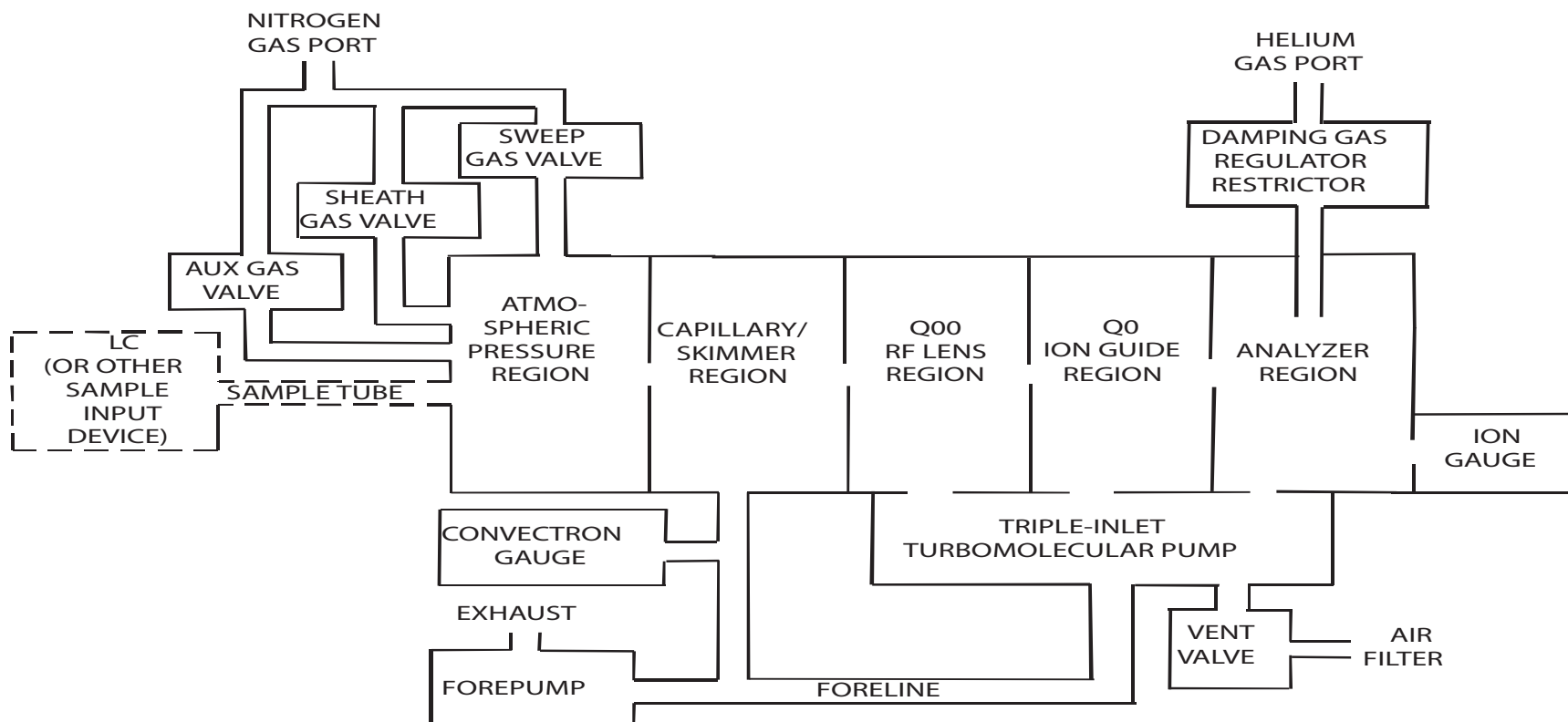
## 2 Functional Description

### Mass Spectrometer (MS) Detector

- Auxiliary gas valve
- Sweep gas valve

A functional block diagram of the vacuum system and inlet gasses hardware is shown in [Figure 20](#).





**Figure 20.** Vacuum system and inlet gasses hardware (functional block diagram)

## Vacuum Manifold

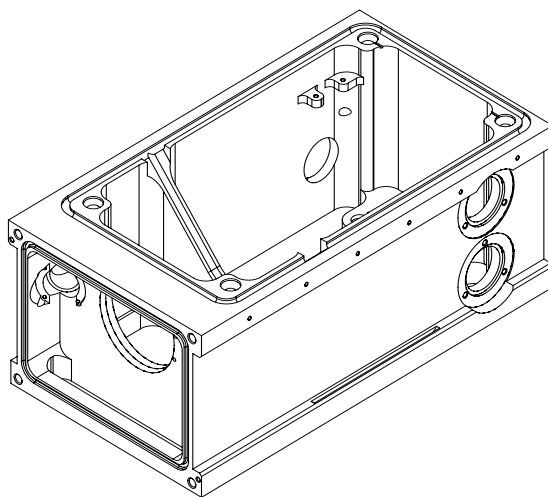
The *vacuum manifold* encloses the ion source interface, ion guides, mass analyzer, and ion detection system assemblies. The vacuum manifold is a thick-walled, aluminum chamber with a removable top cover plate, machined flanges on the front, sides, and bottom, and various electrical feedthroughs and gas inlets.

The vacuum manifold is divided into four chambers by three baffles. See [Figure 21](#). The region inside the first chamber, called the *capillary/skimmer region*, is evacuated by the rotary-vane pump. The region inside the second chamber, called the *Q00 RF lens region*, is evacuated by the third inlet in the molecular drag section of the triple-inlet turbomolecular vacuum pump. The region inside the third chamber, called the *Q0 ion guide region*, is evacuated by the interstage port of the turbomolecular vacuum pump. The region inside the fourth chamber, called the *analyzer region*, is evacuated by the high vacuum port of the turbomolecular pump. The turbomolecular pump in turn discharges into the rotary-vane pump through the foreline.

Three high-voltage electrical feedthroughs pass through the vacuum manifold:

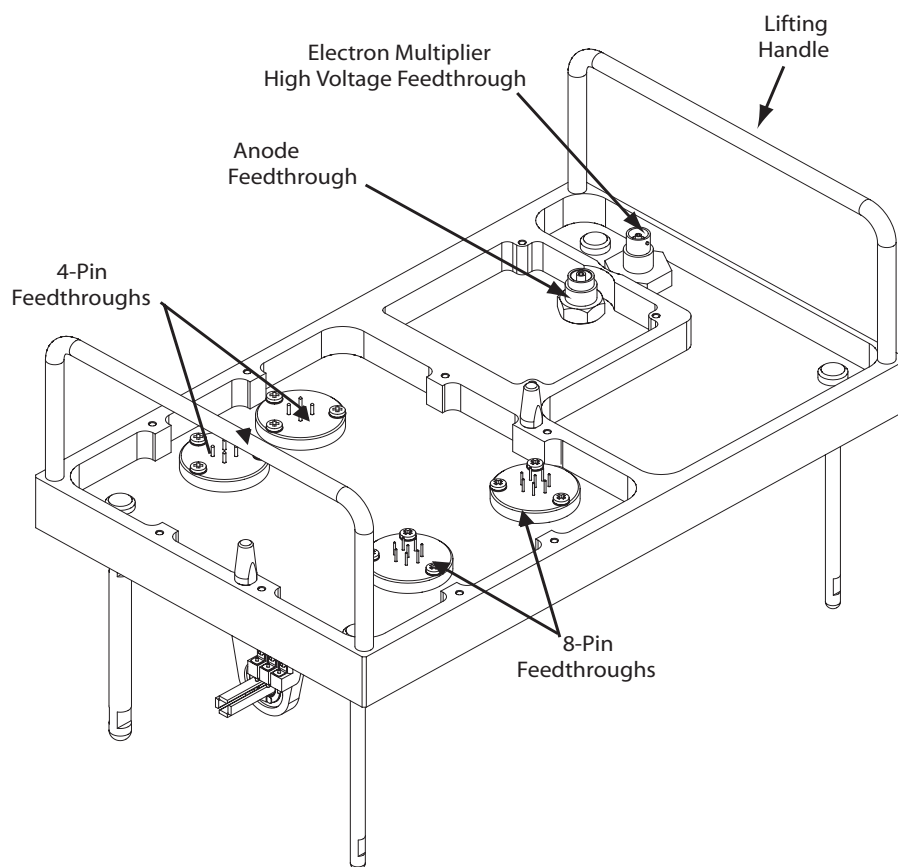
- One feed-through for the high voltage for the conversion dynode
- Two feed-throughs for the RF AC voltages of the mass analyzer

The vacuum manifold also has an opening for the ion gauge.



**Figure 21.** Vacuum manifold

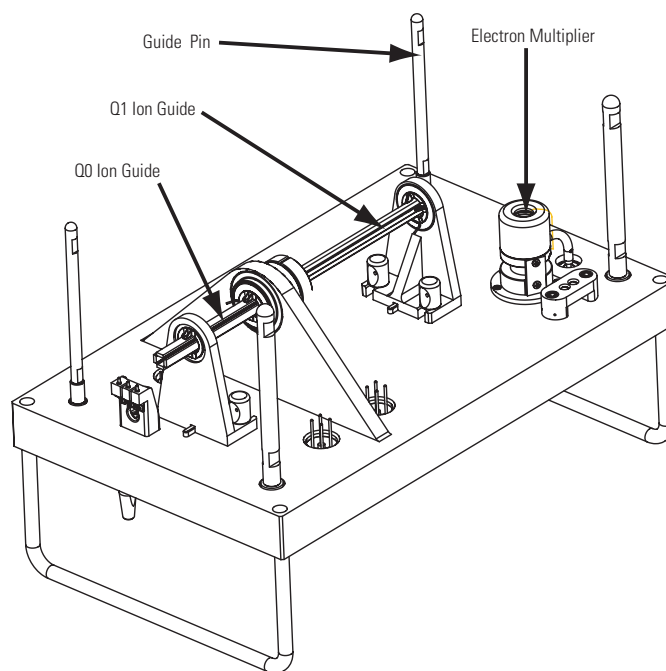
The removable *top cover plate* of the vacuum manifold holds the Q0 and Q1 ion guides and the electron multiplier (part of the ion detection system). Removal of the top cover plate enables access to these assemblies. Two handles on the top and four guide posts on the underside of the top cover plate facilitate its removal and installation. An O-ring provides a vacuum-tight seal between the top cover plate and the vacuum manifold. The top cover plate and its attached assemblies are shown in [Figure 22](#) and [Figure 23](#).



**Figure 22.** Top cover plate of the vacuum manifold (topside)

Six electrical feedthroughs pass through the top cover plate:

- Two 4-pin and two 8-pin feed-throughs for the RF and DC voltages to the ion optics
- One feed-through for the high voltage to the cathodes of the electron multiplier
- A feed-through for the ion current signal from the electron multiplier anode



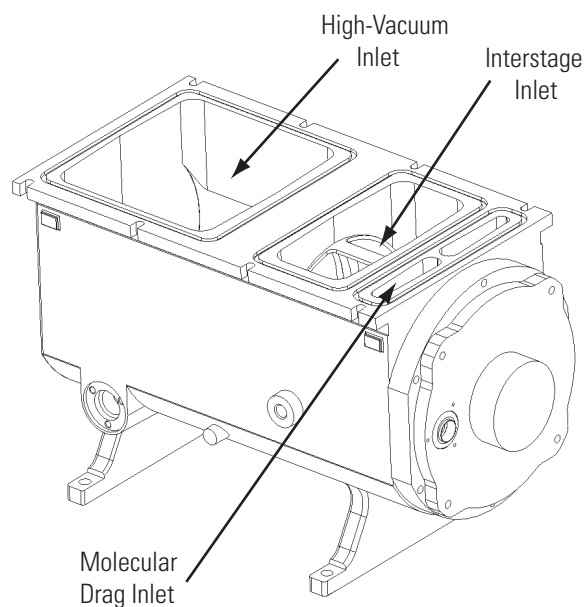
**Figure 23.** Top cover plate of the vacuum manifold (underside), and attached assemblies

### **Turbomolecular Pump**

A Leybold TW220/150/15S triple-inlet *turbomolecular pump* provides the vacuum for the Q00 RF lens region, Q0 ion guide region, and analyzer region of the vacuum manifold. The turbomolecular pump mounts onto the bottom of the vacuum manifold.

The turbomolecular pump has three pumping inlets (see [Figure 24](#)):

- A 220 L/s high-vacuum inlet at the top of the rotor stack, which evacuates the analyzer chamber
- A 150 L/s interstage inlet about half way down the rotor stack, which evacuates the Q0 ion guide chamber
- A 15 L/s third inlet in the molecular drag section of the pump, which evacuates the Q00 RF lens chamber



**Figure 24.** Turbomolecular pump

The turbomolecular pump is controlled by a Leybold TDS controller and powered by a +24 V dc (250 W) power supply. Power for the turbomolecular pump is turned off by the main power circuit breaker switch, but not by the electronics service switch. The pump is air cooled by a fan that draws air in from the front of the instrument.

The Leybold TDS *Turbomolecular Pump Controller* provides power to and control of the turbomolecular pump. The turbomolecular pump status (such as temperature or rotational speed) is sent from the Turbomolecular Pump Controller to the embedded computer over a serial line. Power to the turbomolecular pump is shut off if the pump temperature is too high.

### **Forepump**

An Edwards E2M30 *forepump* (or mechanical pump) establishes the vacuum necessary for the proper operation of the turbomolecular pump. The forepump also evacuates the ion transfer capillary-skimmer region of the vacuum manifold. The pump has a maximum displacement of 650 L/min and maintains a minimum pressure of approximately 1 Torr.

The forepump is connected to the turbomolecular pump by a section of 1.27 cm (0.5 in.) ID reinforced PVC tubing. The power cord of the forepump is plugged into the outlet labeled *Mech. Pump* on the power panel

(See [Figure 13](#) on [page 36](#)). This outlet supplies power to the pump and is controlled by the main power circuit breaker switch and not by the electronics service switch.



**CAUTION** Always plug the forepump power cord into the outlet labeled *Mech. Pump* on the right side of the MS detector. Never plug it into a wall outlet.

### **Convectron® Gauge**

The *Convectron gauge* measures the pressure in the ion transfer capillary-skimmer region of the vacuum manifold and the foreline, which connects the turbomolecular pump and the forepump.

### **Ion Gauge**

The pressure in the analyzer region of the vacuum manifold is measured by a Granville-Phillips® 342™ mini ion gauge. The *ion gauge* produces energetic electrons that cause the ionization of molecules in the ion gauge. Positive ions formed in the ion gauge are attracted to a collector. The collector current is related to the pressure in the vacuum manifold. The ion gauge is also used in vacuum protection.

### **Vent Valve**

The *vent valve* allows the vacuum manifold to be vented to air that has been filtered through a sintered nylon filter. The vent valve is a solenoid-operated valve. The vent valve is closed when the solenoid is energized.

The vacuum manifold is vented when external power is removed from the MS detector. (Power is removed from the MS detector by a power failure or by placing the main power circuit breaker in the Off (O) position.) Power is provided to the vent valve for a short time after the external power is removed. If external power is not restored to the MS detector in 10 s, power to the vent valve solenoid is shut off. When power to the vent valve solenoid is shut off, the vent valve opens and the manifold is vented to filtered air. The vent valve closes after power is restored to the MS detector.

### **Damping Gas Inlet Assembly**

The *damping gas inlet assembly* controls the flow of helium into the mass analyzer cavity. Helium ( $40 \pm 10$  psig [ $275 \pm 70$  kPa], 99.999% [ultra-high] purity) enters the MS detector through a 1/8-in. port on the rear of the MS detector. LXQ regulates the flow of helium by use of an “open split” helium line. The helium enters the mass analyzer through a nipple on the ion trap mount.

Helium in the mass analyzer cavity dampens ionic motion and improves the performance of the MS detector. See [“Helium Damping Gas in the Mass Analyzer Cavity”](#) on [page 46](#).

## Sheath Gas, Auxiliary Gas, and Sweep Gas Valves

The *sheath gas, auxiliary gas, and sweep gas valves* control the flow of nitrogen into the API source. *Sheath gas* is nitrogen gas that flows through the inner coaxial of the API probe. The sheath gas converts the sample solution into a fine mist as the solution exits the sample tube. *Auxiliary gas* is the outer coaxial nitrogen gas that assists the sheath gas in the evaporation of the sample solution. *Sweep gas* flows out from behind the sweep cone in the ion source interface. The sweep gas aids in solvent declustering and adduct reduction.

Dry nitrogen ( $100 \pm 20$  psig [ $690 \pm 140$  kPa], 99% purity) enters the MS detector through a 1/4-in. port in the rear of the MS detector. The nitrogen pressure is regulated by valves that are controlled by the data system. You can set the flow rates from the Tune Plus window. Sheath gas is not used with an NSI source. The sheath gas, auxiliary gas, and sweep gas enter the API source through 1/4-in. ID tubing.

## Cooling Fans

Five fans provide cooling for the MS detector. One 100 ft.<sup>3</sup>/min. fan cools the RF voltage coil. One 21 ft.<sup>3</sup>/min. fan cools the turbomolecular pump. Three 100 ft.<sup>3</sup>/min. fans cool the electronics in the tower. Air is drawn in from the rear of the MS detector. The exhaust air is expelled from the vent slots on the sides of the MS detector.



**CAUTION** To ensure proper cooling, the MS detector must always be operated with its covers in place.

## Electronic Assemblies

The electronic assemblies that control the operation of the MS detector are distributed among various printed circuit boards (PCBs) and other modules located in the electronics rack and on or around the vacuum manifold of the MS detector.

The electronic assemblies of the MS detector include the following:

- Power Entry Module and power distribution assemblies
- System control and monitoring circuitry
- RF/waveform voltage generation electronic assemblies
- Ion detection system electronic assemblies

## Power Entry Module and Power Distribution

The *Power Entry Module* provides system power control, a contact closure interface, an Ethernet 100 Base T connection from the Power/Signal Distribution PCB to the data system PC, and a system reset button. See [Figure 13](#) on [page 36](#).

The Power Entry Module accepts line power, filters it, and provides it to various components of the MS detector. The Power Entry Module includes the following components:

- Main power circuit breaker switch
- Line filter
- Electronics service switch
- Interlock PCB

A functional block diagram of the Power Entry Module and MS detector power distribution is shown in [Figure 25](#).

Line power (230 V ac  $\pm$  10%, 15 A, 50/60 Hz, single phase) enters the power panel on the right side panel of the MS detector, passes through the main power circuit breaker and then to a line filter (see [Figure 13](#) on [page 36](#)).

The *main power circuit breaker switch*, located on the right side panel of the MS detector (see [Figure 13](#) on [page 36](#)), shuts off all power to the MS detector, including the vacuum system. After the main power circuit breaker switch, power goes to the line filter.

The *line filter* removes noise from the line power.

After the line filter, power goes to the Power/Signal Distribution PCB and to the electronics service switch.

The *electronics service switch* is a circuit breaker that allows service of the non-vacuum system components of the MS detector with the vacuum system still in operation (see [Figure 13](#) on [page 36](#)). In the Service position, the switch removes power to all components of the MS detector other than the fans and vacuum system. In the Electronics Normal position, power is supplied to all components of the MS detector.



**CAUTION** For emergency shutoff of all power to the MS detector, place the main power circuit breaker switch in the Off (O) position. Do not use the electronics service switch to remove power to the system in an emergency.



The *Interlock PCB*, which resides in the Power Module, receives 220 V ac from the electronics service switch (called *service 220 V ac*) and +24 V dc from PS2 power supply via the Power/Signal Distribution PCB. If the safety interlock switch on the API source is closed, then the Interlock PCB distributes 220 V ac to the APCI vaporizer heater and +24 V dc (called interlock +24 V dc) to the Power/Signal Distribution PCB, which distributes it to the 8 KV power supply and the conversion dynode/electron multiplier power supply.

The *Power/Signal Distribution PCB* receives 220 V ac and service 220 V ac from the Power Module. The Power/Signal Distribution PCB distributes the 220 V ac to power supply PS2 and the service 220 V ac to power supply PS1. It then distributes the power produced by PS1 and PS2 to other power supplies, PCBs, turbomolecular pump, vent valve, and fans. The Power/Signal Distribution PCB also receives the interlock +24 V dc from the Interlock PCB and distributes it to the 8 KV power supply and the conversion dynode/electron multiplier power supply.

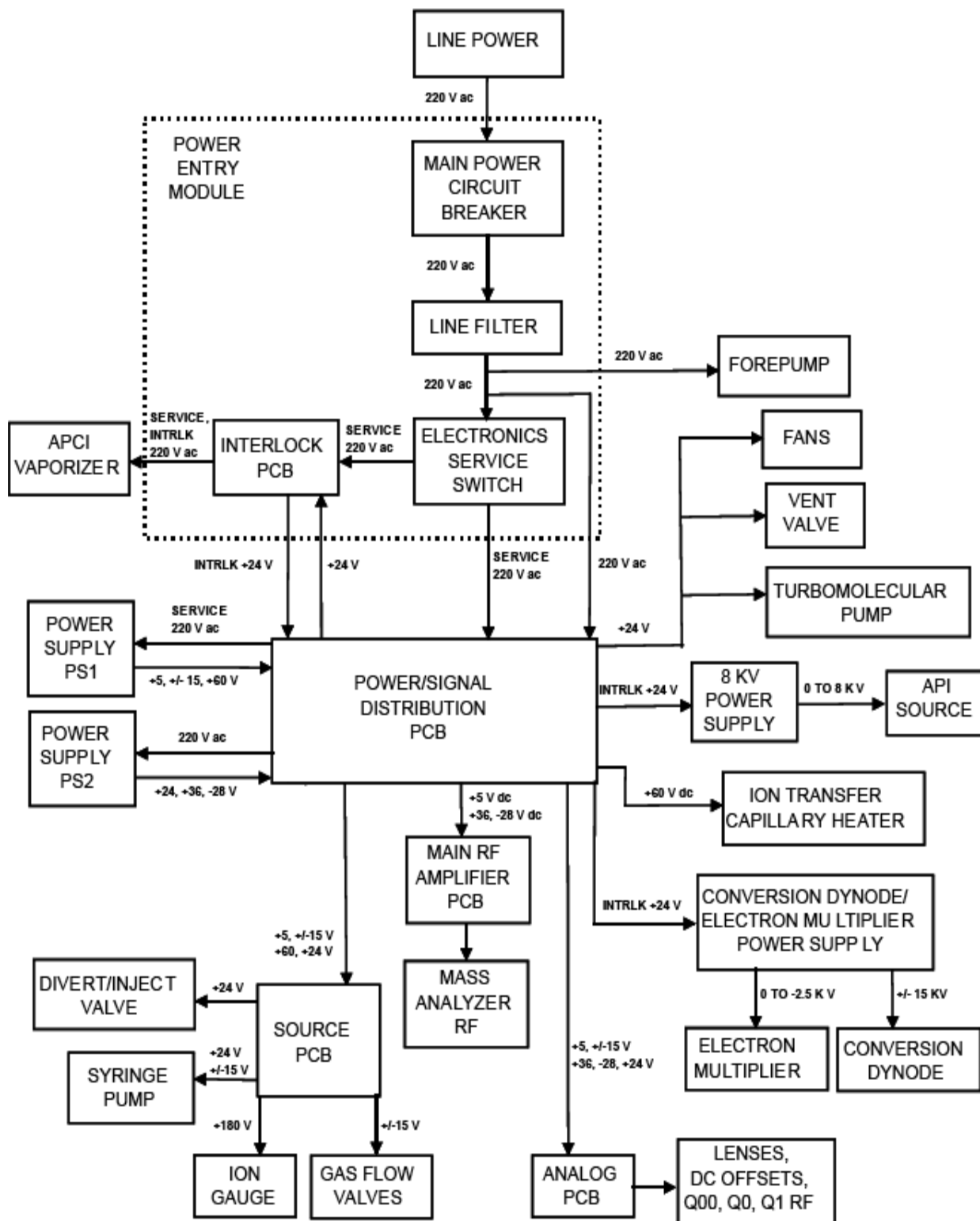
*Power supply PS1* provides +5 V dc,  $\pm 15$  V dc for analog and digital circuits and +60 V dc for the heater that heats the ion transfer capillary.

*Power supply PS2* provides +24 V dc for the turbomolecular pump, fans, vent valve, divert/inject valve, syringe pump, 8 KV power supply, conversion dynode/electron multiplier power supply, Main RF PCB, and Analog PCB. It also provides +36 V dc and -28 V dc that is used for RF generation for the ion guides and mass analyzer.

The *Source PCB* distributes power to the ion gauge, divert/inject valve, syringe pump and nitrogen gas valves.

The *8 kV power supply* delivers voltage to either the ESI needle in the ESI mode, or the corona discharge needle in the APCI mode. Typical operating voltages range between  $\pm 3$  to  $\pm 6$  kV. In the ESI mode, the voltage is regulated, whereas in the APCI mode, the current is regulated.

The *conversion dynode / electron multiplier power supply* provides  $\pm 15$  kV to the conversion dynode and 0 to -2.5 KV to the electron multiplier in the ion detection system.



**Figure 25.** Power Entry Module and power distribution of the MS detector (functional block diagram)

## System Control and Monitoring Circuitry

The LXQ electronics contains the following circuits for controlling and monitoring the operation of the MS detector:

- DC voltage control circuitry
- Divert/inject valve control circuit
- API source control circuit
- Electron multiplier control circuit
- Conversion dynode control circuit
- Ion transfer capillary heater/sensor control circuit
- APCI vaporizer heater/sensor control circuit/safety interlock relay
- Ion gauge control circuit
- Convectron® gauge control circuit
- Vacuum protection circuitry
- RF voltage control circuitry
- Temperature monitoring circuitry
- Diagnostic circuitry

The *dc voltage control circuitry* controls and monitors the dc voltages that are applied to the ion transfer capillary heater, tube lens, ion optics, lenses, and mass analyzer electrodes.

The *divert/inject valve control circuit* controls and monitors the divert/inject valve.

The *API source control circuit* controls and monitors the high voltage that is applied to the ESI needle, the APCI corona discharge needle, and the NSI capillary.

The *electron multiplier control circuit* sends a signal to the electron multiplier power supply that is proportional to the voltage to be applied to the electron multiplier cathode. It also reads back a signal that is proportional to the actual voltage applied to the electron multiplier cathode. The electron multiplier control circuit lowers the electron multiplier voltage when mass analysis is not occurring.

The *conversion dynode control circuit* controls and monitors the polarity of the 15 kV potential that is applied to the conversion dynode.

The *ion transfer capillary heater/sensor control circuit* monitors the temperature of the ion transfer capillary via a platinum probe temperature sensor. It also provides the voltage needed by the ion transfer capillary heater.

The *APCI vaporizer heater/sensor control circuit* controls the temperature of the APCI vaporizer via a thermocouple sensor. It also provides 230 V ac line voltage to the heater in the APCI vaporizer.

The *ion gauge control circuit* controls the ion gauge and reads back the pressure signal. (The ion gauge measures the pressure in the analyzer region of the vacuum manifold.)

The *Convectron gauge control circuit* controls the Convectron gauge and reads back the pressure signal. (The Convectron gauge measures the pressure in the foreline and the ion transfer capillary-skimmer region of the vacuum manifold.)

The *vacuum protection circuitry* monitors the pressure in the ion transfer capillary-skimmer region of the vacuum manifold, as measured by the Convectron gauge, and in the analyzer region of the vacuum manifold, as measured by the ion gauge. The vacuum protection circuitry turns off power to the ion optics and mass analyzer RF and waveform generation circuitry, 8 kV power supply (for the API source), electron multiplier and conversion dynode power supply, APCI vaporizer heater, and dc voltages to the ion transfer capillary heater, tube lens, ion optics, and mass analyzer if one or more of the following conditions arise:

- The pressure in the ion transfer capillary-skimmer region is above 3 Torr
- The pressure in the analyzer region is above  $5 \times 10^{-4}$  Torr
- The high-voltage safety interlock switch on the API source is open (that is, the API Probes have been removed)

The LED labeled *Vacuum* on the LXQ front panel is illuminated green when the vacuum protection circuitry detects adequate vacuum.

The *RF voltage control circuitry* controls and monitors the PCBs that are responsible for RF voltage generation.

The *temperature monitoring circuitry* monitors the temperatures at several PCBs in the MS detector.

The *diagnostic circuitry* monitors the outputs of various components and circuits on the LXQ. Information on voltages, currents, temperatures, flow rates, logic, etc. is sent to the data system, where it can be accessed via diagnostics views of Tune Plus.

### **RF / Waveform Voltage Generation Electronic Assemblies**

The *RF/waveform voltage generation electronic assemblies* produce the RF voltages for the mass analyzer, Q00 RF lens and Q0 quadrupole, and Q1 octapole. They also produce the ion isolation waveform voltage, resonance excitation RF voltage, and resonance ejection RF voltage that are applied to the exit rods of the mass analyzer.

The main RF voltage generation involves the following components:

- RF oscillator
- RF Voltage Amplifier PCB
- Low Pass Filter PCB
- RF voltage coil
- RF voltage detector
- Mass DAC
- Integrating amplifier

The *RF oscillator* on the Digital PCB provides a 1.2 MHz sine wave reference signal that it uses to produce the RF voltage.

The *RF Voltage Amplifier PCB* produces the RF primary voltage for the RF voltage coil. To produce the RF primary voltage, the RF Voltage Amplifier PCB takes the sine wave reference signal and amplifies it by an amount based on a 0 to 10 V dc RF modulation signal from the integrating amplifier.

The *Low Pass Filter PCB* removes second and third harmonics from the RF primary voltage.

The *RF voltage coil* amplifies the RF primary voltage to produce a secondary voltage of 0 to 10,000 V ac (zero to peak) that is supplied to the rods of the mass analyzer.

The *RF voltage detector* senses the 0 to 10,000 V RF voltage signal applied to the rods of the mass analyzer and converts this sensed signal into a 0 to -10 V dc output signal.

The *integrating amplifier* (also called an error amplifier) produces the 0 to 10 V dc RF modulation signal that is used by the RF Voltage Amplifier PCB. The magnitude of the RF modulation signal is proportional to the difference between the detected RF signal and the mass set signal requested by the *Mass DAC* (digital-to-analog converter). The integrating amplifier adjusts the RF modulation signal until the detected RF signal equals the requested RF signal.

The *Waveform AWG* (*arbitrary waveform generator*), which is part of the Digital PCB, provides the reference waveforms that are used to create the ion isolation waveform voltage, resonance excitation RF voltage, and resonance ejection RF voltage. The reference waveforms are amplified by a waveform amplifier on the Analog PCB.

The *embedded computer*, which is also part of the Digital PCB, is where the computations that are required to produce the waveforms take place.

### **Ion Detection System Electronic Assemblies**

The *ion detection system electronic assemblies* provide high voltage to the electron multiplier and conversion dynode of the ion detection system. The ion detection system electronic assemblies also receive the electron multiplier output current signal, convert it to a voltage (by the electrometer circuit), and pass it to the data system. A functional block diagram of the ion detection system electronic assemblies is shown in [Figure 26](#).

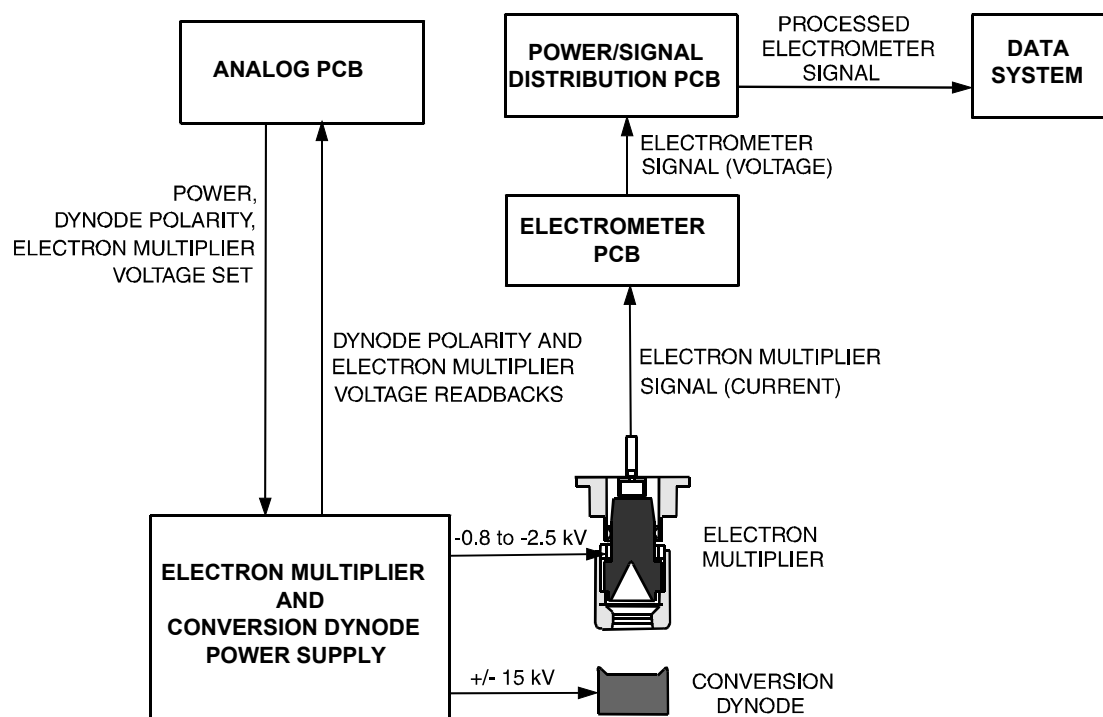
The ion detection system electronic assemblies include the following:

- Electron multiplier/conversion dynode power supply
- Electrometer circuit

The *electron multiplier/conversion dynode power supply* supplies the -0.8 kV to -2.5 kV dc high voltage to the cathode of the electron multiplier. The high voltage set control signal for the electron multiplier power supply comes from the Analog PCB. This signal controls a feedback control circuit and is proportional to the final high voltage to be applied to the electron multiplier cathode. The electron multiplier voltage is lowered by the Analog PCB during sample ionization to prolong the life of the electron multiplier.

The electron multiplier/conversion dynode power supply also supplies +15 kV and -15 kV dc high voltage to the conversion dynode. The polarity of the voltage applied to the conversion dynode is determined by a control signal from the Analog PCB.

The *electrometer circuit*, located in a shielded enclosure on the Electrometer PCB, receives the amplified ion current from the anode of the electron multiplier, converts the current into a voltage, and then integrates the voltage over time. The integrated voltage is then passed to the Power/Signal Distribution PCB where it is processed and sent to the data system.



**Figure 26.** Ion detection system electronic assemblies (functional block diagram)

## Data System

The *data system* controls and monitors the LXQ. The data system also processes data that is acquired by the LXQ. The data system is composed of the following:

- Computer hardware
- Data system/MS detector/LC interface
- Data system/local area network interface
- Printer (optional)

## Computer Hardware

The data system computer has the following major features:

- 1 Ghz Intel® Pentium® IV processor
- 1 GB of random access memory (RAM)
- High capacity hard disk drive
- Recordable/rewriteable CD drive
- Primary Ethernet adapter (data system to MS detector)
- Secondary Ethernet adapter (data system to local area network)
- 1.44-MB, 3.5-in. diskette drive
- Integrated video graphics card with 48 MB RAM
- 19-in., 1280 × 1024 resolution, flat panel LCD monitor
- Keyboard and mouse

For more information about the computer, refer to the manuals that come with the computer.

The minimum hardware and software requirements for the installation of Xcalibur 2.0 are:

- Intel Pentium IV 1 GHz processor
- 256 MB RAM for processing
- 256 MB RAM for acquisition
- 20 GB hard drive (NTFS) or more recommended
- CD-ROM drive



- Video card and monitor capable of 1280 × 1025 resolution and 65,536 colors
- Microsoft Windows XP
- Microsoft Office XP

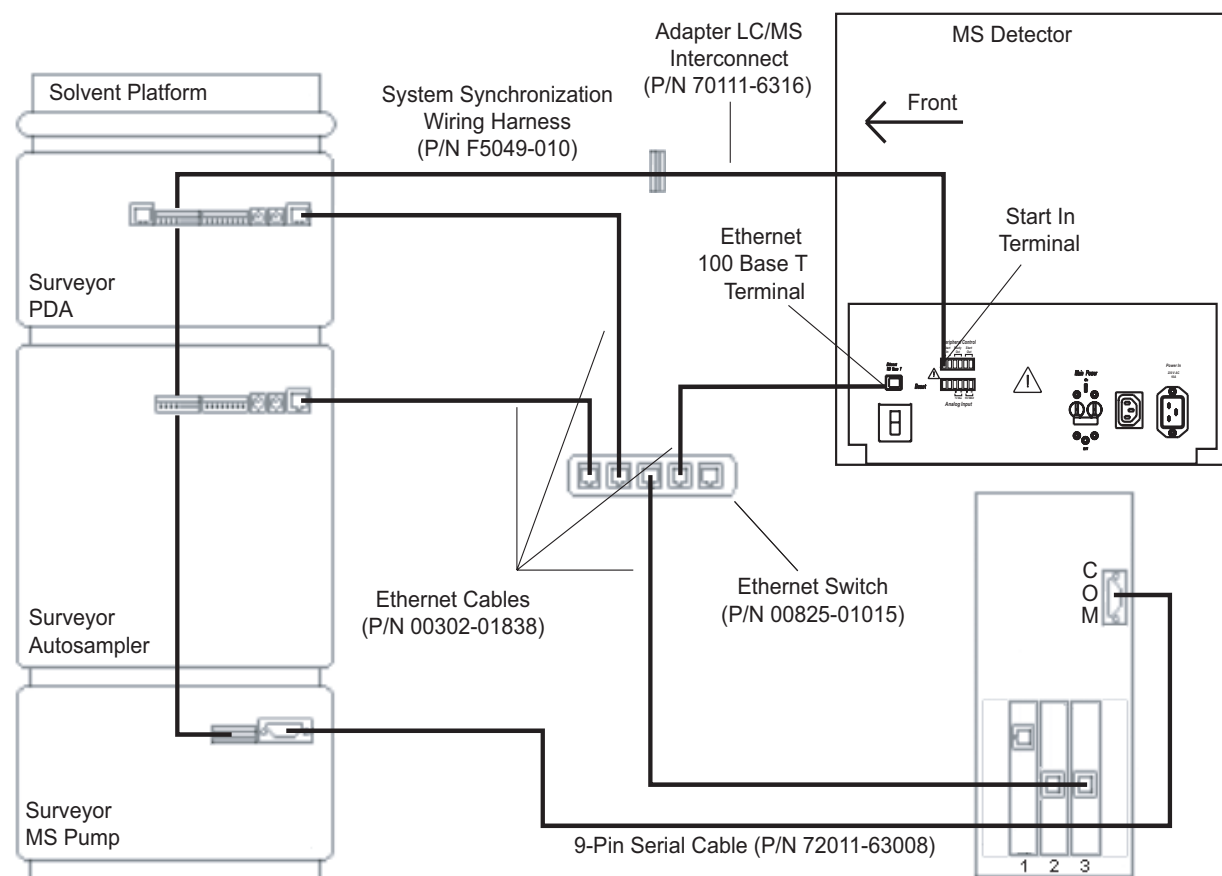
## **Data System / MS Detector / LC Interface**

The data system computer contains a 100 base T Ethernet adapter (called the primary Ethernet adapter) that is dedicated to data system/MS detector/LC communications. This primary Ethernet adapter communicates with the MS detector, autosampler, and PDA detector via a 10/100 base T Ethernet switch. The Ethernet adapter on the MS detector resides on the on the Digital PCB.

Communication between the data system and the MS pump is established by way of an RS232 connection. A synchronization cable assembly is used to coordinate the run control signals between the LC modules and the MS detector. Refer to **Finnigan LXQ Getting Connected** for information on connecting the LXQ with other LC modules.

## 2 Functional Description

### Data System



**Figure 27.** Surveyor LC system with an MS pump, LXQ MS detector, and data system computer (cable diagram)

### Data System / Local Area Network Interface

The data system computer contains a secondary Ethernet adapter. This secondary Ethernet adapter is not involved in data system/MS detector or LC communications. You can use this secondary Ethernet adapter to access your local area network.

### Printer

A high-resolution laser printer is available with the LXQ as an option. The printer communicates with the PC via the local area network. Refer to the manual supplied by the manufacturer for details about the printer.

Set up the printer from the Print Setup dialog box. To open the Print Setup dialog box, choose **File > Print Setup** in any window.

## Chapter 3 Daily Operation

This chapter outlines the checks and cleaning procedures of the LXQ system that should be performed every day to insure the proper operation of your system. It contains the following sections:

- [Before Operating the LXQ](#)
- [After Operating the LXQ](#)

**Note** You do not need to tune and calibrate the LXQ as part of your daily routine.

*Calibration parameters* are instrument parameters that affect the mass accuracy and resolution. *Tune parameters* are instrument parameters that affect the intensity of the ion signal. You need to tune and calibrate the LXQ (that is, optimize the tune and calibration parameters) perhaps once a quarter. See the *Automatic Tuning and Calibrating in the ESI/MS Mode* chapter in *Finnigan LXQ Getting Started* for a procedure for tuning and calibrating the LXQ. To check the tuning and calibration, follow the procedure described in the topic *Testing the Operation of the MS Detector in the ESI/MS Mode* in *Finnigan LXQ Getting Started*.

You need to optimize the tune parameters (or change the Tune Method) whenever you change the type of experiment. See the *Optimizing the MS Detector with Your Compound in ESI/MS Mode* or *Optimizing the MS Detector with Your Compound in APCI/MS Mode* chapter in *Finnigan LXQ Getting Started* for a procedure for optimizing the tune parameters for your ESI or APCI experiment.

## Before Operating the LXQ

The following checks should be performed every day before you begin your first analysis:

- [Check the Helium and Nitrogen Supplies](#)
- [Check the ESI Fused-Silica Sample Tube for Elongation](#)
- [Check the System Vacuum Levels](#)
- [Check the Disk Space](#)

### Check the Helium and Nitrogen Supplies

Check the helium supply on the regulator of the gas tank. Make sure that you have sufficient gas for your analysis. If necessary, install a new tank of helium. Verify that the pressure of helium reaching the MS detector is between 200 and 350 kPa (30 to 50 psig). If necessary, adjust the pressure with the tank pressure regulator.

Check the nitrogen supply on the regulator of the nitrogen gas tank or liquid nitrogen boil-off tank. Make sure that you have sufficient gas for your analysis. Typical nitrogen consumption is 100 cubic feet per day (nitrogen On 24 hours per day). If necessary, replace the tank. Verify that the pressure of nitrogen reaching the MS detector is between 550 and 830 kPa (80 to 120 psig). If necessary, adjust the pressure with the tank pressure regulator.

**Note** Before you begin normal operation each day, make sure that you have sufficient nitrogen for your API source. The presence of oxygen in the ion source when the MS detector is On could be unsafe. LXQ displays a popup message if the nitrogen pressure is too low.

### Check the ESI Fused-Silica Sample Tube for Elongation

Using acetonitrile in the mobile phase can cause elongation of the polyimide coating on the fused-silica sample tube. Elongation of the polyimide coating can degrade signal intensity and signal stability over time.

If you are running in ESI mode with a fused-silica sample tube, verify the sample tube is not elongated past the tip of the ESI spray needle.

#### **Cut and reposition the end of the sample tube 1 mm inside the end of the ESI needle**

1. Remove the ESI probe from the Ion Max ion source by following the procedure described in the section *Removing the ESI Probe* in the *Finnigan Ion Max API Source Hardware Manual*.

2. Loosen the sample inlet fitting.
3. Gently pull back on the sample tube to free it from the fitting.
4. Push the sample tube forward so that it extends beyond the end of the electrospray needle.
5. Use a fused-silica cutting tool to cut off a small length of sample tube. Ensure that you cut the end of the sample tube squarely.
6. Pull the sample tube backwards until the exit end of the sample tube is recessed just inside the ESI needle by approximately 1 mm.
7. Tighten the sample inlet fitting securely to hold the sample tube in place.

**Note** The sample tube might move forward when you tighten the sample inlet fitting. Ensure that the sample tube is retracted into the ESI needle approximately 1 mm. If necessary, loosen the fitting and reposition the sample tube.

8. Reinstall the ESI probe as described in the section *Installing the ESI Probe* in the *Finnigan Ion Max API Source Hardware Manual*.

## Check the System Vacuum Levels

For proper performance, your LXQ system must operate at the proper vacuum levels. Operation of the system with poor vacuum levels can cause reduced sensitivity, tuning problems, and reduced lifetime of the electron multiplier. You should check your system for air leaks by checking the system vacuum levels before you begin your first acquisition.

**Note** Major air leaks are often identifiable merely by listening for a rush of air or a hissing sound somewhere on the instrument. A major leak might be caused, for example, by a loose or disconnected fitting, by an O-ring that is not properly seated, or by an open valve.

You can check the current values of the pressures in the capillary-skimmer region and foreline (labeled *Convectron Gauge Pressure*) and in the analyzer region (labeled *Ion Gauge Press*) in the Vacuum dialog box of the Tune Plus window. To display the Tune Plus window choose **Start > Programs > Xcalibur > LXQ Tune**. Choose **Setup > Vacuum** to display the Vacuum dialog box.

Compare the current values of the pressures in the vacuum manifold with the values listed in Table 3-1. If the current values are higher than normal, you may have an air leak.

**Table 1.** Typical Pressure Readings

Conditions	Convectron gauge reading (foreline, capillary skimmer region)	Ion gauge reading (analyzer region)
Ion transfer capillary orifice open, ion transfer capillary at 250 °C	1.0 to 1.5 Torr	$0.75 \times 10^{-5}$ to $1.5 \times 10^{-5}$ Torr

If the pressure is high (above  $5 \times 10^{-5}$  Torr in the analyzer region), and you have restarted the system within the last 30 to 60 minutes, wait an additional 30 minutes and recheck the pressure. If the pressure is decreasing with time, check the pressure periodically until it is within the typical pressure range of the MS detector.

If the pressure remains high, your system may have an air leak. If you suspect an air leak, shut down the system as described in [Shutting Down the System Completely](#) on [page 131](#). Make a visual inspection of the vacuum system and vacuum lines for leaks. Check each fitting and flange on the system for tightness, and tighten the fittings or flanges that are loose. Do not tighten fittings indiscriminately. Pay particular attention to fittings that have been changed recently or to fittings that have been subjected to heating and cooling. Make sure that the cover plates of the vacuum manifold are properly seated.

## Check the Disk Space

Periodically you should verify that your hard disk drive has enough free space for data acquisition. The amount of available disk space is shown in the Disk Space dialog box.

### Determine the amount of available disk space

1. From the Home Page window (which is available by choosing **Start > Programs > Xcalibur > Xcalibur**), choose **Actions > Check Disk Space** to open the Disk Space dialog box. The Disk Space dialog box lists the following:
  - Current drive and directory  
(for example, C:\Xcalibur\system\programs)
  - Number of Mb that are available (free) on the current drive

- Percentage of the current drive that is available
  - Total capacity of the current drive
2. To select another disk drive so that you can determine its disk space, click **Directory**.
  3. When you have completed this procedure, choose **OK** to close the dialog box.

If necessary, you can free space on the hard disk by deleting obsolete files and by moving files from the hard disk drive to a backup medium. First, copy files to the backup medium. After you have copied the files, you can delete them from the hard disk.

## After Operating the LXQ

After operating the LXQ perform the following steps in sequence:

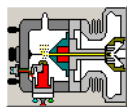
- Flush the Sample Transfer Line, Sample Tube, and API Probe
- Place the System in Standby Condition
- Flush the Ion Sweep Cone and Ion Transfer Capillary
- Purge the Oil in the Rotary-Vane Pump
- Empty the Solvent Waste Bottle

### Flush the Sample Transfer Line, Sample Tube, and API Probe

You should flush the sample transfer line, sample tube, and API probe at the end of each working day (or more often if you suspect they are contaminated) by flowing a 50:50 methanol:distilled water solution from the LC through the API source.

To flush the sample transfer line, sample tube, and API probe, proceed as follows:

1. Wait until data acquisition, if any, is complete.
2. Make sure that the lid to the API chamber is closed and secured.
3. Choose **Start > Programs > Xcalibur > LXQ Tune** to open the LXQ Tune Plus window.
4. From the Tune Plus window, choose **Control > On** (or click on the On/Standby button to toggle it to On) to turn on the voltages and gas flows to the API source.
  - If you are operating in APCI or APPI mode, go to step 5.
  - If you are operating in ESI mode, go to step 6.
5. Set up the APCI source as follows.
  - a. In the LXQ Tune Plus window, choose **Setup > APCI Source** to (or click on the APCI source button) to display the APCI Source dialog box.
  - b. Set the APCI vaporizer temperature to 500 °C. In the APCI Source dialog box, enter **500** in the Vaporizer Temperature text box.

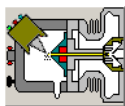




- c. Set the sheath gas flow rate to 30.  
In the APCI Source dialog box, enter **30** in the Sheath Gas Flow Rate text box.
- d. Set the auxiliary gas flow rate to 5.  
In the APCI Source dialog box, enter **5** in the Aux Gas Flow Rate text box.
- e. Set the sweep gas flow rate to 0.  
In the APCI Source dialog box, enter **0** in the Sweep Gas Flow Rate text box.
- f. Set the APCI spray current to 0.  
In the APCI Source dialog box, enter **0** in the Spray Current text box.
- g. Click **OK**.

Go to step 7.

6. Set up the ESI source as follows.





- a. In the LXQ Tune Plus window, choose **Setup > ESI Source** to (or click on the ESI source button) to display the ESI Source dialog box.
- b. Set the sheath gas flow rate to 30.  
In the ESI Source dialog box, enter **30** in the Sheath Gas Flow Rate text box.
- c. Set the auxiliary gas flow rate to 5.  
In the ESI Source dialog box, enter **5** in the Aux Gas Flow Rate text box.
- d. Set the sweep gas flow rate to 0.  
In the ESI Source dialog box, enter **0** in the Sweep Gas Flow Rate text box.
- e. Set the ESI spray voltage to 0.  
In the ESI Source dialog box, enter **0** in the Spray Voltage text box.
- f. Click **OK**.

7. Set up and start a flow of 50:50 methanol:water solution from the LC to the API source, as follows:



- a. In the LXQ Tune Plus window, choose **Setup > Inlet Direct Control** (or click **AS/LC direct control**). The Inlet Direct Control view appears.
- b. Select the LC tab.
- c. Set the Flow Rate to a value that is typical for your experiments.

- d. Set the solvent proportions to 50% methanol and water.
  - e. Click  (or **Pump On** or **Start Pump**) to start the LC pump.
8. Let the solution flow through the sample transfer line, sample tube, and API probe for 15 min. After 15 min, turn off the flow of liquid from the LC to the API source, as follows. Leave the API source (including the APCI vaporizer, sheath gas, and auxiliary gas) on for an additional 5 min. Click  (or **Pump Off** or **Stop Pump**) to stop the LC pump.
  9. After 5 min, turn off the API source by placing the MS detector in Standby: From the LXQ Tune Plus window, choose **Control > Standby** (or click **On/Standby**) to put the MS detector in Standby.

## Place the System in Standby Condition




Use the following procedure to place the LXQ system in the standby condition:

1. From the LXQ Tune Plus window, choose **Control > Standby** (or click **On/Standby**) to put the MS detector in Standby. The System LED on the front panel of the MS detector is illuminated yellow when the system is in Standby.
2. Leave the MS detector power On.
3. Leave the LC power On.
4. Leave the autosampler power On.
5. Leave the data system power On.

## Flush the Ion Sweep Cone and Ion Transfer Capillary

You need to clean the ion sweep cone (or spray cone) and the ion transfer capillary on a regular basis to prevent corrosion and to maintain optimum performance of your API source. A good practice is to flush the ion sweep cone and ion transfer capillary at the end of each operating day after you flush the sample transfer line, sample tube, and API probe with a 50:50 methanol:water solution from the LC (see [Flush the Sample Transfer Line, Sample Tube, and API Probe](#) on [page 76](#).) If you are operating the system with nonvolatile buffers in your solvent system or high concentrations of sample, you might need to clean the ion sweep cone and ion transfer capillary more often. It is not necessary to vent the system to flush the ion sweep cone and ion transfer capillary.

## To clean the ion sweep cone and the ion transfer capillary

1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source. To turn off the flow of liquid from the LC to the API source:
  - a. Choose **Start > Programs > Xcalibur > LXQ Tune** to open the LXQ Tune Plus window.
  - b. In the LXQ Tune Plus window, choose **Setup > Inlet Direct Control** (or click **AS/LC direct control**). The Inlet Direct Control view appears.
  - c. Select the LC tab and click  (or **Pump Off** or **Stop Pump**) to stop the LC pump.
2. From the LXQ Tune Plus window, choose **Control > Standby** (or click **On/Standby**) to put the MS detector in Standby.



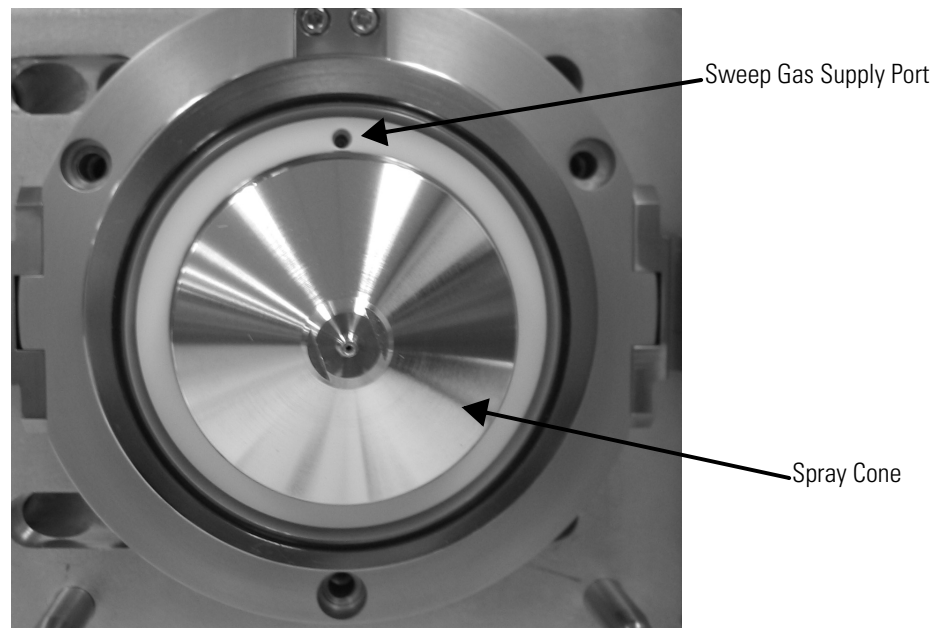
**CAUTION AVOID BURNS.** At operating temperatures, the APCI vaporizer and ion transfer capillary can severely burn you! The APCI vaporizer typically operates at 400 to 600 °C and the ion transfer capillary typically operates at 100 to 300 °C. Allow the vaporizer and ion transfer capillary to cool for approximately 20 min. to room temperature before you touch or remove either component.

3. Remove the Ion Max ion source from the front of the MS detector as described in the topic **Removing the Ion Max Ion Source Housing** on page 4-12.
4. Fill a spray bottle with a 50:50 solution of HPLC-grade methanol:distilled water. Spray approximately 5 mL of the solution at the opening of the ion transfer capillary. Do not touch the ion transfer capillary with the tip of the spray bottle.
5. Use the spray bottle filled with the 50:50 solution of methanol:water to flush contaminants from the accessible surfaces of the ion source chamber and the spray cone or ion sweep cone (if installed).
6. Ensure that you have removed any salt or other contaminants that may have been deposited on the ion sweep cone or spray cone.
7. Remove the ion sweep cone (if it is installed) as follows:
  - a. Put on a pair of talc-free gloves.

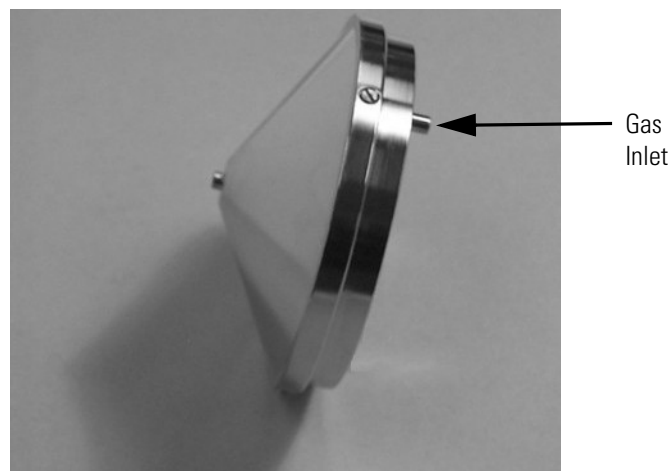
- i. Grasp the outer ridges of the ion sweep cone and pull the cone straight off of the API cone seal. Note, you might need to loosen the set screws on the ion sweep cone in order to remove it.

**Note** This is a good point to remove and clean the ion transfer capillary. You remove the ion transfer capillary by unscrewing it counter clockwise with the custom removal tool. See [Removing and Cleaning the Ion Transfer Capillary](#) on page 89.

- b. Clean the ion sweep cone as follows:
  - i. Place the ion sweep cone and the ion capillary tube in a beaker of 50:50 methanol/water.
  - ii. Sonicate it for 15 min.
  - iii. Dry the ion sweep cone.
- c. Clean the spray cone with a Kimwipe soaked in methanol.
- d. Reinstall the ion sweep cone as follows:
  - i. Note the location of the sweep gas supply port in the API cone seal. The gas inlet on the ion sweep cone is placed in this port. See [Figure 28](#) and [Figure 29](#).
  - ii. Carefully align the gas inlet on the ion sweep cone with the sweep gas supply port in the API cone seal. Firmly press the ion sweep cone into position.
  - iii. If necessary to achieve a proper ion sweep cone installation, adjust the set screws around the perimeter of the ion sweep cone.



**Figure 28.** Sweep gas supply port in the API cone seal




**Figure 29.** Ion sweep cone, showing the gas inlet

- e. Reinstall the Ion Max ion source as described in the topic [Reinstalling the Ion Max Ion Source Housing](#) on [page 101](#).

## Purge the Oil in the Rotary-Vane Pump

You need to purge (decontaminate) the oil in the rotary-vane pump on a daily basis to remove water and other dissolved chemicals from the pump oil. Water and other chemicals in the rotary-vane pump can cause corrosion and decrease the lifetime of the pump. A good time to purge the oil is at the end of the working day after you flush the API probe, ion sweep cone, and ion transfer capillary.

### To purge the oil in the rotary-vane pump

1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source. To turn off the flow of liquid from the LC to the API source:
  - a. Choose **Start > Programs > Xcalibur > LXQ Tune** to open the LXQ Tune Plus window.
  - b. In the LXQ Tune Plus window, choose **Setup > Inlet Direct Control** (or click on the AS/LC direct control button). The Inlet Direct Control view appears.
  - c. Select the LC tab and click  (or **Pump Off** or **Stop Pump**) to stop the LC pump.
2. From the LXQ Tune Plus window, choose **Control > Standby** (or **On/Standby**) to put the MS detector in Standby. Ensure that a septum seals the entrance to the ion transfer capillary.
3. Open the gas ballast valve on the rotary-vane pump by turning it to position |. Refer to the manual that came with the pump for the location of the gas ballast valve.
4. Allow the pump to run for 30 min with the gas ballast valve open.
5. After 30 min, close the gas ballast valve by turning it to position O.



On Standby



## Empty the Solvent Waste Bottle

The solvent level in the solvent waste bottle should be checked on a daily basis. If necessary, empty the solvent waste bottle. Dispose of the solvent waste in accordance with local and national regulations.

## Chapter 4 MS Detector Maintenance

LXQ performance depends on the maintenance of all parts of the instrument. **It is your responsibility to maintain your system properly by performing the system maintenance procedures on a regular basis.**

This chapter describes routine MS detector maintenance procedures that must be performed to ensure optimum performance of the instrument. Most of the procedures involve cleaning. Maintenance procedures include cleaning the API source, ion guides, mass analyzer, and ion detection system. Procedures are also provided for replacing the API sample tube, ion transfer capillary, and API source, ion optics, and mass analyzer assemblies.

This chapter contains the following sections:

- [Tools and Supplies](#)
- [Frequency of Cleaning](#)
- [API Source Maintenance](#)
- [Cleaning the Q00-L0 RF Lens](#)
- [Cleaning the Q0 and Q1 Ion Guides](#)
- [Maintaining the Mass Analyzer](#)
- [Replacing the Electron Multiplier](#)
- [Replacing the Turbomolecular Pump Cartridge](#)
- [Cleaning the Fan Filter](#)

MS detector maintenance procedures are listed in [Table 2](#).

**Table 2.** MS detector maintenance procedures

MS Detector Component	Procedure	Frequency	Procedure Location
API source	Flush (clean) sample transfer line, sample tube, and API probe	Daily	Page 3-6
Ion source interface	Flush (clean) ion sweep cone and ion transfer capillary	Daily (or more often <sup>1</sup> )	Page 3-8
Rotary-vane pump	Purge (decontaminate) oil	Daily	Page 3-11
Ion source interface	Remove and clean ion transfer capillary	Weekly, or if ion transfer capillary bore is contaminated or obstructed	Page 4-89
PhotoMate light source	Clean or polish VUV lamp window	If VUV lamp window is dirty	Finnigan Ion Max API Source Hardware Manual
Ion source interface	Clean tube lens and skimmer	As needed <sup>1</sup>	Page 4-95
Cooling fans	Clean fan filters	Every 4 months	Page 4-125
Q00 RF lens	Clean Q00 RF lens and lens L0	As needed <sup>1</sup>	Page 4-104
ESI probe	Trim sample tube	If polyimide coating on the end of the sample tube has elongated	Page 3-3
APCI or ESI probe	Replace sample tube	If sample tube is broken or obstructed	Finnigan Ion Max API Source Hardware Manual
Ion source interface	Replace ion transfer capillary	If ion transfer capillary bore is corroded	Finnigan Ion Max API Source Hardware Manual
PhotoMate light source	Replace VUV lamp	If lamp fails	Finnigan Ion Max API Source Hardware Manual
Q0 ion guide	Clean Q0 quadrupole and intermultiple lens L1 <sup>2</sup>	As needed <sup>1</sup>	Page 4-110
Q1 ion guide	Clean Q1 octapole and gate lens <sup>2</sup>	As needed <sup>1</sup>	Page 4-110
Ion detection system	Clean ion detection system (electron multiplier and conversion dynode)	Whenever the top cover plate of the vacuum manifold is removed	Page 4-117
Mass analyzer	Clean mass analyzer <sup>2</sup>	Very rarely (if ever) <sup>1</sup>	Page 4-120
Rotary-vane pump	Add oil	If oil level is low	Manufacturer's documentation
Rotary-vane pump	Change oil	Every 3 months or if oil is cloudy or discolored	Manufacturer's documentation
Ion detection system	Replace electron multiplier assembly <sup>2</sup>	If noise in spectrum is excessive or proper electron multiplier gain can not be achieved	Page 4-121
Turbomolecular pump	Replace turbomolecular pump insert <sup>2</sup>	Every 20,000 to 30,000 hours or if bearings fail	Page 4-124



**Table 2.** MS detector maintenance procedures, continued

MS Detector Component	Procedure	Frequency	Procedure Location
Electronic modules	Replace electronic module <sup>2</sup>	If electronic module fails	<b>Diagnostics and PCB and Assembly Replacement</b> chapter
PCBs	Replace PCB <sup>2</sup>	If PCB fails	<b>Diagnostics and PCB and Assembly Replacement</b> chapter
<sup>1</sup> Frequency depends on analytical conditions			
<sup>2</sup> We recommend that this maintenance procedure be performed by a Thermo Electron Field Service Engineer			

For instructions on maintaining LCs or autosamplers, refer to the manual that comes with the LC or autosampler.

**Note** When following the procedures in this chapter,

- Proceed methodically.
- Always wear clean, lint-free gloves when handling the components of the API source, ion guides, mass analyzer, and ion detection system.
- Always place the components on a clean, lint-free surface.
- Never overtighten a screw or use excessive force.

## Tools and Supplies

The LXQ requires very few tools to perform routine maintenance procedures. You can remove and disassemble many of the components by hand. The tools, equipment, and chemicals listed in [Table 3](#) are needed for the maintenance of the API source, ion guides, mass analyzer, and ion detection system.

**Table 3.** Tools, equipment, and chemicals

Description	Part Number
Screwdrivers, set, ball point, Allen (also referred to as ball drivers)	00025-03025
Hex ball Driver, 3/16-in.	00025-01700
Hex ball Driver, 7/64-in.	00025-01800
Hex ball driver, 5/16-in., 9.5 in. long	00025-10015
Hex ball driver, 5/32, 7.4 in. long	00025-10020
Ion transfer capillary removal tool	70111-20258
Screwdriver, slot head, large	
Screwdriver, slot head, small	
Screwdriver, Phillips, small	
Fused-silica cutting tool	
Spray bottle	
Beaker, 450 mL	
Gloves, nylon	00301-09700
Kimwipes or other lint-free industrial tissue	
Applicators (swabs), cotton-tipped	00301-02000
Detergent	
Clean, dry, compressed nitrogen gas	
Distilled water	
Methanol, HPLC grade or better	
Nitric acid, dilute	



**CAUTION** As with all chemicals, solvents and reagents should be stored and handled according to standard safety procedures and disposed of according to applicable local and national regulations.

## Frequency of Cleaning

The frequency of cleaning the components of the MS detector depends on the types and amounts of samples and solvents that are introduced into the instrument. In general, for a given sample and ionization technique, the closer a MS detector component is to the source of the ions, the more rapidly it becomes dirty.

- The sample tube, API probe, ion transfer capillary bore, and ion sweep cone of the API source should be cleaned at the end of each operating day to remove any residual salts from buffered mobile phases or other contamination that might have accumulated during normal operation. See [Flushing the Sample Transfer Line, Sample Tube, and API Probe on page 88](#) and [Flushing the Ion Sweep Cone and Ion Transfer Capillary on page 88](#).
- The tube lens and skimmer of the Q00 RF lens become dirty at a slower rate than the API probe, ion sweep cone, and ion transfer capillary. The Q00 RF lens and lens L0 require cleaning less often than the tube lens and skimmer. See [Cleaning the Q00-L0 RF Lens on page 104](#).
- The Q0 quadrupole, Q1 octapole, and lenses of the Q0 and Q1 ion guides become dirty at a rate significantly slower than the API source and Q00 RF lens. See [Cleaning the Q0 and Q1 Ion Guides on page 110](#).
- The rods of the mass analyzer require cleaning very rarely (if ever). See [Maintaining the Mass Analyzer on page 120](#).
- Clean the electron multiplier and conversion dynode whenever you remove the top cover plate of the vacuum manifold by blowing them with a clean, dry gas. See [Cleaning the Ion Detection System on page 117](#).

When the performance of your system decreases significantly due to contamination, clean the components of the MS detector in the following order:

1. Clean the API probe, ion sweep cone (if installed), spray cone, and ion transfer capillary
2. Clean the tube lens and skimmer
3. Clean the quadrupole and lens of the Q00 RF lens
4. Clean the quadrupole and lens of the Q0 ion guide and the octapole and lens of the Q1 ion guide
5. Clean the mass analyzer

## API Source Maintenance

The API source requires a minimum of maintenance. Periodically, you need to clean the components of the API source to remove salts or other contaminants. The frequency of cleaning the API source depends on the types and amounts of samples and solvents that are introduced into the instrument.

Maintenance procedures are provided for the following:

- Flush the sample transfer line, sample tube, and API probe
- Flush the ion sweep cone (or spray cone) and the bore of the ion transfer capillary
- Remove and clean the ion transfer capillary
- Maintain the API probes, including replacing the sample tube
- Maintain the PhotoMate light source, including replacing the VUV lamp
- Maintain the ion source interface, including replacing the ion transfer capillary and heater



**CAUTION AVOID EXPOSURE TO POTENTIALLY HARMFUL MATERIALS.** Always wear protective gloves and safety glasses when you use solvents or corrosives. Also, contain waste streams and use proper ventilation. Refer to your supplier's Material Safety Data Sheets (MSDS) for procedures that describe how to handle a particular solvent.

### Flushing the Sample Transfer Line, Sample Tube, and API Probe

You should flush the sample transfer line, sample tube, and API probe at the end of each working day (or more often if you suspect they are contaminated) by flowing a 50:50 methanol:distilled water solution from the LC through the API source.

To flush the sample transfer line, sample tube, and API probe, follow the procedure described in [Flush the Sample Transfer Line, Sample Tube, and API Probe](#) on [page 76](#).

### Flushing the Ion Sweep Cone and Ion Transfer Capillary

You need to clean the ion sweep cone (or the spray cone, if the ion sweep cone is not installed) and the ion transfer capillary on a regular basis to prevent corrosion and to maintain optimum performance of your API source. A good practice is to flush the ion sweep cone and ion transfer capillary at the end of each operating day after you flush the sample transfer line, sample tube, and API probe with a 50:50 methanol:water solution


from the LC. To clean the ion sweep cone and the ion transfer capillary follow the procedure described in [Flush the Ion Sweep Cone and Ion Transfer Capillary](#) on page 78.

## Removing and Cleaning the Ion Transfer Capillary

The bore of the ion transfer capillary can become blocked by buffer salts or high concentrations of sample. The ion transfer capillary can be easily removed for cleaning. You do not have to vent the system to remove the ion transfer capillary.

If the pressure in the ion transfer capillary-skimmer region (as measured by the convectron gauge) drops considerably below 1 Torr, you should suspect a blocked ion transfer capillary. You can check the Convectron gauge pressure in the Vacuum dialog box of the Tune Plus window. To display the Tune Plus window choose **Start > Programs > Xcalibur > LXQ Tune**. Choose **Setup > Vacuum** to display the Vacuum dialog box.

To remove and clean the ion transfer capillary, do the following:

1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source. To turn off the flow of liquid from the LC to the API source, do the following:
  - a. Choose **Start > Programs > Xcalibur > LXQ Tune** to open the Tune Plus window.
  - b. In the LXQ Tune Plus window, choose **Setup > Inlet Direct Control** (or click **AS/LC direct control**). The Inlet Direct Control view appears.
  - c. Select the LC tab and click  (or **Stop Pump** or **Pump Off**) to stop the LC pump.
2. Place the electronics service switch (located on the right side of the MS detector) in the Service position to turn off the non-vacuum system voltages.



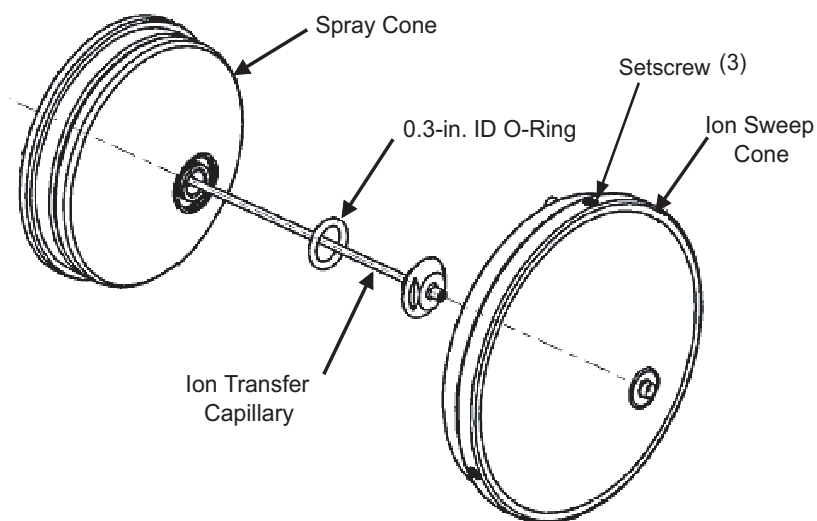
**CAUTION** Make sure that the LXQ electronics service switch is in the Service position before you proceed.

3. Remove the Ion Max ion source housing from the front of the MS detector as described in the topic [Removing the Ion Max Ion Source Housing](#) on [page 93](#).



**CAUTION** The ion transfer capillary typically operates at 250 to 400 °C. Allow the ion transfer capillary and ion sweep cone to cool before you remove them.

4. Remove the ion sweep cone by grasping its outer ridges and pulling the cone straight off of the API cone seal. Note, you might need to loosen the set screws on the ion sweep cone in order to remove it. See [Figure 30](#).
5. Remove the ion transfer capillary (P/N 97055-20198) by turning it counterclockwise with the custom removal tool (P/N 70111-20258) until you can pull it free from the ion source interface.
6. Soak the ion transfer capillary in a dilute solution of nitric acid to remove contaminants.
7. Sonicate the ion transfer capillary in distilled water.
8. Clean the ion sweep cone by wiping the inside and outside with methanol and a Kimwipe.
9. Remove, clean with methanol, and inspect the 0.3-in. ID Kalrez<sup>®</sup> O-ring (P/N 00107-12750) that seats in the spray cone under the entrance end of the ion transfer capillary. Replace it if necessary.



**Figure 30.** Ion sweep cone, ion transfer capillary, O-ring, and spray cone of the ion source interface

10. Reseat the O-ring in the spray cone.



**CAUTION** Be careful not to bend the ion transfer capillary. Rotate the capillary as you insert it.

11. Insert the ion transfer capillary into the heater block. Rotate the capillary as you insert it. Once inserted, turn the capillary clockwise until it is finger tight.
12. Reinstall the ion sweep cone on the ion source interface.
13. Reinstall the Ion Max ion source housing on the MS detector as described in the topic [Reinstalling the Ion Max Ion Source Housing](#) on [page 101](#).

**Note** If you have unblocked the ion transfer capillary, the Convectron gauge pressure should increase to a normal value (approximately 1 Torr). If you cannot clear the ion transfer capillary by this method, replace the ion transfer capillary.

14. Place the electronics service switch in the Electronics Normal position to turn on the non-vacuum system voltages.

## Maintaining the API Probes

The API probes of the Ion Max ion source requires a minimum of maintenance. If the sample tube becomes obstructed with salt precipitates or is broken, you need to replace it. Also, you may need to disassemble an API probe so you can clean it or to replace a part.

See the *Finnigan Ion Max API Source Hardware Manual* for procedures for maintaining the API probes.

**Note** You should flush the API probe at the end of each working day by flowing a 50:50 HPCL-grade methanol:distilled water solution from the LC through the APCI probe. See [Flushing the Sample Transfer Line, Sample Tube, and API Probe](#) on page 88.

## Maintaining the PhotoMate Light Source

Maintaining the PhotoMate light source involves the following:

- Cleaning and polishing the VUV lamp
- Replacing the VUV lamp

Refer to *Maintaining the APPI Probe* in the *Finnigan Ion Max API Source Hardware Manual* for procedures for maintaining the APPI probe.

## Maintaining the Ion Source Interface

The ion source interface includes the ion sweep cone, ion transfer capillary, capillary heater, tube lens, and skimmer. The ion transfer capillary has a finite lifetime. You need to replace the ion transfer capillary if the ion transfer capillary bore becomes corroded.

You should flush the ion sweep cone and the bore of the ion transfer capillary at the end of each working day with a 50:50 methanol:water solution. See [Flushing the Ion Sweep Cone and Ion Transfer Capillary](#) on page 88.

The ion transfer capillary can be easily removed for cleaning or replacement without venting the system. Refer to the topic [Removing and Cleaning the Ion Transfer Capillary](#) on page 89.

To access the tube lens and skimmer for cleaning or to replace ion source interface components other than the ion transfer capillary and ion sweep cone:



- Shut down and vent the system
- Remove the Ion Max ion source housing
- Remove the ion source interface
- Clean or replace ion source interface components
- Reinstall the ion source interface
- Reinstall the Ion Max ion source
- Start up the system

### **Shutting Down the System**

Shut down and vent the system as described in the topic [Shutting Down the System Completely](#) on [page 131](#). Wait several minutes for the LXQ to vent.

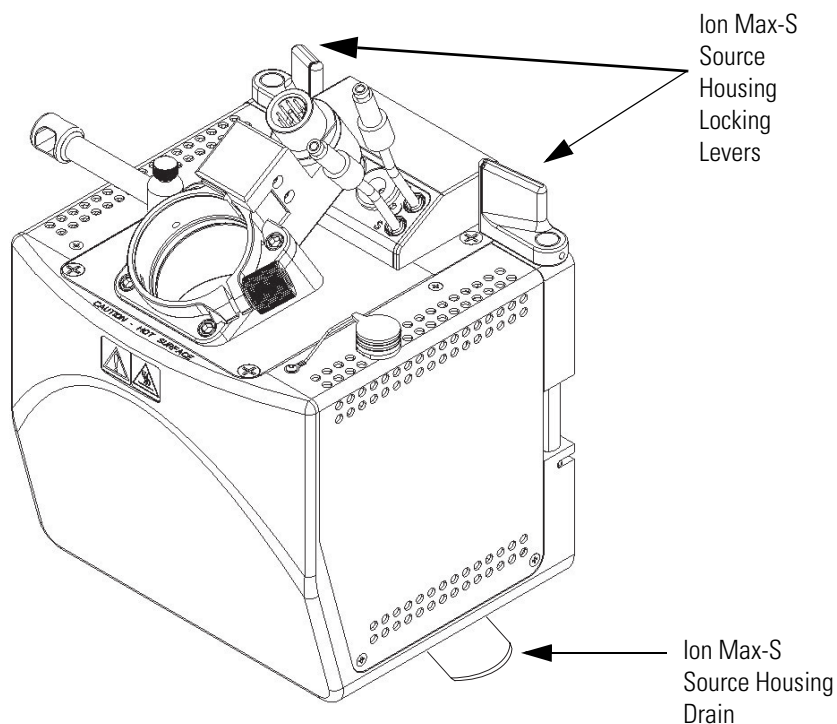
### **Removing the Ion Max Ion Source Housing**

You need to remove the Ion Max ion source to access the ion source interface and Q00 RF lens.

**Note** If an ion source probe is still installed in the ion source housing, the external liquid lines should first be disconnected before removing the ion source housing.

### **To remove the Ion Max ion source housing**

1. Remove the drain tube from the ion source housing drain. See [Figure 31](#).



**Figure 31.** Ion Max-S ion source, showing the locking levers and drain

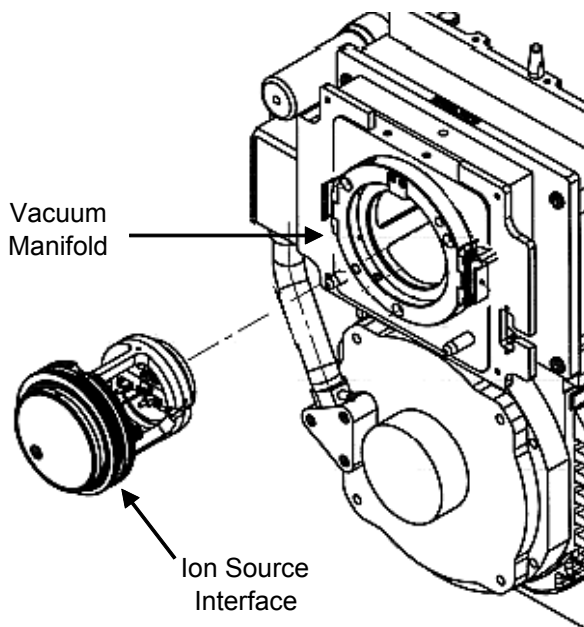
2. Rotate the ion source housing locking levers 90° to release the ion source housing from the ion source mount assembly.
3. Remove the ion source housing by pulling straight off of the ion source mount assembly, and place the housing in a safe location for temporary storage.

### Removing the Ion Source Interface

To remove the ion source interface, grasp the ridges on either side of the ion source interface and carefully pull it free from the vacuum manifold. Place it on a clean surface. Observe the following caution before performing this procedure.



**CAUTION** Make sure that the LXQ power cord is unplugged before you proceed.



**Figure 32.** Ion source interface removal

### Cleaning the Tube Lens and Skimmer

An accumulation of chemicals on the surfaces of the tube lens and skimmer forms an insulating layer that can modify the electrical fields that control ion transmission. The tube lens and skimmer require cleaning less often than the ion sweep cone and the ion transfer capillary.

#### To clean the tube lens and skimmer



**CAUTION** Wait for the ion source interface to cool to ambient temperature before disassembling it.

**Note** Wear clean gloves when you handle the tube lens and skimmer.

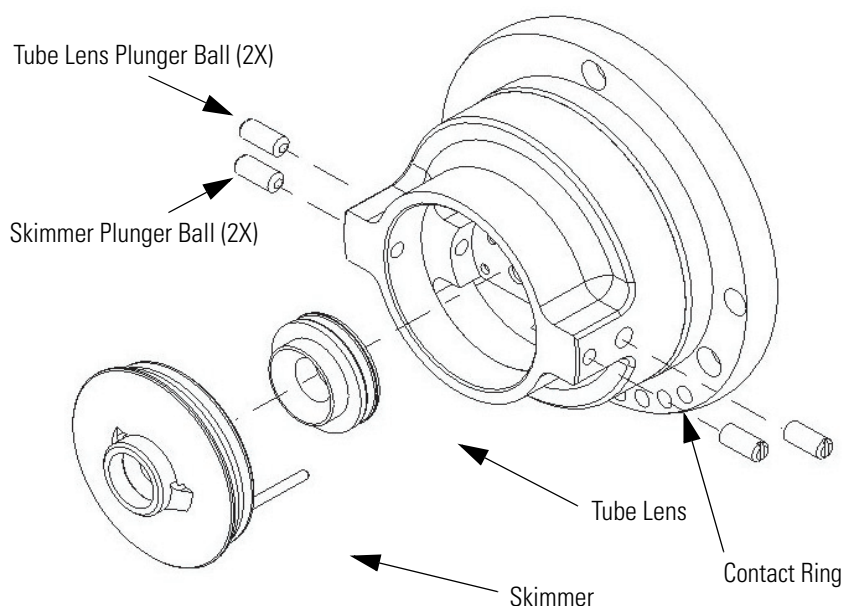


**CAUTION** Take care not to scratch or nick the skimmer cone.

1. Remove the skimmer by carefully pulling it free from the rear of the ion source interface. Note the orientation of the skimmer.
2. Remove the tube lens by carefully pulling it free from the rear of the ion source interface. Note the orientation of the tube lens.

**Note** For most cleaning applications, HPLC grade methanol is the solvent of choice. However, use of buffers or salt solutions may require that you use an acidic, aqueous solution. If you need to use a solvent other than methanol, after cleaning the component, flush the component with distilled water and then flush it with methanol as a final wash. In all cases, ensure that all solvent has evaporated from the component(s) before reassembly.

3. Clean the tube lens inside and out with HPLC-grade methanol and a cotton-tipped applicator (swab).
4. Clean the skimmer inside and out with HPLC-grade methanol and a cotton-tipped applicator (swab).



**Figure 33.** Rear of the ion source interface showing the tube lens and skimmer

5. Reinstall the tube lens in the ion source interface:
  - a. Orient the tube lens such that the lead pin points toward the socket.
  - b. Push the tube lens until it snaps into place.



**CAUTION** Take care not to scratch or nick the skimmer cone.

6. Reinstall the skimmer in the ion source interface:
  - a. Orient the skimmer such that the lead pin points toward the socket.
  - b. Push the skimmer until it snaps into place.

**Note** There are no leads to connect to the tube lens and skimmer.

## Replacing Ion Source Interface Components



Use the following procedure when replacing the Ion Source Interface components. The capillary heater assembly must be replaced as a unit.

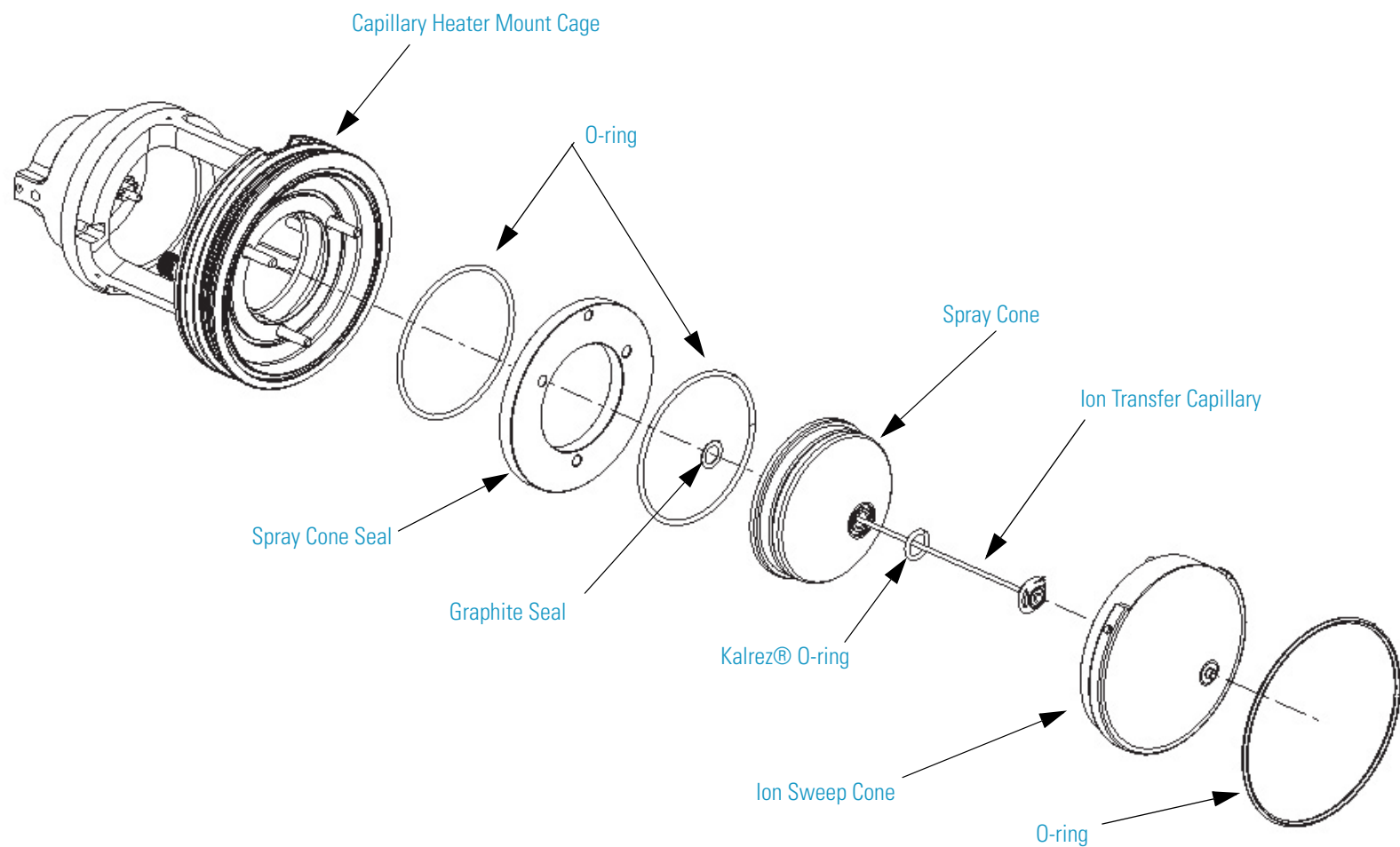
**CAUTION** Wait for the ion source interface to cool to ambient temperature before you disassemble it.

**Note** Wear clean gloves when you handle the ion source interface components.

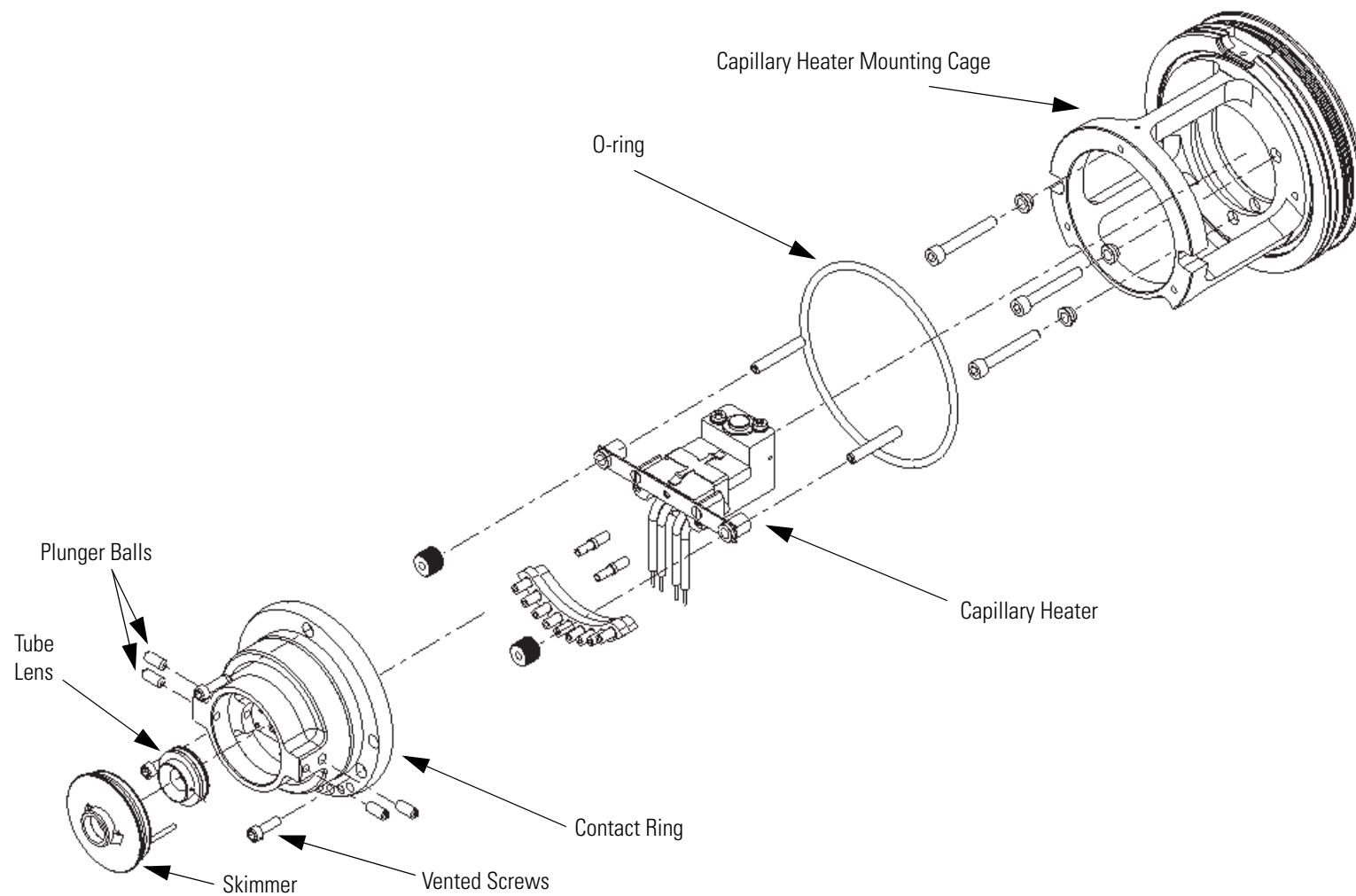
### Removing capillary heater assembly

1. Remove the ion transfer capillary by turning it counterclockwise until you can pull it free from the ion source interface.
2. Disconnect the capillary heater cable from the connector.
3. Disconnect the grounding wire.
4. Loosen the two screws that hold the capillary heater mount to the ion source interface housing.
5. Remove the capillary heater assembly.
6. To install a new capillary heater assembly (P/N 97055-20074), reverse steps 1 through 4.

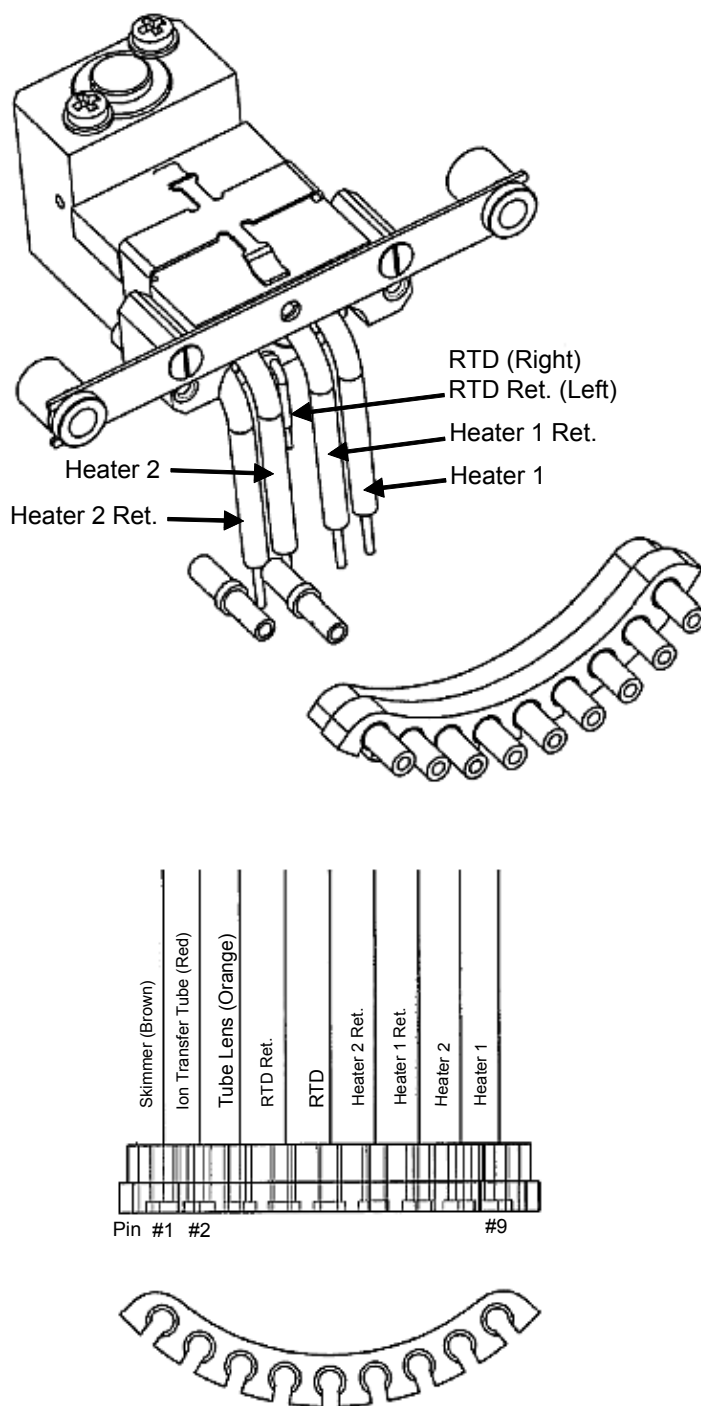
To replace other ion source interface component, refer to the exploded diagrams shown in [Figure 34](#) and [Figure 35](#).



**Figure 34.** Exploded view of the ion source interface (front)



**Figure 35.** Exploded view of the ion source interface (rear)



**Figure 36.** Wiring diagram for the ion source interface



## Reinstalling the Ion Source Interface

## Reinstalling the ion source interface

1. Orient the ion source interface as shown in [Figure 32](#).
2. Carefully insert the ion source interface into the vacuum manifold until it seats in the Q00 RF lens.

## Reinstalling the Ion Max Ion Source Housing

## Reinstalling the Ion Max ion source housing

1. Carefully align the two guide pin holes on the rear of the source housing with the ion source housing guide pins on the mass spectrometer, and carefully press the ion source housing onto the ion source mount. See [Figure 37](#) and [Figure 38](#).
  - a. Rotate the ion source housing locking levers 90 degrees to lock the ion source housing onto the ion source mount assembly.



**CAUTION** Prevent solvent waste from backing up into the ion source and mass spectrometer. Always ensure that liquid in the drain tube is able to drain to a waste container and that the outlet of the drain tube is above the level of liquid in the waste container.

2. Reinstall the source drain tube as follows:

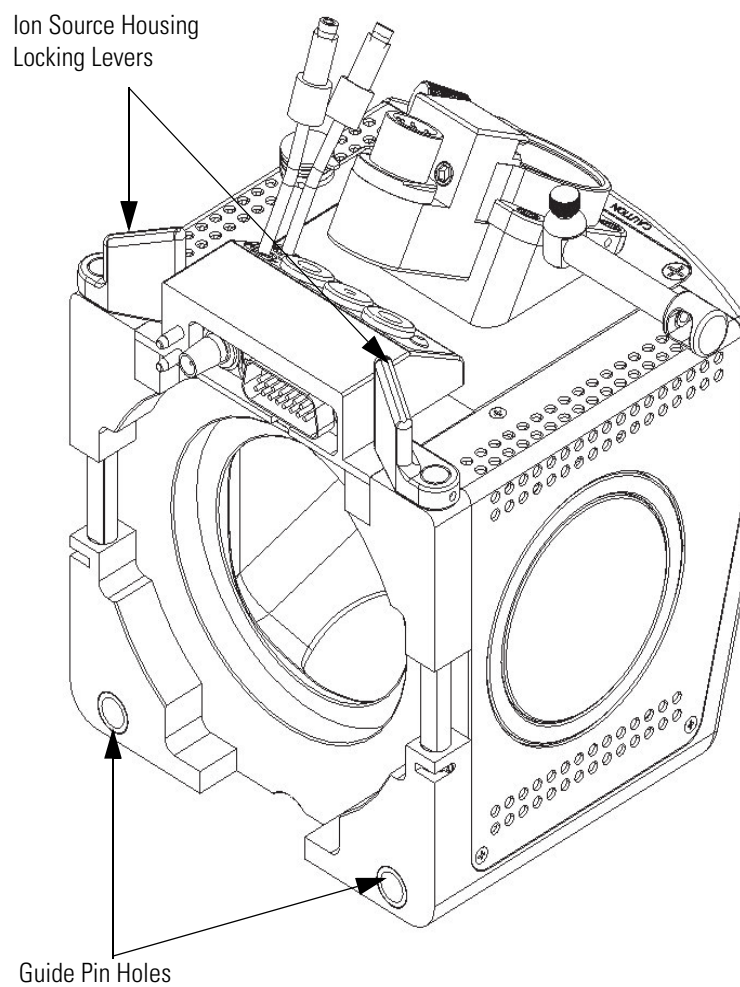


**CAUTION** Do not vent the Ion Max ion source drain tube (or any vent tube connected to the waste container) to the same fume exhaust system to which you have connected the forepumps. The analyzer optics can become irreversibly contaminated with pump oil residue if the Ion Max ion source drain tube and the blue forepump exhaust tubing are connected to the same fume exhaust system.

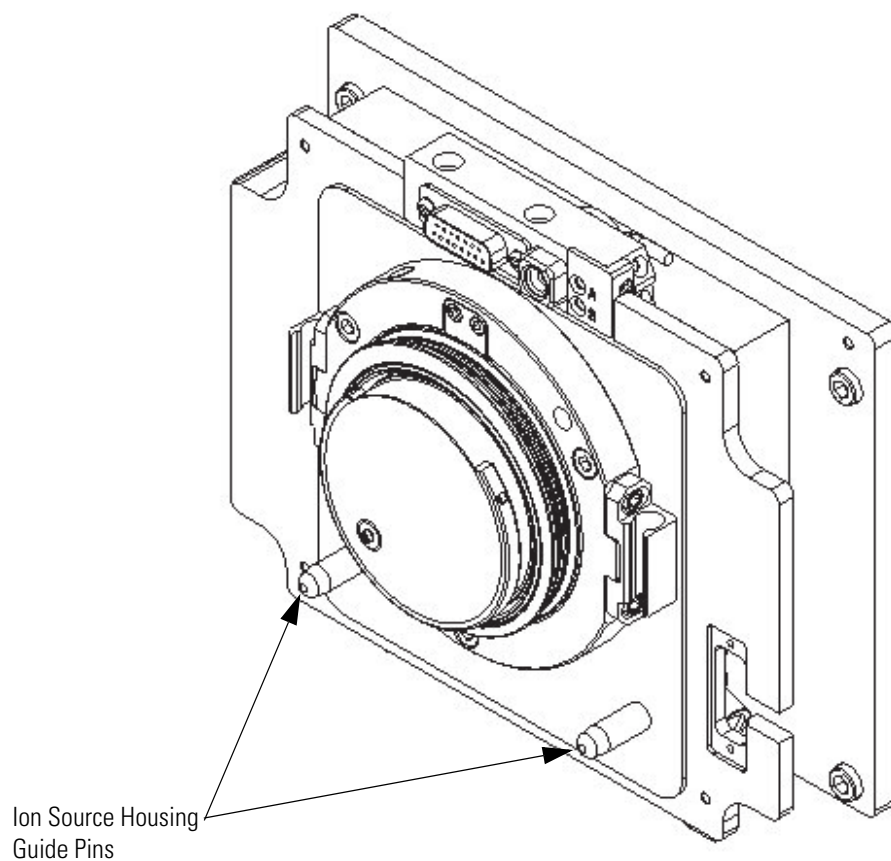


**CAUTION** Your laboratory must be equipped with at least two independent fume exhaust systems. Route the (blue) forepump exhaust tubing to the first dedicated fume exhaust system. Route the drain tube from the Ion Max ion source to a waste container. Vent this waste container to the second dedicated fume exhaust system.

- a. Connect the 1-in. ID Tygon tubing (P/N 00301-22922) to the ion source housing drain fitting.
- b. Attach the free end of the hose to a waste container. Ideally, the waste container should be vented to a fume exhaust system.



**Figure 37.** Rear view of the Ion Max-S ion source housing



**Figure 38.** Ion source mount showing ion source housing guide pins

### Starting Up the System

Start up the system as described in [“Starting the System after a Complete Shutdown”](#) on [page 133](#).

## Cleaning the Q00-L0 RF Lens

An accumulation of chemicals on the surfaces of the Q00 segments and lens L0 forms an insulating layer that can modify the electrical fields that control ion transmission. Therefore, clean ion guide components are essential for the proper operation of the instrument. The Q00 segments and lens L0 require cleaning less often than the tube lens and skimmer. The frequency of cleaning depends on the type and quantity of the compounds that you analyze.

To clean or replace the Q00 RF lens components, do the following:

- [Shutting Down and Venting the System](#)
- [Removing the Ion Max Ion Source Housing](#)
- [Removing the Ion Source Interface](#)
- [Removing the Q00-L0 RF Lens](#)
- [Disassembling the Q00-L0 RF Lens](#)
- [Cleaning the Q00-L0 RF Lens Components](#)
- [Reassembling the Q00-L0 RF Lens](#)
- [Reinstalling the Q00-L0 RF Lens](#)
- [Reinstalling the Ion Source Interface](#)
- [Reinstalling the Ion Max Ion Source Housing](#)
- [Starting Up the System](#)

## Shutting Down and Venting the System

Shut down and vent the system as described in the topic [“Shutting Down the System Completely”](#) on page 131.



**CAUTION** Make sure that the LXQ power cord is unplugged before you proceed.

## Removing the Ion Max Ion Source Housing

Remove the Ion Max ion source to access the ion source interface and Q00-L0 RF lens. Remove the Ion Max ion source from the front of the MS detector as described in [Removing the Ion Max Ion Source Housing](#) on page 93.

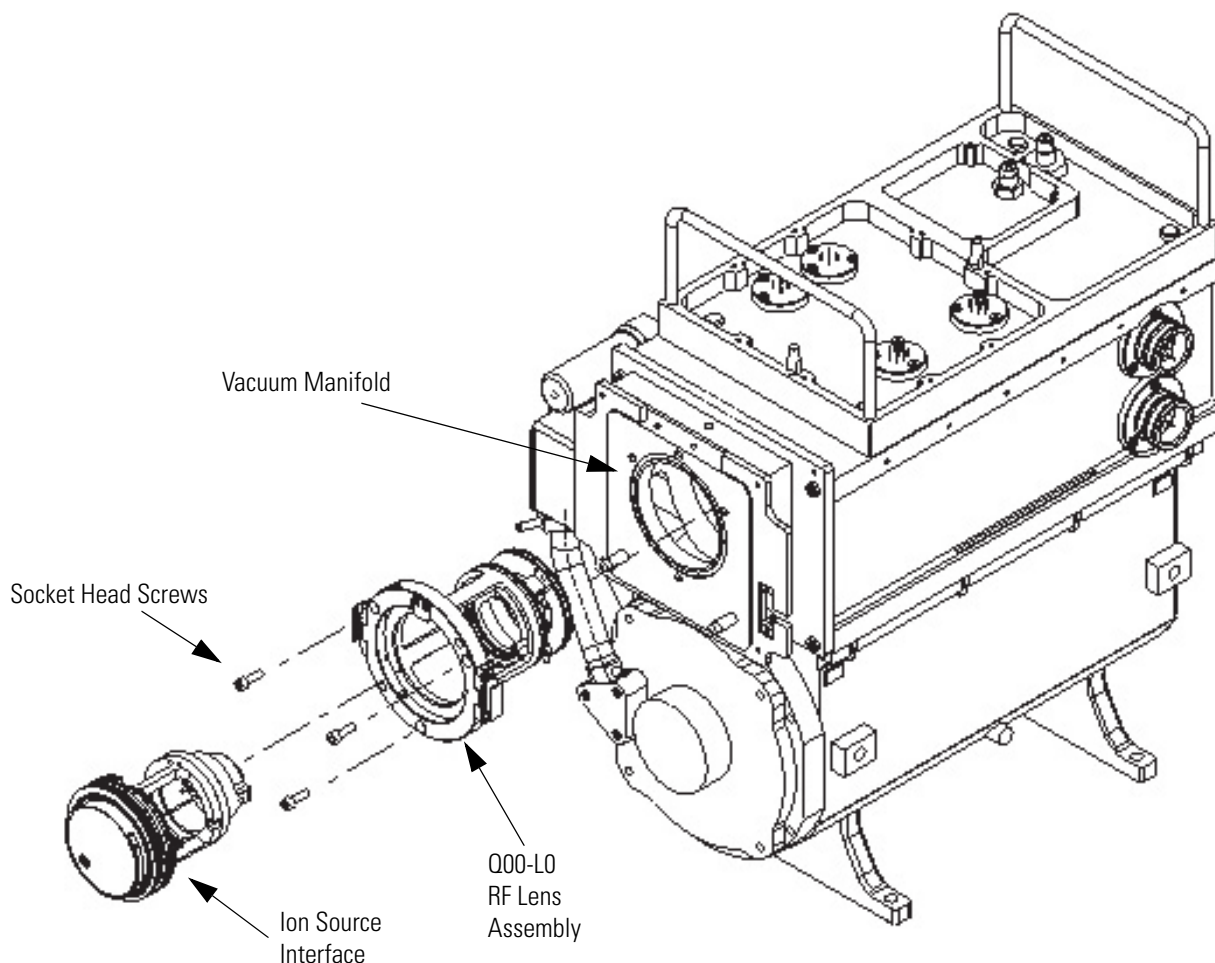
## Removing the Ion Source Interface

You need to remove the ion source interface to access the Q00-L0 RF lens. Remove the ion source interface as described in the topic [Removing the Ion Source Interface](#) on [page 94](#).

## Removing the Q00-L0 RF Lens

### To remove the Q00-L0 RF lens

1. Reach into the opening in the vacuum manifold (where the ion source interface was) and disconnect the electrical connector to the Q00-L0 RF lens.
2. Loosen the three mounting bolts that hold the Q00-L0 RF lens housing to the vacuum manifold. See [Figure 39](#).
3. Carefully remove the Q00-L0 RF lens and place it on a clean surface.



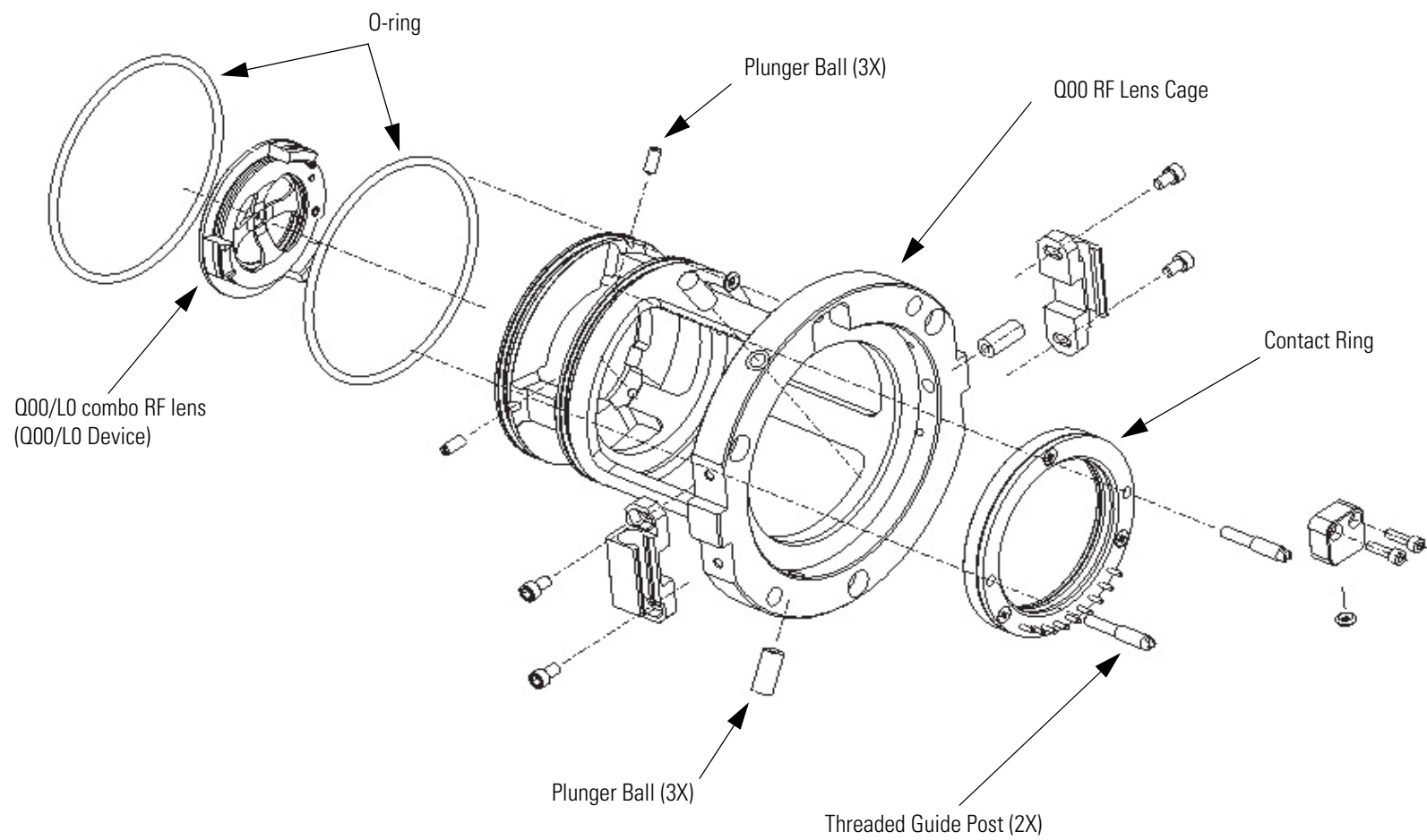
**Figure 39.** Q00-L0 RF Lens assembly removal

## Disassembling the Q00-L0 RF Lens

### Disassembling the Q00-L0 RF lens

**Note** Prepare a clean work area by covering the area with lint-free paper. Wear clean gloves when you handle the Q00-L0 RF lens components.

Remove the Q00-L0 device from the rear of the Q00 RF lens cage. (The Q00-L0 device is secured to the Q00 RF lens cage by plunger balls). See [Figure 40](#) for the location of the Q00-L0 RF lens components.



**Figure 40.** Exploded view of the Q00-L0 RF Lens

## Cleaning the Q00-L0 RF Lens Components

### Cleaning the Q00-L0 RF lens

1. With a soft toothbrush or lint-free swab, scrub the part with a solution of detergent and water.
2. Rinse the part with tap water to remove the detergent.
3. Rinse the part with distilled water.
4. Place the part in a beaker and immerse it completely in HPLC-grade methanol. Move the part up and down in the methanol for 15 s.

**Note** Wear clean gloves to handle the parts after you clean them in methanol.

5. Remove the part from the methanol bath; then rinse it thoroughly with fresh methanol.
6. Dry the part with a rapid stream of nitrogen gas.
7. Inspect each part for contamination and dust. If necessary, repeat the cleaning procedure.

## Reassembling the Q00-L0 RF Lens

### Reassembling the Q00-L0 RF lens

Insert the Q00-L0 device through the rear of the Q00 RF lens cage until it seats in the cage.

## Reinstalling the Q00-L0 RF Lens

### Reinstall the Q00-L0 RF lens in the vacuum manifold

1. Insure that the two 2.148-in. O-rings (P/N 00107-15542) are properly installed on the rear of the Q00 RF lens cage.
2. Orient the Q00-L0 RF lens assembly as shown in [Figure 39](#) on [page 106](#).
3. Carefully insert the Q00-L0 RF lens assembly into the vacuum manifold.
4. Reconnect the electrical connections.



## **Reinstalling the Ion Source Interface**

Reinstall the ion source interface as described in the topic **Reinstalling the Ion Source Interface** on [page 101](#).

Go on to the next topic: **Reinstalling the Ion Max Ion Source Housing**.

## **Reinstalling the Ion Max Ion Source Housing**

Reinstall the Ion Max ion source housing as described in the topic **Reinstalling the Ion Max Ion Source Housing** on [page 101](#).

## **Starting Up the System**

Start up the system as described in the topic **Starting the System after a Complete Shutdown** on [page 133](#).

## Cleaning the Q0 and Q1 Ion Guides

An accumulation of chemicals on the surfaces of the Q0 and Q1 ion guides forms an insulating layer that can modify the electrical fields that control ion transmission. Therefore, clean ion guide components are essential for the proper operation of the instrument. The Q0 and Q1 ion guides require cleaning less frequently than the Q00 RF lens. The frequency of cleaning depends on the type and quantity of the compounds that you analyze.

Cleaning or replacing Q0 and Q1 ion guide components involves the following steps:

- [Shutting Down and Venting the System](#)
- [Removing the Top Cover of the MS Detector](#)
- [Removing the Top Cover Plate of the Vacuum Manifold](#)
- [Removing the Q0 and Q1 Ion Guides](#)
- [Cleaning the Q0 and Q1 Ion Guides](#)
- [Reinstalling the Q0 and Q1 Ion Guides](#)
- [Cleaning the Ion Detection System](#)
- [Reinstalling the Top Cover Plate of the Vacuum Manifold](#)
- [Reinstalling the Top Cover of the MS Detector](#)
- [Starting Up the System](#)

### Shutting Down and Venting the System

Shut down and vent the system as described in the topic [“Shutting Down the System Completely”](#) on [page 131](#).



**CAUTION** Make sure that the LXQ power cord is unplugged before you proceed.

### Removing the Top Cover of the MS Detector

#### Removing the top cover of the MS detector

1. Open the front door of the MS detector by loosening the Allen screw on the right side of the door with an Allen wrench.
2. Remove the top cover of the MS detector.

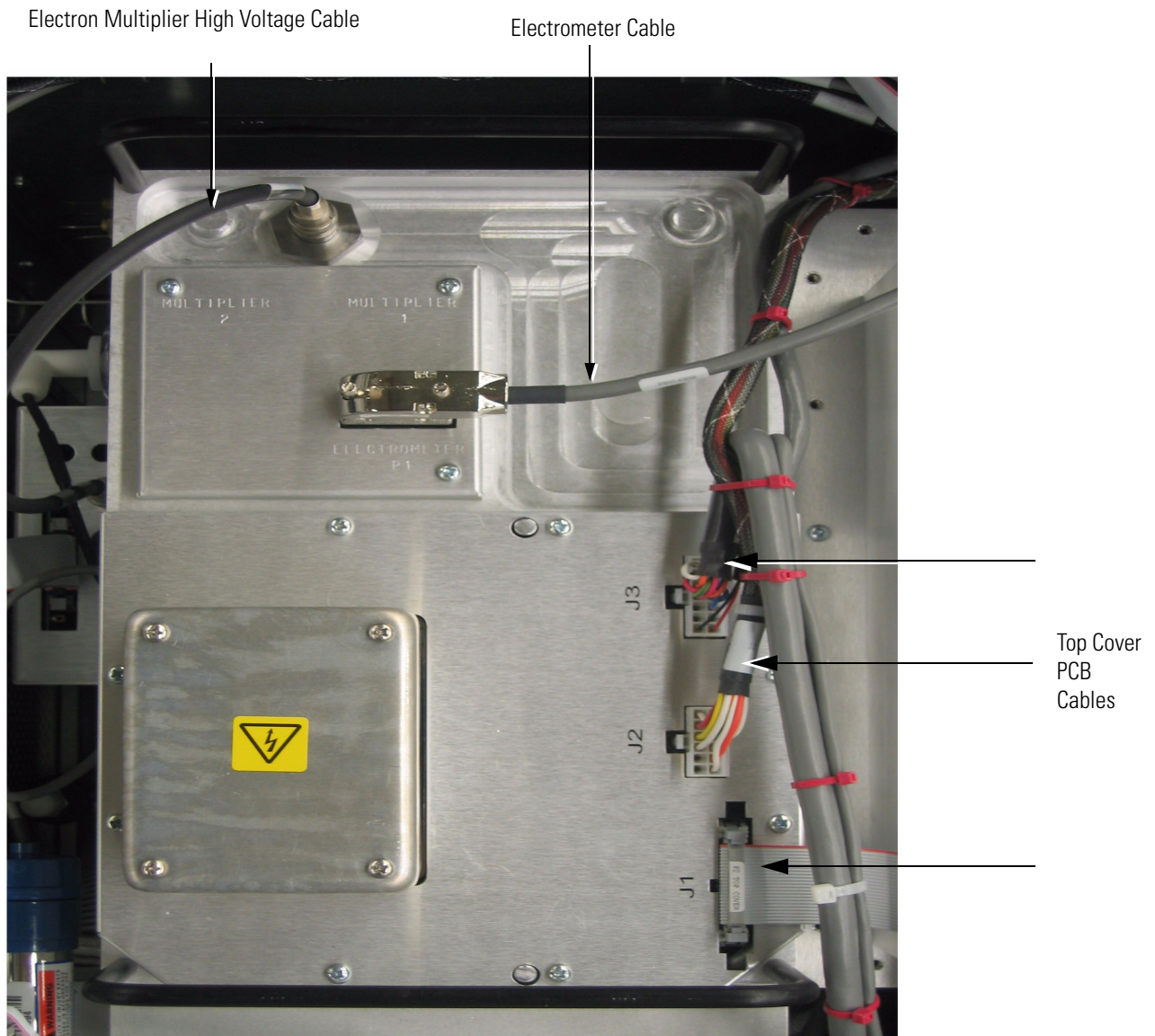
- a. Loosen the two fasteners that hold the top cover to the MS detector chassis. The fasteners are located in the upper right and left corners of the chassis.
- b. Slide the top cover back by about 1.2 cm (0.5 in.).
- c. With one hand under the center of the top cover, lift the top cover up and away from the MS detector.

## **Removing the Top Cover Plate of the Vacuum Manifold**

You need to remove the top cover plate of the vacuum manifold to access the Q0 and Q1 ion guides, mass analyzer, and ion detection system. The top cover plate is held in place by gravity and by the air pressure differential between the vacuum manifold and atmospheric pressure. Five cables are connected to the top cover plate. See [Figure 41](#).

### **Removing the top cover plate**

1. Disconnect the electron multiplier high voltage coaxial cable that originates from the electron multiplier power supply.
2. Disconnect the electrometer cable from the Electrometer PCB. (If necessary, use a small screw driver to loosen the screws that secure the cable.)
3. Disconnect the three cables that connect to the Top Cover PCB.
4. Carefully lift the top cover plate straight up by its two handles. Take care not to damage the components on the underside of the cover plate. Place the cover plate upside down (supported on its handles) on a flat surface.
5. Cover the opening in the top of the vacuum manifold with a large, lint-free tissue.



**Figure 41.** Electrical connections to the top cover of the vacuum manifold

## Removing the Q0 and Q1 Ion Guides

Two adjustable mounting brackets hold the Q0 and Q1 ion guides in position against the baffle on the top cover plate of the vacuum manifold. See [Figure 42](#).

## Removing the Q0 and Q1 ion guides from the top cover plate

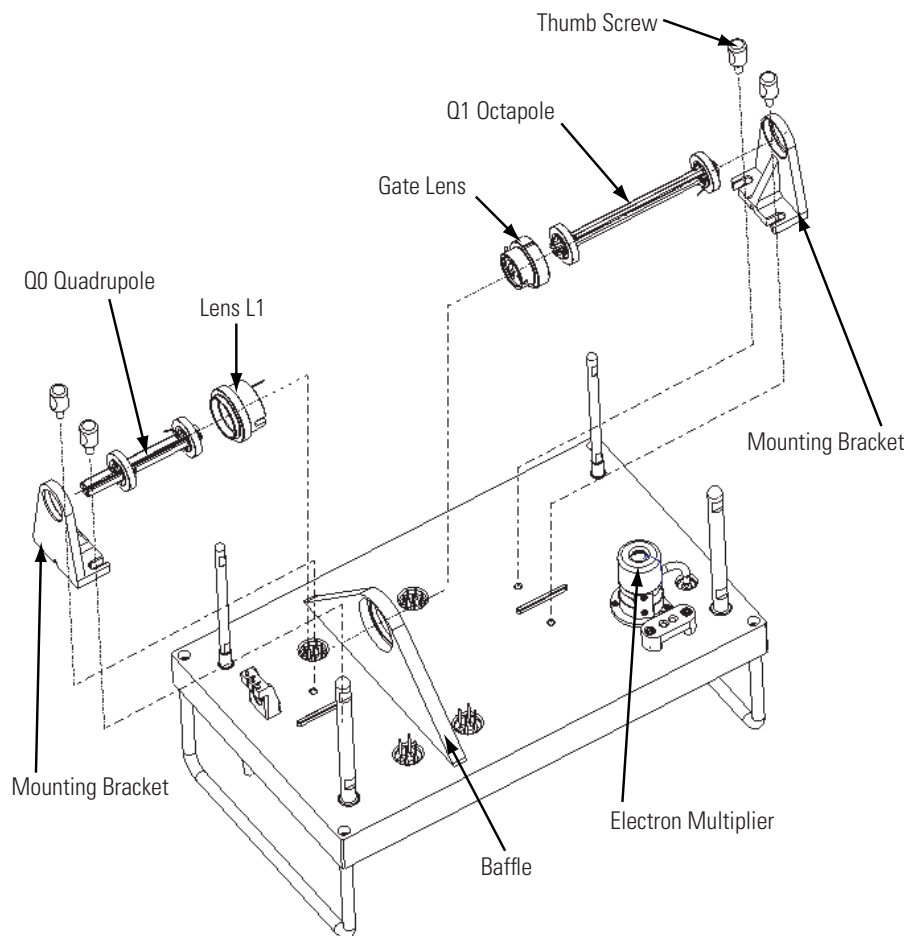
**Note** Wear clean, lint-free, nylon or cotton gloves when you handle the ion guides.

1. Prepare a clean work area by covering the area with lint-free paper. Place each part on the paper as you remove it.



**CAUTION** Be careful not to bend or break the lead pins on the Q0 quadrupole and Q1 octapole.

2. Disconnect the electrical leads to the Q0 quadrupole, lens L1, gate lens, and Q1 octapole.
3. Hold the Q0 quadrupole and lens L1 with one hand; loosen and remove the two thumb screws that hold the Q0 ion guide mounting bracket to the top cover plate of the vacuum manifold. See [Figure 42](#).
4. Remove the Q0 quadrupole and lens L1.
5. Hold the Q1 octapole and gate lens with one hand; loosen and remove the two thumb screws that hold the Q1 ion guide mounting bracket to the top cover plate of the vacuum manifold. See [Figure 42](#).
6. Remove the Q1 octapole and gate lens.



**Figure 42.** Exploded view of the Q0 and Q1 ion guides

## Cleaning the Q0 and Q1 Ion Guides

Remove contamination from the Q0 quadrupole, Q1 octapole, lens L1, and the gate lens. Clean each part in turn. After cleaning, place each part on a clean, lint free surface.



**CAUTION** Take care not to bump or jar the Q0 quadrupole and Q1 octapole.

**Note** When you clean the ion guide parts, pay particular attention to the inside surfaces.

### Removing contamination from the Q0 quadrupole, Q1 octapole, lens L1, and the gate lens

1. With a soft tooth brush or lint-free swab, scrub the ion guide part with a solution of detergent and water.
2. Rinse the part with tap water to remove the detergent.
3. Rinse the part with distilled water.
4. Place the part in a tall beaker and immerse it completely in HPLC-grade methanol. Move the part up and down in the methanol for 15 s.

**Note** Wear clean, lint-free, nylon or cotton gloves to handle the parts after you clean them in methanol.

5. Remove the part from the methanol bath; then rinse it thoroughly with fresh methanol.
6. Dry the part with a rapid stream of nitrogen gas.
7. Inspect each part for contamination and dust. If necessary, repeat the cleaning procedure.

### Reinstalling the Q0 and Q1 Ion Guides

Two adjustable mounting brackets hold the Q0 and Q1 ion guides in position against the baffle on the top cover plate of the vacuum manifold. See [Figure 42](#).

#### Reinstalling the Q0 and Q1 ion guides on the top cover plate.

**Note** Wear clean, lint-free, nylon or cotton gloves when you handle the ion guides.

1. To install the Q1 ion guide,
  - a. Insert the gate lens into the opening in the baffle ([Figure 42](#)).
  - b. With one hand, hold the Q1 octapole against the gate lens; with the other hand, install the Q1 ion guide mounting bracket so that the octapole is held between the mounting bracket and the gate lens.
  - c. Tighten the two thumb screws that hold the Q1 ion guide mounting bracket to the top cover plate.
2. To install the Q0 ion guide,

- a. Insert lens L1 into the opening in the baffle ([Figure 42](#)).
- b. With one hand, hold the Q0 quadrupole against the lens L1; with the other hand, install the Q0 ion guide mounting bracket so that the quadrupole is held between the mounting bracket and the lens L1.
- c. Tighten the two thumb screws that hold the Q0 ion guide mounting bracket to the top cover plate.

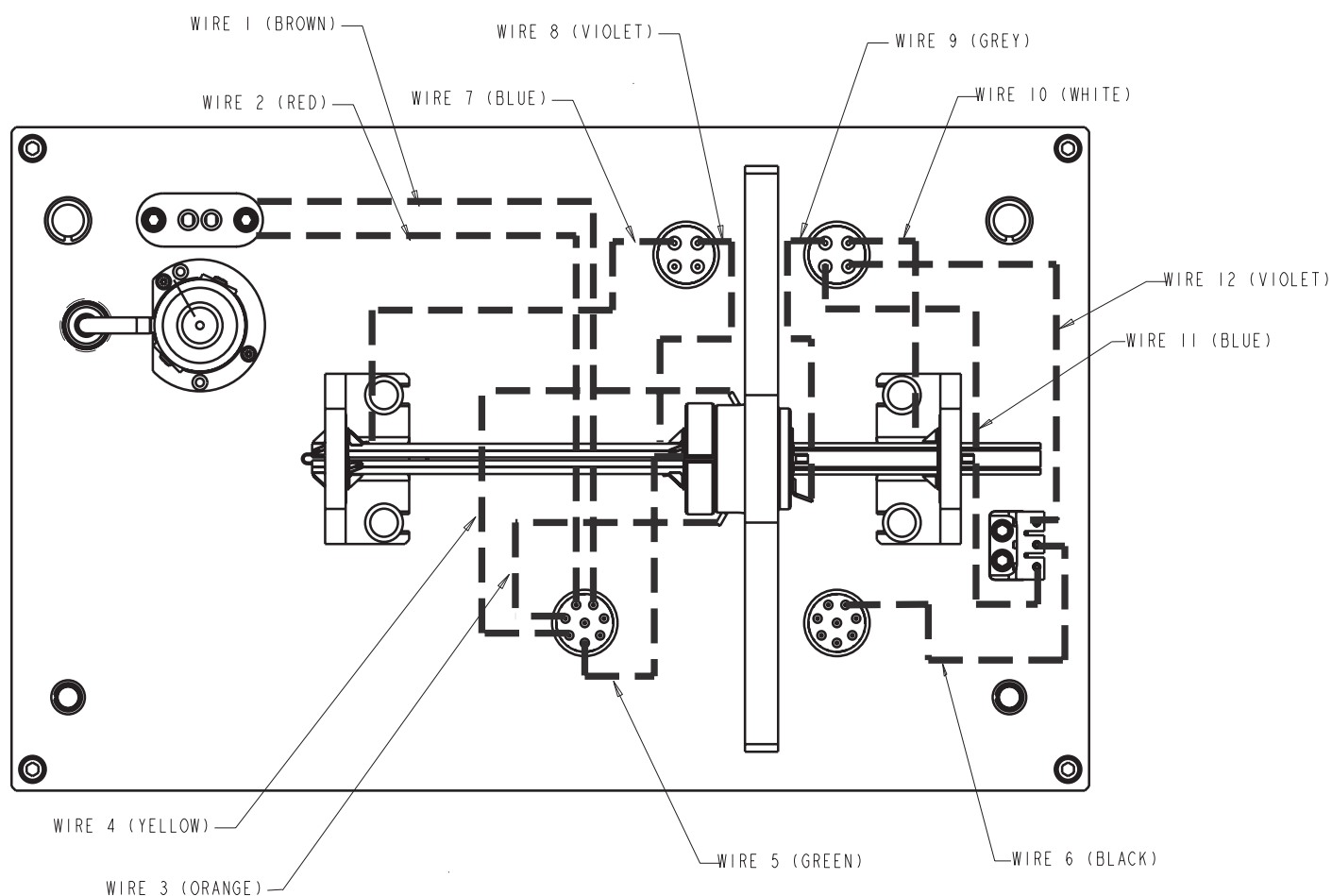


**CAUTION** Be careful not to bend or break the lead pins on the Q0 quadrupole and Q1 octapole.

3. Reconnect the electrical leads to the Q0 quadrupole, lens L1, gate lens, and Q1 octapole according to the wiring diagram shown in [Figure 43](#).

**Note** Check all leads and ensure that they are secure and that they are attached to the proper electrodes.





**Figure 43.** Wiring diagram for the Q0 and Q1 ion guides

## Cleaning the Ion Detection System

The conversion dynode and electron multiplier of the ion detection system must be kept dust free. Clean the conversion dynode and electron multiplier whenever you remove the top cover plate of the vacuum manifold. Cleaning the conversion dynode and electron multiplier involves only blowing them with a clean, dry gas such as nitrogen. Freon gas is not recommended. **Do not use liquids to clean the ion detection system components.** Always cover the opening in the top of the vacuum manifold with a large, lint-free tissue whenever you remove the top cover plate of the vacuum manifold.

## Reinstalling the Top Cover Plate of the Vacuum Manifold

### Reinstalling the top cover plate of the vacuum manifold

1. Remove the tissue from the opening in the top of the vacuum manifold.

2. Check the O-ring that surrounds the opening for signs of wear, and replace it if necessary (P/N 97055-40005). Make sure that the O-ring is seated properly.

**Note** Periodically, remove any contamination that might be on the inner walls of the manifold by wiping the inner walls with a lint-free tissue soaked in HPLC-grade methanol. Use a cotton-tipped applicator soaked in methanol to clean around inlets and feedthroughs.

3. Carefully lift the top cover plate up by its two handles and turn it over. Orient the top cover plate such that the electron multiplier is over the conversion dynode. Carefully insert the guide posts on the underside of the top cover plate into the guide holes in the vacuum manifold. Slowly lower the cover plate onto the opening in the vacuum manifold. Take care not to damage the components on the underside of the cover plate. Ensure that the cover plate is seated properly on the vacuum manifold.
4. Reconnect the three cables to the Top Cover PCB. See [Figure 41](#).
5. Reconnect the electron multiplier high voltage coaxial cable that comes from the electron multiplier power supply.
6. Reconnect the electrometer cable to the Electrometer PCB.

## Reinstalling the Top Cover of the MS Detector

### Reinstall the top cover of the MS detector

1. Open the front door of the MS detector by loosening the Allen screw on the right side of the door with an Allen wrench or hex-head ball driver.
2. With one hand under the center of the top cover, place the top cover over the MS detector such that the front of the cover is about 1.2 cm (0.5 in.) behind the front of the MS detector.
3. Slide the cover forward until it is flush with the front doors (when they are closed).
4. Tighten the two fasteners to secure the top cover to the chassis.
5. Close the front door of MS detector. Tighten the screw on the right side of the door.
6. Reconnect any tubing between the syringe pump and the API source to accommodate your instrument configuration.

## Starting Up the System

Start up the system as described in the topic [“Starting the System after a Complete Shutdown”](#) on [page 133](#).

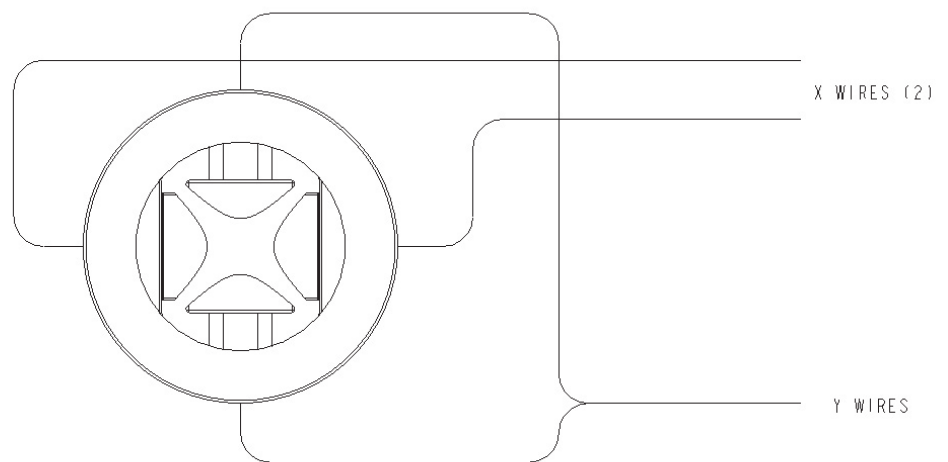
# Maintaining the Mass Analyzer



The mass analyzer very rarely, if ever, requires cleaning.

**CAUTION** The hyperbolic rods of the mass analyzer are precision-aligned at the factory. Due to the delicate nature of the mass analyzer, mass analyzer maintenance should only be performed by a Thermo Electron Field Service Engineer.

A wiring diagram for the mass analyzer is shown in [Figure 44](#).



**Figure 44.** Wiring diagram for the mass analyzer

## Replacing the Electron Multiplier

The electron multiplier of the ion detection system includes an anode and a cathode. The anode and cathode have finite lifetimes. The anode loses sensitivity over time due to contamination of its surface. Things that decrease the lifetime of the cathode are: heat, electron flow (which produces internal heat), air (which causes oxidation and arcing) and water (which causes arcing).

The following symptoms suggest that the electron multiplier may need replacing:

- Excessive noise in the mass spectrum
- Inability of the multiplier gain calibration procedure to achieve a gain of  $4 \times 10^5$  electrons per ion with an electron multiplier voltage less than or equal to 2.5 kV

You can read the current value of the electron multiplier voltage in the Ion Detection System dialog box, which can be reached from the Tune Plus window by choosing **Setup > Ion Detection System**.

If you are having problems with the ion detection system, you need to replace the electron multiplier assembly.

### Replacing the electron multiplier assembly

1. Shut down and vent the system as described in the topic [“Shutting Down the System Completely”](#) on [page 131](#).



**CAUTION** Make sure that the LXQ power cord is unplugged before you proceed.

2. Remove the top cover of the MS detector as described in the topic [“Removing the Top Cover of the MS Detector”](#) on [page 110](#).
3. Remove the top cover plate of the vacuum manifold as described in the topic [“Removing the Top Cover Plate of the Vacuum Manifold”](#) on [page 111](#).

**Note** Wear clean, lint-free, nylon or cotton gloves when you handle the electron multiplier components.

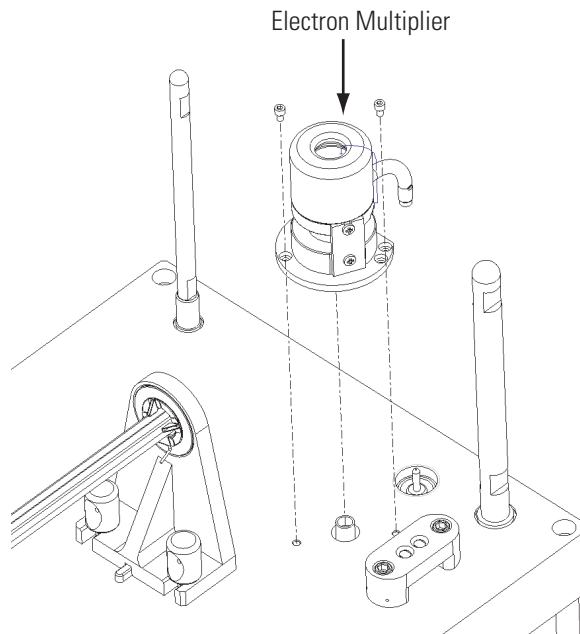
4. With an Allen wrench, remove the two socket-head screws that hold the electron multiplier support to the top cover plate of the vacuum manifold. See [Figure 45](#).

5. With one hand hold the high voltage tube and with the other hand hold the electron multiplier support. Then, detach the high voltage tube from the high voltage feedthrough in the top cover plate and remove the electron multiplier as a unit. (The anode remains in the anode feedthrough in the top cover plate.).



**CAUTION** Be careful not to damage the surface of the electron multiplier shield. The electron multiplier shield has been electropolished to prevent field emission.

6. With one hand holding the high voltage tube and the other hand holding the electron multiplier support, install the new electron multiplier (P/N 96000-60036) on the top cover plate. Ensure that the high voltage tube is properly inserted in the high voltage feedthrough and that the screw holes in the electron multiplier support are aligned with the screw holes in the top cover plate.



**Figure 45.** Electron multiplier

7. Reinstall the two socket-head screws that secure the electron multiplier support to the top cover plate. Tighten the screws with an Allen wrench.
8. Reinstall the top cover plate of the vacuum manifold over the opening in the vacuum manifold as described in [“Reinstalling the Top Cover Plate of the Vacuum Manifold”](#) on [page 117](#).

9. Reinstall the top cover of the MS detector as described in “[Reinstalling the Top Cover of the MS Detector](#)” on page 118.
10. Start up the LXQ system as described in “[Starting the System after a Complete Shutdown](#)” on page 133.
11. Set the electron multiplier voltage to -800 V as follows:
  - a. First, make sure that the system is in MS/MS mode.
  - b. Choose **Start > Programs > Xcalibur > LXQ Tune** to open the Tune Plus window.
  - c. From the Tune Plus window, choose **Diagnostics > Diagnostics**.
  - d. Select (General) Graphs to display the Graphs page.
  - e. In the Set Device Value option box, select Multiplier 1 (V).
  - f. In the text box to the right of the Set Device Value option box, enter **-800**.
  - g. Click on the **Set** button to set the electron multiplier voltage to -800 V.
  - h. Click **OK** button to return to Tune Plus.
12. Calibrate the electron multiplier voltage as follows:
  - a. Allow the system to pump down for at least one hour before you turn on the high voltages.
  - b. Set up for the infusion of the tuning solution into the MS detector as described in *LXQ Getting Started*.
  - c. From the Tune Plus window, choose **Control > Calibrate**. The Calibrate dialog box appears.
  - d. Click the **Semi-Automatic** tab to display the Semi-Automatic page.
  - e. Select the Electron Multiplier Gain option. Click **Start** to start the multiplier gain procedure.
13. After the Electron Multiplier Gain program is finished, set up for operation as described in the *LXQ Getting Started* manual.

# Replacing the Turbomolecular Pump Cartridge

The rotating, interior portion of the turbomolecular pump, referred to as the turbomolecular pump *cartridge*, should be replaced after 20,000 to 30,000 hours of operation or if the bearings fail.

## Replacing the turbomolecular pump cartridge

1. Shut down the system.
2. Remove the left front panel.
3. Disconnect the power cable from the turbomolecular pump.
4. Disconnect the foreline from the turbomolecular pump.
5. Loosen and remove the six 4 mm socket-head screws that hold the insert to the pump.
6. Remove the old cartridge.
7. Install a new cartridge.
8. Install and tighten the six screws that hold the cartridge to the pump.
9. Connect the foreline to the turbomolecular pump.
10. Connect the power cable to the turbomolecular pump.
11. Reinstall the left front panel.
12. Start up the system.



**CAUTION** The turbomolecular pump insert is very delicate. It is recommended that a Thermo Electron Field Service Engineer replace the turbomolecular pump insert.



## **Cleaning the Fan Filter**

You need to clean the fan filter (P/N 97055-20254) every four months. The fan filter is located on the rear of the MS detector on the right side (viewing from the front).

### **Cleaning the fan filter**

1. Remove the fan filter from the rear of the MS detector by pulling it up and out of its fan filter bracket.
2. Wash the fan filter in a solution of soap and water.
3. Rinse the fan filter with tap water.
4. Squeeze the water from the fan filter and allow it to air dry.
5. Reinstall the fan filter in its fan filter bracket.



## Chapter 5 System Shutdown, Startup, and Reset

Many maintenance procedures for the LXQ system require that the MS detector be shut down completely. In addition, the LXQ can be placed in Standby mode if the system is not to be used for 12 hours or more.

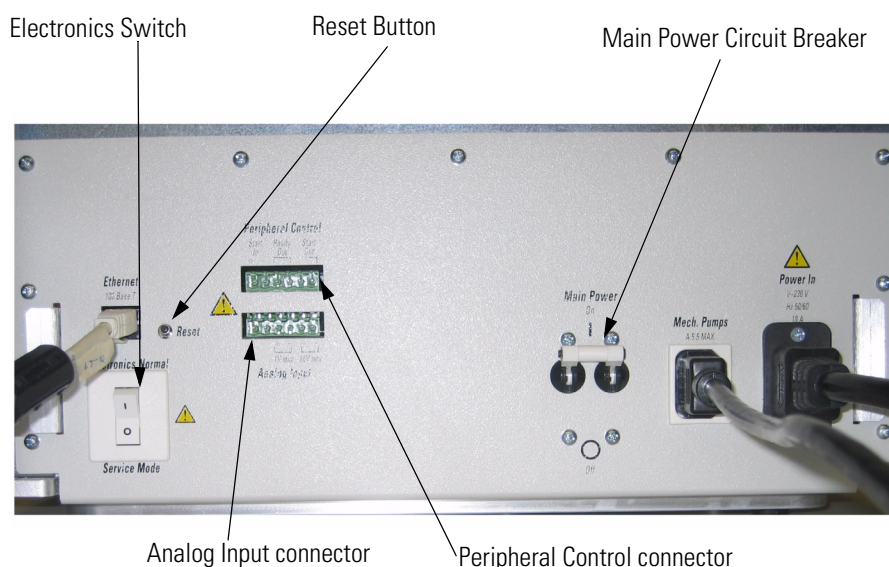
This chapter contains the following procedures :

- [Shutting Down the System in an Emergency](#)
- [Placing the System in Standby Condition](#)
- [Shutting Down the System Completely](#)
- [Starting the System after a Complete Shutdown](#)
- [Resetting the MS Detector](#)
- [Resetting the Tune and Calibration Parameters to their Default Values](#)
- [Resetting the Data System](#)
- [Turning Off Selected MS Detector Components](#)

## Shutting Down the System in an Emergency

If you need to turn off the MS detector in an emergency, place the main power circuit breaker switch, located on the power panel on the right side panel of the MS detector (see [Figure 46](#)), in the Off (O) position. This turns off all power to the MS detector, including the vacuum pumps. Although removing power abruptly will not harm any component within the system, this is not the recommended shutdown procedure to follow. See [“Shutting Down the System Completely”](#) on [page 131](#).

To turn off the LC, autosampler, and computer in an emergency, use the on/off switches on the LC, autosampler, and computer, respectively.



**Figure 46.** View of the power panel showing the Reset button and the main power circuit breaker.


## Placing the System in Standby Condition

The LXQ system does not need to be shut down completely if you are not going to use it for a short period of time, such as overnight or over weekends. When you are not going to operate the system for 12 hours or more, you can leave the system in a standby condition.

Use the following procedure to place the LXQ system in the standby condition:

6. Wait until data acquisition, if any, is complete.
7. Turn off the flow of sample solution from the LC to the API source, as follows:



- a. In the Tune Plus window, click on the LC button. The Inlet Direct Control dialog box appears.
- b. Click on  (or **Pump Off** or **Stop Pump**) to stop the LC pump.



**CAUTION** If you are using APPI do not leave the LC or other liquid delivery device ON while the mass spectrometer is in Standby mode. The absence of sheath and auxiliary gas can cause the hot VUV lamp to break upon contact with liquids.



8. From the Tune Plus window, choose **Control > Standby** (or click **On/Standby** to toggle it to Standby) to put the MS detector in Standby. When you choose Control > Standby, the LXQ turns off the electron multiplier, conversion dynode, 8 kV power to the API source, main RF voltage, and ion guide RF voltages. The LXQ also turns off the auxiliary and sheath gas flows. See [Table 4](#) on [page 140](#) for the On/Off status of MS detector components when the MS detector is in the standby condition. The System LED on the front panel of the MS detector is illuminated yellow when the system is in Standby mode.
9. Flush the spray cone and the entrance end of the ion transfer capillary of the API source as described in the topic [“Flushing the Ion Sweep Cone and Ion Transfer Capillary”](#) on [page 88](#).
10. Purge the rotary-vane pump oil as described in the topic [“Purge the Oil in the Rotary-Vane Pump”](#) on [page 82](#).
11. Leave the MS detector power on.
12. Leave the LC power on.
13. Leave the autosampler power on.

## **5 System Shutdown, Startup, and Reset**

### Placing the System in Standby Condition

14. Leave the data system power on.

## Shutting Down the System Completely

The LXQ system does not need to be shut down completely if you are not going to use it for a short period of time, such as overnight or over weekends (see “[Placing the System in Standby Condition](#)” on [page 129](#)). Shut down the system completely only if it is to be unused for an extended period or if it must be shut down for a maintenance or service procedure.

### Shutting down the LXQ system completely

1. Turn off the flow of sample solution from the LC (or other sample introduction device).

**Note** For instructions on how to operate the LC from the front panel, refer to the manual that came with the LC.

2. From the Tune Plus window, choose **Control > Standby** (or click **On/Standby**) to put the MS detector in Standby. When you place the MS detector in Standby mode, LXQ turns off the electron multiplier, conversion dynode, 8 kV power to the API source, main RF voltage, and octapole RF voltage, sheath and auxiliary gasses.
3. Place the electronics service switch, located on the power panel (see [Figure 46](#) on [page 128](#)), in the Service position. Power to the non-vacuum system electronics is turned off when you place the electronics service switch in the Service position.
4. Place the main power circuit breaker switch, located on the power panel ([Figure 46](#)) in the Off (O) position. When you place the main power circuit breaker switch in the Off (O) position, the following occurs:
  - All power to the MS detector, including the turbomolecular pump and rotary vane pump, is turned off. (All LEDs on the front panel of the MS detector are off.)
  - Power to the vent valve solenoid is shut off. When power to the vent valve solenoid is shut off, the vent valve opens and the vacuum manifold is vented to filtered air. You can hear a hissing sound as the air passes through the air filter.
  - After about 5min, the vacuum manifold is at atmospheric pressure.

5. Unplug the power cord for the MS detector.



**CAUTION** Allow heated components to cool before servicing them.

**Note** If you are planning to perform routine or preventive system maintenance on the MS detector only, you do not need to turn off the LC, data system, and autosampler. In this case, the shutdown procedure is completed. However, if you do not plan to operate your system for an extended period of time, we recommend that you turn off the LC, data system, and autosampler as described in steps 6 through 11 below.

6. Turn off the LC (if it is a part of your system). Follow the procedure described in the manual that came with the LC.
7. Turn off the helium damping gas supply at the tank.
8. Turn off the nitrogen supply at the tank.
9. Turn off the data system as follows:
  - a. Choose **Start > Shut Down** from the Windows XP task bar. The Shut Down Windows dialog box appears.
  - b. Select **Shut Down The Computer**, and then click **Yes** to start the Windows XP shutdown procedure.
  - c. When the Windows XP shutdown procedure tells you that it is safe to turn off the computer, turn off the monitor and computer by using the on/off switches.
10. Turn off the printer (if it is a part of your system) by using the printer on/off switch.
11. Turn off the autosampler (if it is a part of your system) by using the autosampler main power on/off switch.



## Starting the System after a Complete Shutdown

To start up the LXQ system after it has been shut down completely, you need to do the following:

- [Starting the LC](#) (if this is a part of the system)
- [Starting the Data System](#)
- [Starting the MS Detector](#)
- [Starting the Autosampler](#) (if this is a part of the system)
- [Setting Up Conditions for Operation](#)

### Starting the LC

To start up the LC, follow the startup procedure described in the manual that came with the LC. If necessary, configure the LC as described in **LXQ Getting Connected**. Do not turn on the liquid flow to the MS detector.

### Starting the Data System

#### Starting the data system

1. Turn on the monitor, computer, and printer.
2. Follow the Windows XP startup procedure on the monitor.
3. Press <Ctrl>-<Alt>-<Del> when you are prompted to do so. Then, click **OK** or enter your password (if you have one) in the Logon Information dialog box to complete the start up procedure.

### Starting the MS Detector

#### Starting the MS detector

**Note** The data system must be running before you start up the MS detector. The MS detector will not operate until software is received from the data system.

1. Turn on the flows of helium and nitrogen at the tanks if they are off.
2. Make sure that the main power circuit breaker switch is in the Off (O) position and the electronics service switch is in the Service position.
3. Plug in the power cord for the MS detector.
4. Place the main power circuit breaker switch in the On (I) position. When you place the main power circuit breaker switch in the On (I)

position, the rotary-vane pump and the turbomolecular pump are started. All LEDs on the MS detector front panel are off.

5. Allow the LXQ to pump down for 5 min.
6. Place the electronics service switch in the Electronics Normal position. When you place the electronics service switch in the Electronics Normal position, the following occurs:
  - The Power LED on the MS detector front panel turns green to indicate that power is provided to the MS detector electronics. (The electron multiplier, conversion dynode, 8 kV power to the API source, main RF voltage, and octapole RF voltage remain off.)
  - The embedded computer reboots. After several seconds the Communication LED on the front panel turns yellow to indicate that the data system and the MS detector have started to establish a communication link.
  - After several more seconds, the Communication LED turns green to indicate that the data system and the MS detector have established a communication link. Ensure that the instrument console window is active. Software for the operation of the MS detector is then transferred from the data system to the MS detector.
  - After three minutes, the System LED turns yellow to indicate that the software transfer from the data system to the MS detector is complete and that the instrument is in Standby.

**Note** The Vacuum LED on the front panel of the MS detector turns green only if the pressure in the vacuum manifold is below the maximum allowable pressure ( $5 \times 10^{-4}$  Torr in the analyzer region, and 2 Torr in the capillary-skimmer region).

If you have an autosampler see [“Starting the Autosampler”](#) on [page 134](#). If you do not have an autosampler, go to the topic: [“Setting Up Conditions for Operation”](#) on [page 135](#).

## Starting the Autosampler

To start up the autosampler, place the main power switch on the autosampler in the on position. If necessary, configure the autosampler. For procedures for placing sample vials, preparing solvent and waste bottles, installing syringes, etc., refer to the manual supplied with the autosampler. Autosampler hook-up procedures are given in the *LXQ Getting Connected* manual.

## Setting Up Conditions for Operation

You need to do the following to set up your LXQ for operation:

1. Before you begin data acquisition with your LXQ system, you need to allow the system to pump down for at least 1 hour. Operation of the system with excessive air and water in the vacuum manifold can cause reduced sensitivity, tuning problems, and reduced lifetime of the electron multiplier.
2. Ensure that the helium pressure and nitrogen pressure are within the operational limits (helium:  $40 \pm 10$  psig [ $275 \pm 70$  kPa], nitrogen:  $100 \pm 20$  psig [ $690 \pm 140$  kPa]).

**Note** Air in the helium line must be purged or given sufficient time to be purged for proper LXQ performance.

3. Look at the status panel in the Tune Plus window. Check to see if the pressure measured by the ion gauge is below about  $5 \times 10^{-5}$  Torr, and the pressure measured by the Convector gauge is around 1 Torr. Compare the values of the other parameters in the status panel with values that you recorded previously.
4. Set up for ESI, APCI, APPI, or NSI operation as described in *Finnigan LXQ Getting Started*.

**Note** You do not need to calibrate or tune the LXQ each time you restart the LXQ.

**Calibration parameters** are instrument parameters whose values do not vary with the type of experiment. You need to calibrate the LXQ perhaps once a month, and check the calibration once a week. Refer to **Finnigan LXQ Getting Started** for a procedure for calibrating the LXQ.

**Tune parameters** are instrument parameters whose values vary with the type of experiment. You need to tune the LXQ (or change the Tune Method) whenever you change the type of experiment. Refer to **Finnigan LXQ Getting Started** for procedures for tuning the LXQ in the ESI or APCI mode. (Note that LXQ comes with several standard Tune Methods specific for various experimental conditions, making tuning unnecessary for many types of experiments.)

# Resetting the MS Detector

If communication between the MS detector and data system computer is lost, it may be necessary to reset the MS detector using the Reset button on the power panel. When you press the Reset button an interruption in the embedded computer is created which causes the embedded computer to restart in a known (default) state. See [Figure 46](#) on [page 128](#) for the location of the Reset button.

**Note** Only a momentary press of the Reset button is needed. The Reset button is a momentary switch.

The procedure given here assumes that the MS detector and data system computer are both powered on and operational. If the MS detector, data system computer, or both are off, see [“Starting the System after a Complete Shutdown”](#) on [page 133](#).

To reset the MS detector, press the Reset button located on the power panel. Make sure the Communication LED is extinguished upon releasing the Reset button. When you press the Reset button, the following occurs:

- An interruption of the embedded computer causes the CPU to reboot. All LEDs on the front panel of the MS detector are off except the Power LED.
- After several seconds, the Communication LED turns yellow to indicate that the data system and the MS detector are starting to establish a communication link.
- After several more seconds, the Communication LED turns green to indicate that the data system and the MS detector have established a communication link. Software for the operation of the MS detector is then transferred from the data system to the MS detector.
- After three minutes the software transfer is complete. The System LED turns either green or yellow. Green indicates that the instrument is functional and the high voltages are on. Yellow indicates that the instrument is functional and is in Standby mode.

## Resetting the Tune and Calibration Parameters to their Default Values

You can reset the LXQ tune and calibration parameters to their default values at any time. This feature may be useful if you have manually set some parameters that have resulted in less than optimum performance.

### Resetting the LXQ tune and calibration parameters to their default values

**Note** Make sure that the problems that you are experiencing are not due to improper API source settings (spray voltage, sheath and auxiliary gas flow, ion transfer capillary temperature, etc.) before resetting the system parameters to their default values.

1. In the Tune Plus window, choose **File > Restore Factory Calibration** to restore the default calibration parameters, or choose **File > Restore Factory Tune Method** to restore the default tune parameters.
2. To optimize the LXQ system parameters (that is, to calibrate or tune the system), perform the calibration procedure described in *LXQ Getting Started*.

## Resetting the Data System

There are two ways to reset the data system:

- By using the Windows XP shutdown and restart procedure
- By pressing the reset button on the personal computer

### Resetting the Data System Using Windows XP

If possible, use the Windows XP shutdown and restart procedure to shut down and restart the data system so that Windows XP can properly close applications and save changes to files.

#### Reset the data system by using Windows XP

1. Choose **Start > Shut Down** from the Windows XP task bar. The Shut Down Windows dialog box appears.
2. Select the **Restart The Computer** button, and then click on **Yes** to start the Windows XP shutdown and restart procedure.
3. Follow the Windows XP shutdown and restart procedure on the monitor.
4. Press **<Ctrl>-<Alt>-<Del>** when you are prompted to do so. Then, click **OK** or enter your password (if you have one) in the Logon Information dialog box to complete the shutdown and restart procedure.

**Note** The communications link between the data system and the MS detector should be automatically reestablished after you reset the data system. When this occurs the Communication LED on the front panel of the MS detector is illuminated yellow and then green. If the system is unable to reestablish the communications link, press the Reset button on the power panel of the MS detector. Only a momentary push of the Reset button is needed as it is a momentary switch.

### Resetting the Data System by Using the Reset Button on the Personal Computer

#### If you are unable to reset the data system by using Windows XP

1. Press the reset button on the personal computer.
2. Observe the Windows XP shutdown and restart procedure on the monitor.
3. Press **<Ctrl>-<Alt>-<Del>** when you are prompted to do so. Then, click on **OK** or enter your password (if you have one) in the Logon

Information dialog box to complete the shutdown and restart procedure.

4. When the shutdown and restart procedure has completed, choose **Start > Programs > Xcalibur > LXQ Tune** to display the Tune Plus window.

**Note** The communications link between the data system and the MS detector should be automatically reestablished after you reset the data system. When this occurs, the Communication LED on the front panel of the MS detector turns yellow and then green. If the system is unable to reestablish the communications link, press the Reset button on the power panel of the MS detector. Only a momentary push of the Reset button is needed as it is a momentary switch.



## Turning Off Selected MS Detector Components

There are five ways that you can turn off some or all of the MS detector components

- Turn off individual MS detector components from the Tune Plus window. Turning off individual MS detector components might be necessary when you are troubleshooting or when you are running certain diagnostic procedures.
- Place the MS detector in Standby. Standby is the normal condition to leave the MS detector in when it is not in use. Choose **Control > Standby** (or toggle the On/Standby button) from the Tune Plus window to place the MS detector in Standby.
- Turn the MS detector Off. Off is similar to Standby, except all high voltage components of the MS detector are turned off. Choose **Control > Off** from the Tune Plus window to place the MS detector in the Off condition.
- Turn the electronics service switch to Service. The electronics service switch allows you to perform maintenance procedures involving nonvacuum system components of the MS detector.
- Place the main power circuit breaker switch in the Off (O) position. Placing the main power circuit breaker switch in the Off (O) position removes all power to the MS detector, including the vacuum system.



The on/off status of MS detector components, voltages, and gas flows is summarized in [Table 4](#).

**Table 4.** On/Off Status of MS Detector Components, Voltages, and Gas Flows in System Standby or System Off modes. On/Off Status of MS Detector Components, Voltages, and Gas Flows when Electronics Service Switch is in the Service Position or when Main Power Breaker Switch is in the Off position.

MS detector component	Standby mode 	Off mode 	Electronics service switch in Service position	Main power circuit breaker switch in Off (O) position
Electron multiplier	Off	Off	Off	Off
Conversion dynode	Off	Off	Off	Off
Mass analyzer RF/waveform voltages	Off	Off	Off	Off
Mass analyzer dc offset voltage	On	Off	Off	Off
Ion optics multipoles RF voltages	Off	Off	Off	Off
Ion optics multipoles dc offset voltages	On	Off	Off	Off



**Table 4.** On/Off Status of MS Detector Components, Voltages, and Gas Flows in System Standby or System Off modes. On/Off Status of MS Detector Components, Voltages, and Gas Flows when Electronics Service Switch is in the Service Position or when Main Power Breaker Switch is in the Off position.

MS detector component	Standby mode 	Off mode 	Electronics service switch in Service position	Main power circuit breaker switch in Off (O) position
Ion optics lens	On	Off	Off	Off
Tube lens	On	Off	Off	Off
Ion transfer capillary heater	On	On	Off	Off
Ion transfer capillary dc offset	On	Off	Off	Off
Corona discharge needle	Off	Off	Off	Off
APCI vaporizer	On	Off	Off	Off
ESI needle	Off	Off	Off	Off
Sheath gas	Off	Off	Off	Off
Auxiliary gas	Off	Off	Off	Off
Sweep gas	Off	Off	Off	Off
Helium damping gas	On	On	On	On
Vent valve	Closed	Closed	Closed	Open
Turbomolecular pump	On	On	On	Off
Rotary-vane pump	On	On	On	Off
Turbomolecular Pump Controller	On	On	On	Off
Power supply, electron multiplier/conversion dynode	Off	Off	Off	Off
Power supply, 8 kV	Off	Off	Off	Off
Power supply PS1	On	On	Off	Off
Power supply PS2	On	On	On	Off
Fan, turbomolecular pump	On	On	On	Off
Fan, RF coil	On	On	Off	Off
Fans, electronics tower	On	On	On	Off
Convector gauge	On	On	Off	Off
Ion gauge	On	On	Off	Off



## Chapter 6 **Diagnostics and PCB and Assembly Replacement**

Many of the MS detector components can be tested by the LXQ diagnostics. Thermo Electron's service philosophy for the LXQ system calls for troubleshooting to the lowest part, assembly, PCB, or module listed in the **Replaceable Parts** chapter. You should replace LXQ components when indicated by the LXQ diagnostics, by Thermo Electron Technical Support, or by a Thermo Electron Customer Support Engineer.

This chapter contains the following topics:

- [Running the LXQ Diagnostics](#)
- [Replacing a Fuse](#)
- [Replacing Power Supplies](#)
- [Replacing PCBs in the MS Detector](#)

## Running the LXQ Diagnostics

The LXQ diagnostics are used to test the major electronic circuits within the instrument and indicate whether the circuits pass or fail the tests. If there is a problem with the instrument electronics, the LXQ diagnostics can often locate the problem. You can then often correct the problem yourself by replacing a faulty PCB or assembly.

The LXQ diagnostics do not diagnose problems that are not electrical in nature. For example, they do not diagnose poor sensitivity due to misaligned or dirty components or to improper tuning. For such reasons, it is important to have someone who is familiar with system operation and basic hardware theory run the diagnostics and use them to assist in isolating any problems.

Before running the diagnostics, consider the following:

- Did the system fail when you were running samples?
- Did problems occur after you performed maintenance on the instrument, data system, or peripherals?
- Did you change the system's configuration, cables, or peripherals just before the problem occurred?

If the answer is yes to the first item above, there is the possibility of a hardware failure, and running the diagnostics is appropriate.

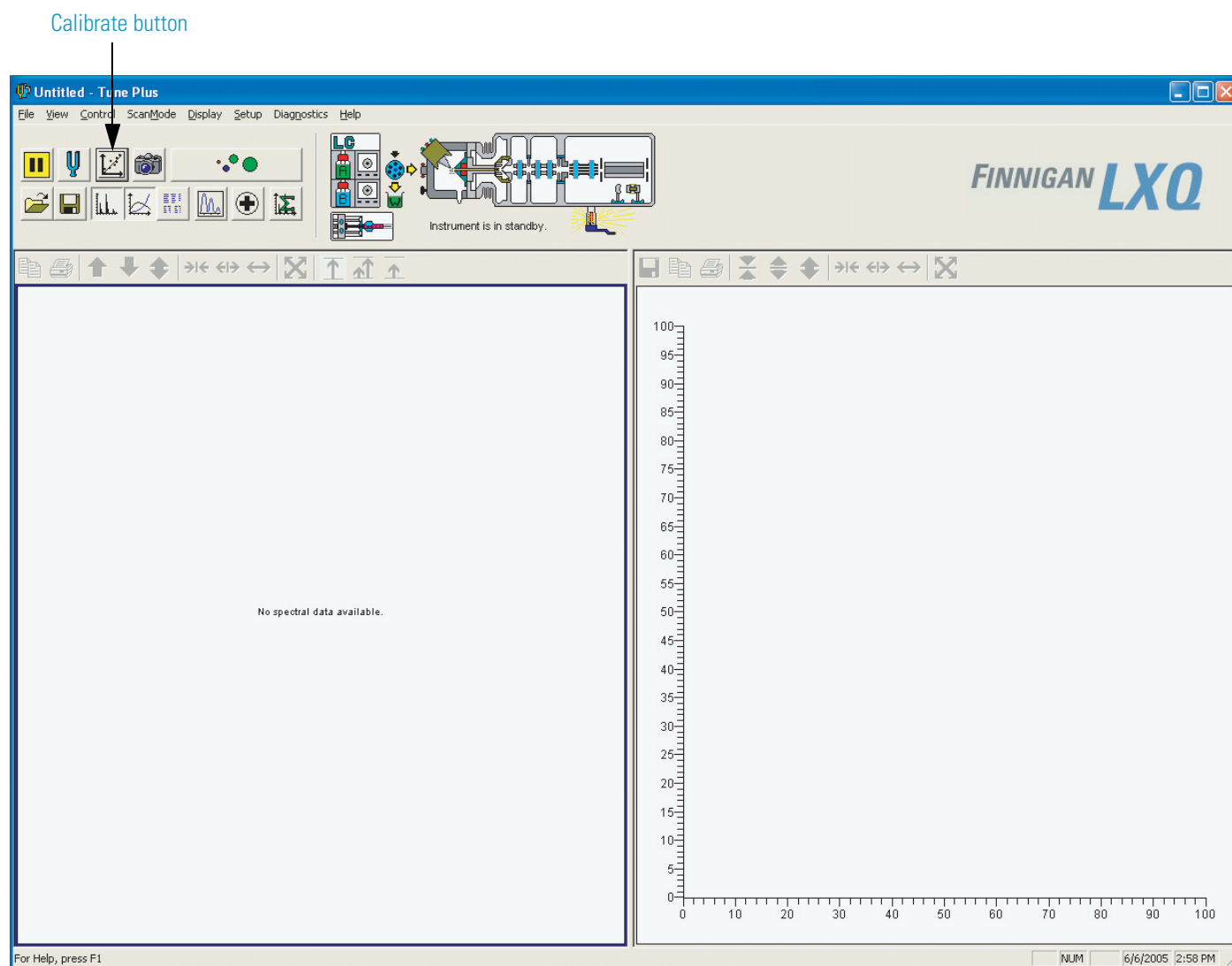
If the answer is yes to one of the last two items above, the problem is probably mechanical, not electrical. Check again that alignment, configurations, and cable connections are correct before you run the LXQ diagnostics.

The LXQ diagnostics procedure starts with Multipole RF and Main RF tuning (steps 1-3 below) and conclude with the diagnostic procedure (steps 4-7 below).

### To run the LXQ diagnostics

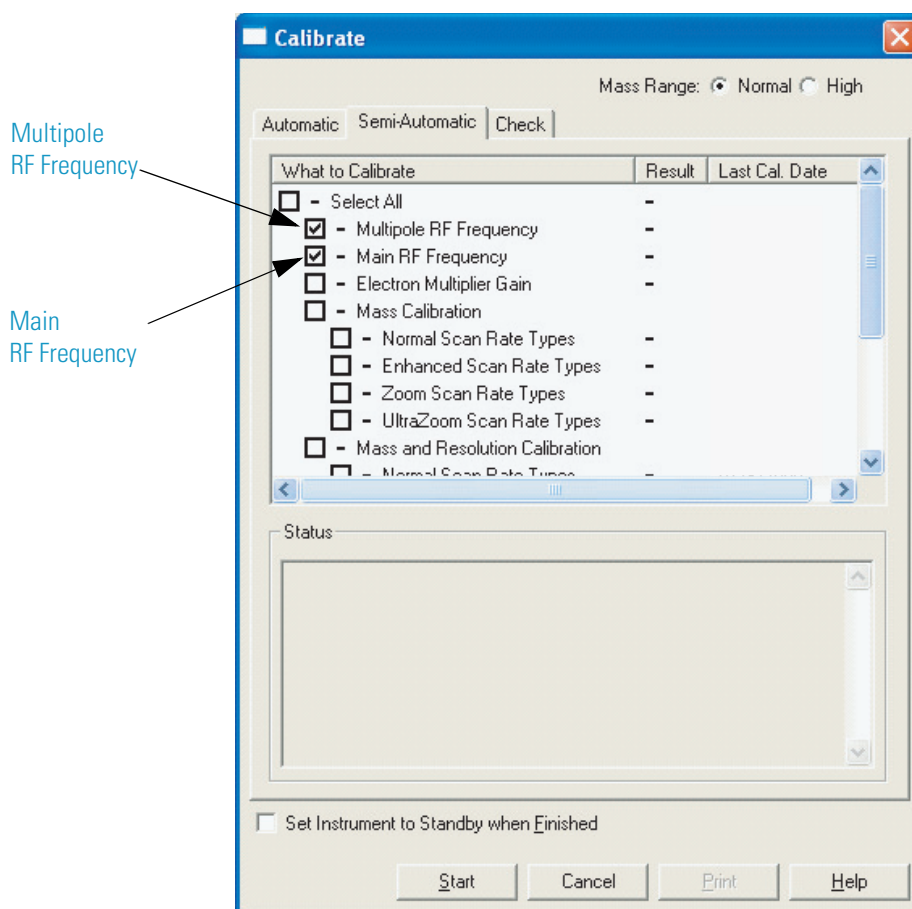
1. Tune the Multipole RF and Main RF. Click **Calibrate** in the Tune Plus window task bar (Figure 47). You may also access Calibrate from the

Control menu at the top of the Tune Plus window by choosing **Control** > **Calibrate**.



**Figure 47.** LXQ Tune Plus window. The Calibrate button is indicated.

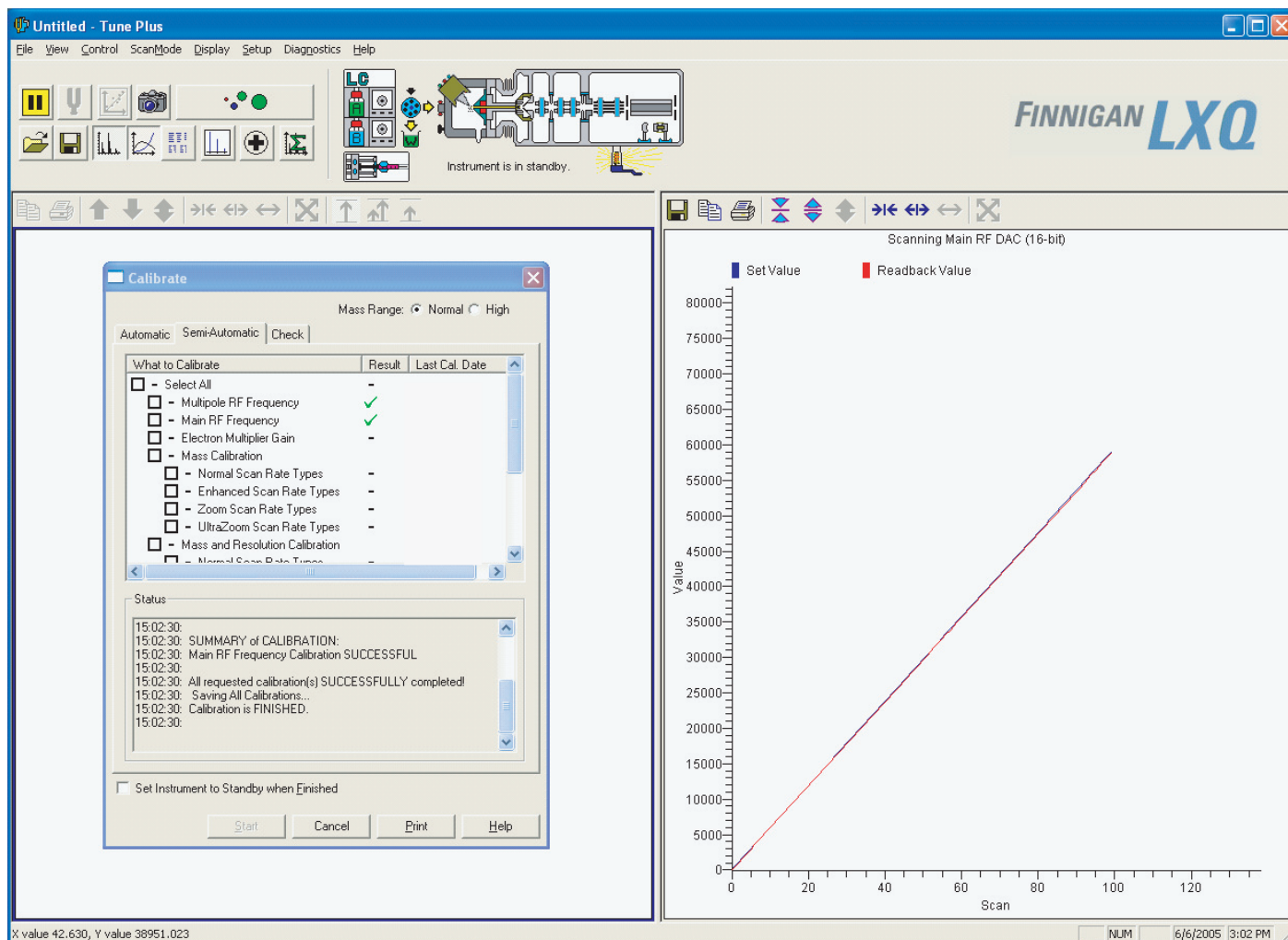
2. The Calibrate dialog box will appear (Figure 48). In this dialog box choose the Semi-Automatic tab. Then click in the boxes to the left of both Multipole RF Frequency and Main RF Frequency in the What to Calibrate section. Check marks will appear in the boxes after you click in them. Finally, click on the Start button at the bottom of the dialog box.



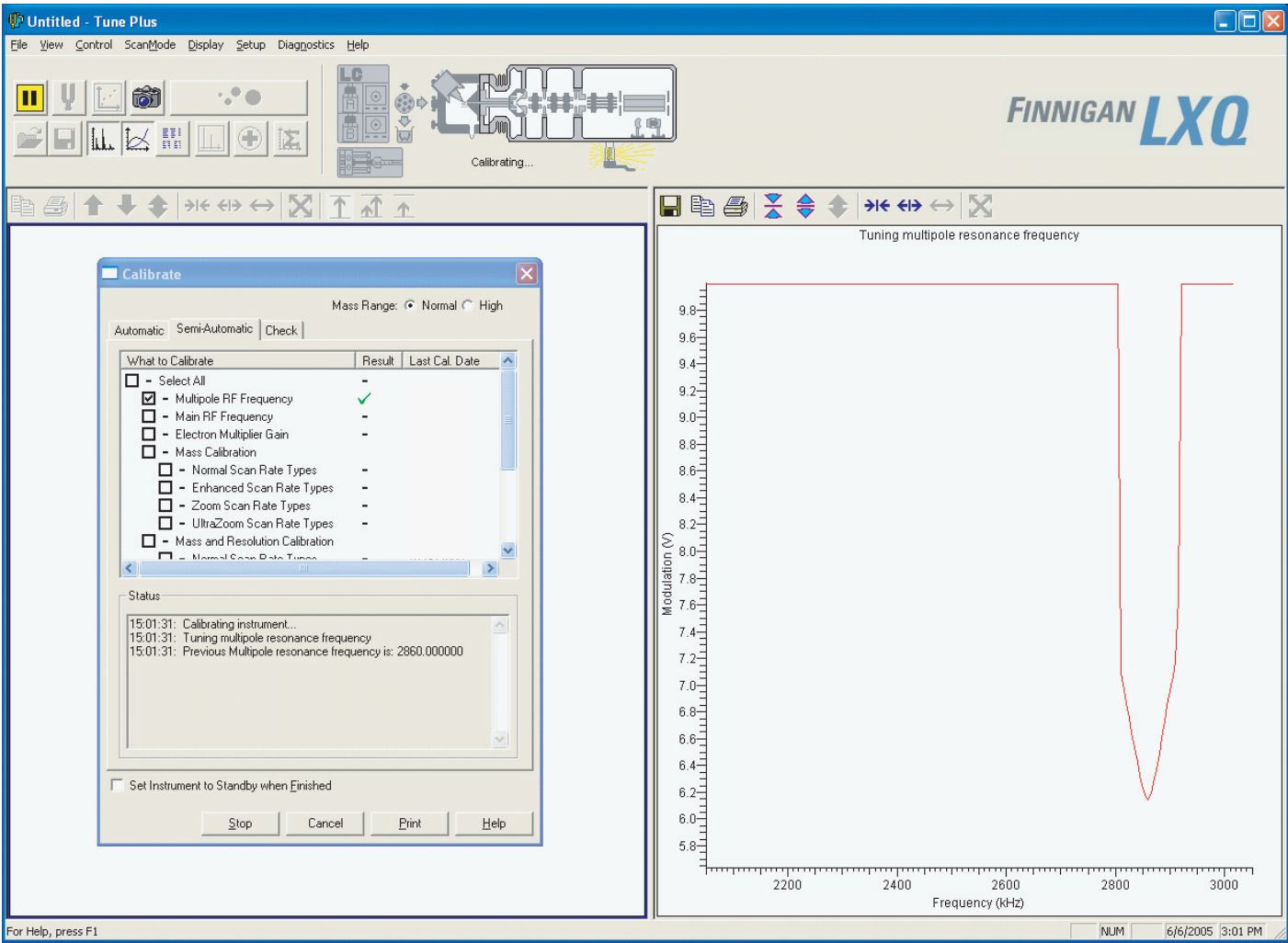
**Figure 48.** Calibrate Dialog Box. Multipole RF Frequency and Main RF Frequency are indicated.

3. Upon pressing the Start button (see Step 2 above) the instrument will carry out an automated sequence of steps. These will be displayed as graphs on the right side of the Tune Plus window. The titles of the graphs are: Scanning Main RF DAC (16-bit) (Figure 49), Tuning Multipole Resonance Frequency (Figure 50), Scanning Multipole Resonance DAC (Figure 51), and Tuning RF Resonance Frequency (Figure 52). The graphs shown in Figure 49 through Figure 52 will appear automatically as the instrument goes through the tuning procedure. Note, ignore the What to Calibrate items checked in the

Calibrate dialog boxes shown in Figure 51 and Figure 52. These were checked specifically to produce the examples shown in the Figures.

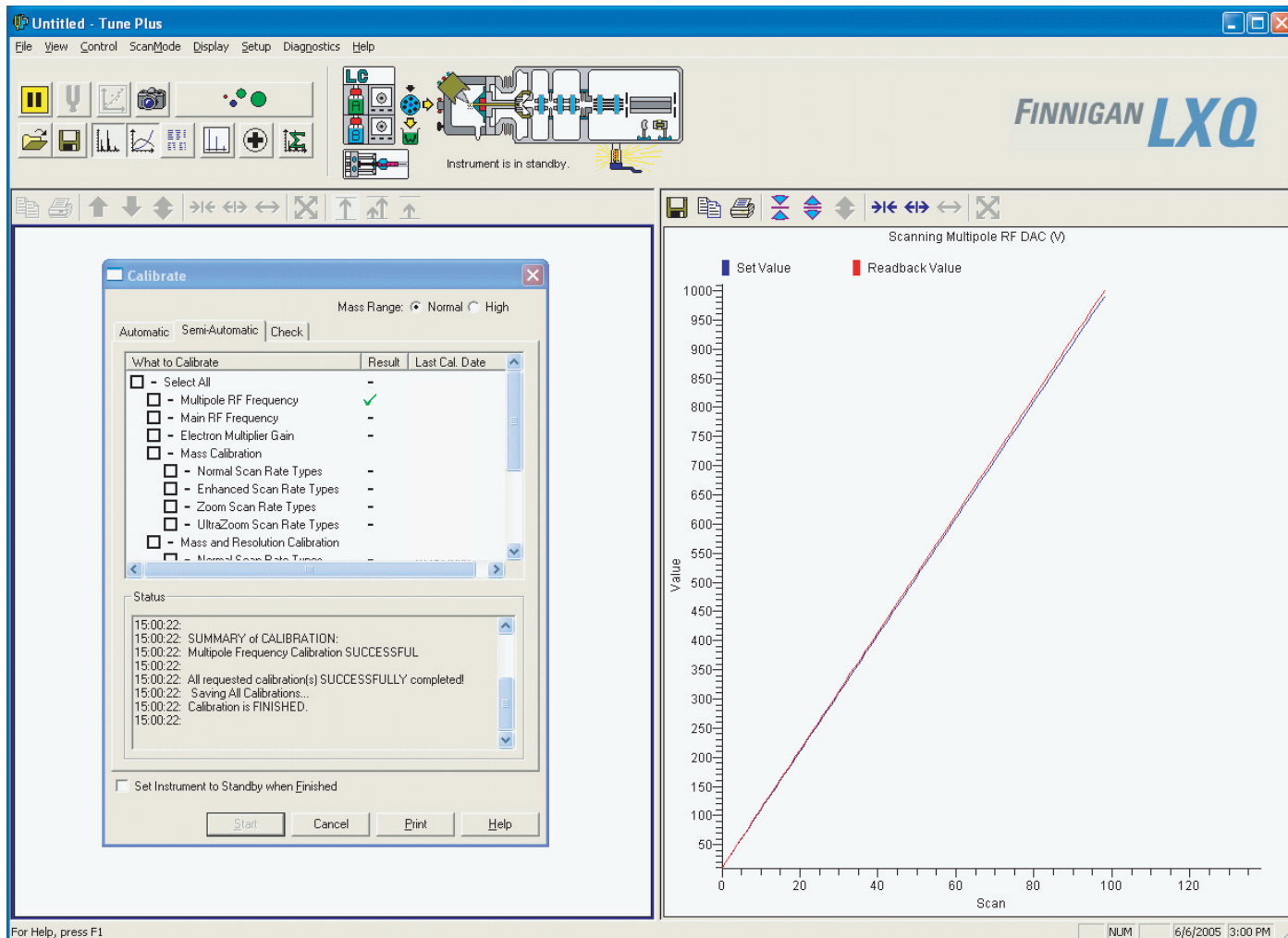


**Figure 49.** Main RF Frequency Tune procedure. Scanning Main RF DAC (16 bit) graph is shown.



**Figure 50.** Multipole RF Frequency Tune procedure. Tuning Multipole Resonance Frequency graph is shown.

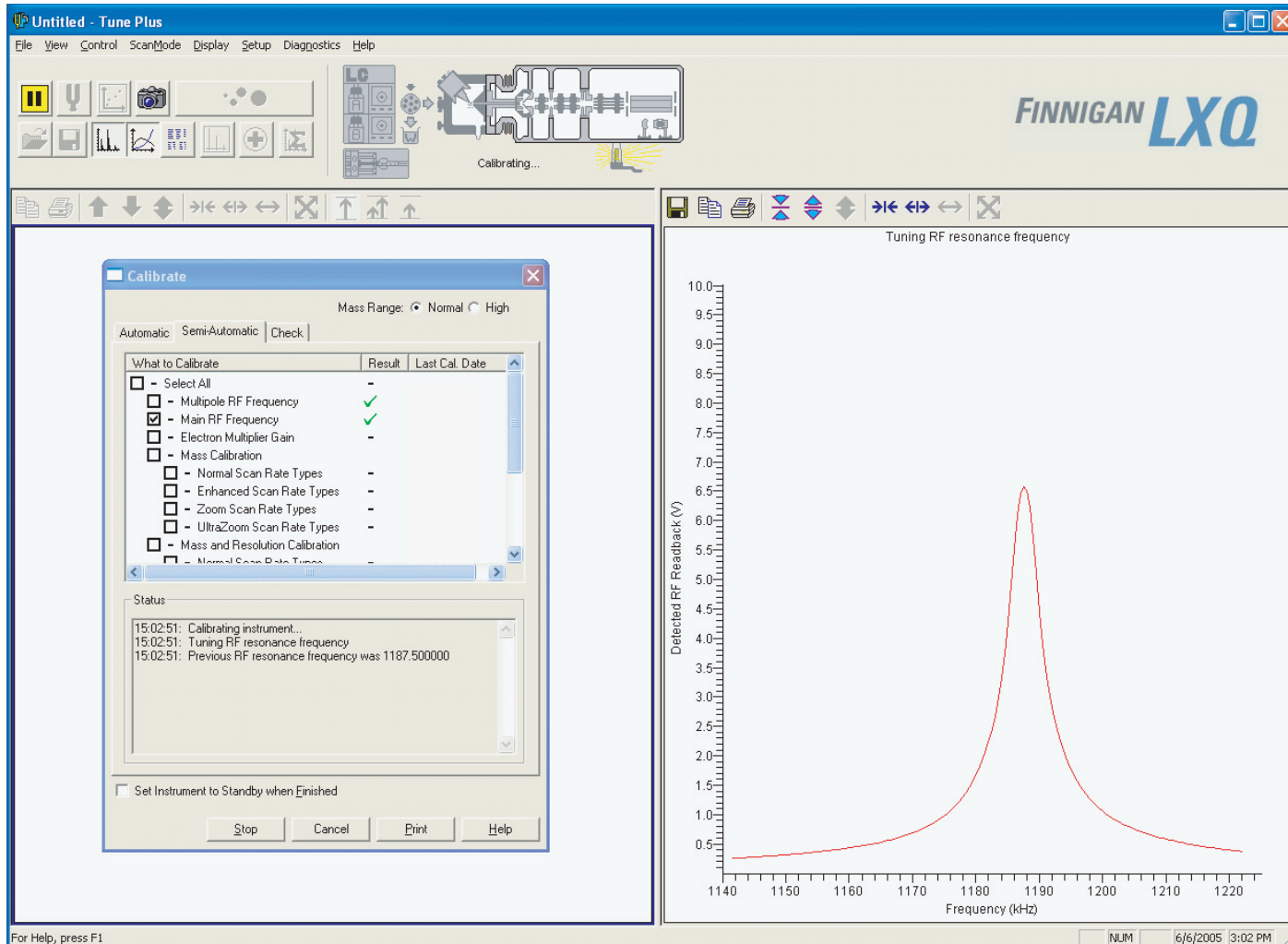




**Figure 51.** Multipole RF Frequency Tune procedure. Scanning Multipole RF DAC graph is shown.

## 6 Diagnostics and PCB and Assembly Replacement

### Running the LXQ Diagnostics



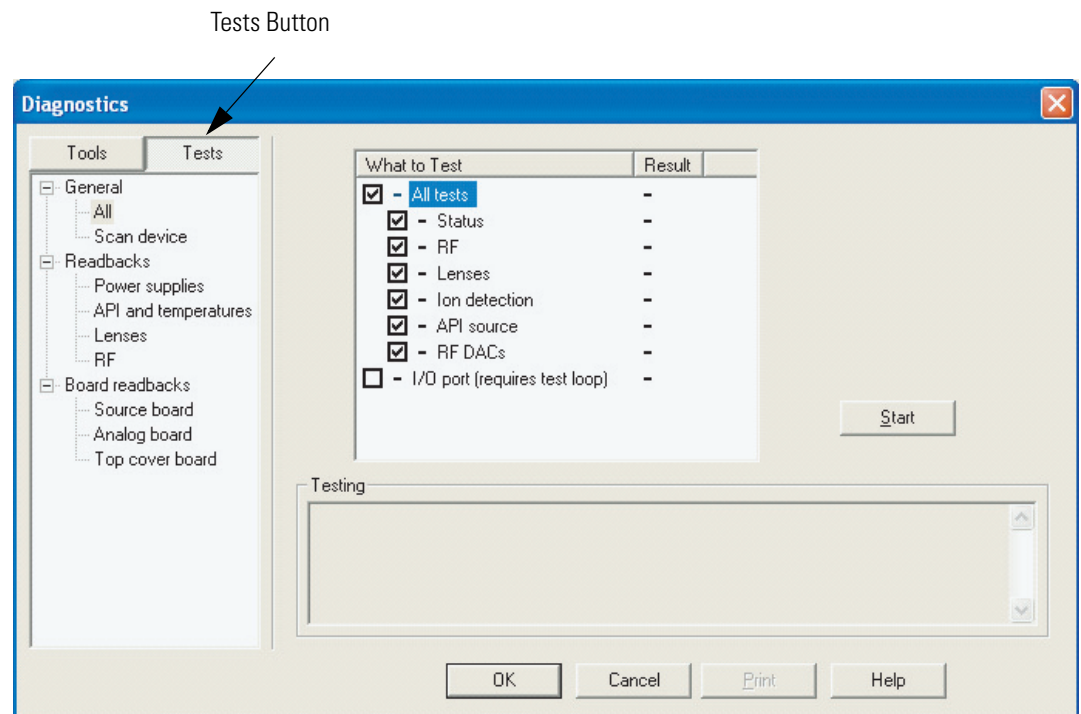
**Figure 52.** Main RF Frequency Tune procedure. Tuning RF Resonance Frequency graph is shown.

4. In the Tune Plus window, choose **Diagnostics > Diagnostics**. (To open Tune Plus, choose **Start > Programs > Xcalibur > LXQ Tune**.) The Diagnostics dialog box appears (Figure 53). Click on the Tests button (Figure 53).
5. Select one of the following options:

- Looking at the text box on the left side of the dialog box (under the Tests button), click on the plus sign beside GENERAL if the choices under GENERAL are not visible. Then, click **ALL** under GENERAL. Next, look at the What to Test group box in the center of the Diagnostics dialog box and click on the check box next to ALL TESTS. The check boxes of the subsystems under ALL TESTS will automatically become checked. This will test all of the electronic subsystems (that is, power supplies, lenses, ion detection system, electronics and RF system) as shown in Figure 54.
- To test an individual subsystem, click on the box corresponding to that subsystem in the What to Test page.

6. Click the **Start** button to start the diagnostics.

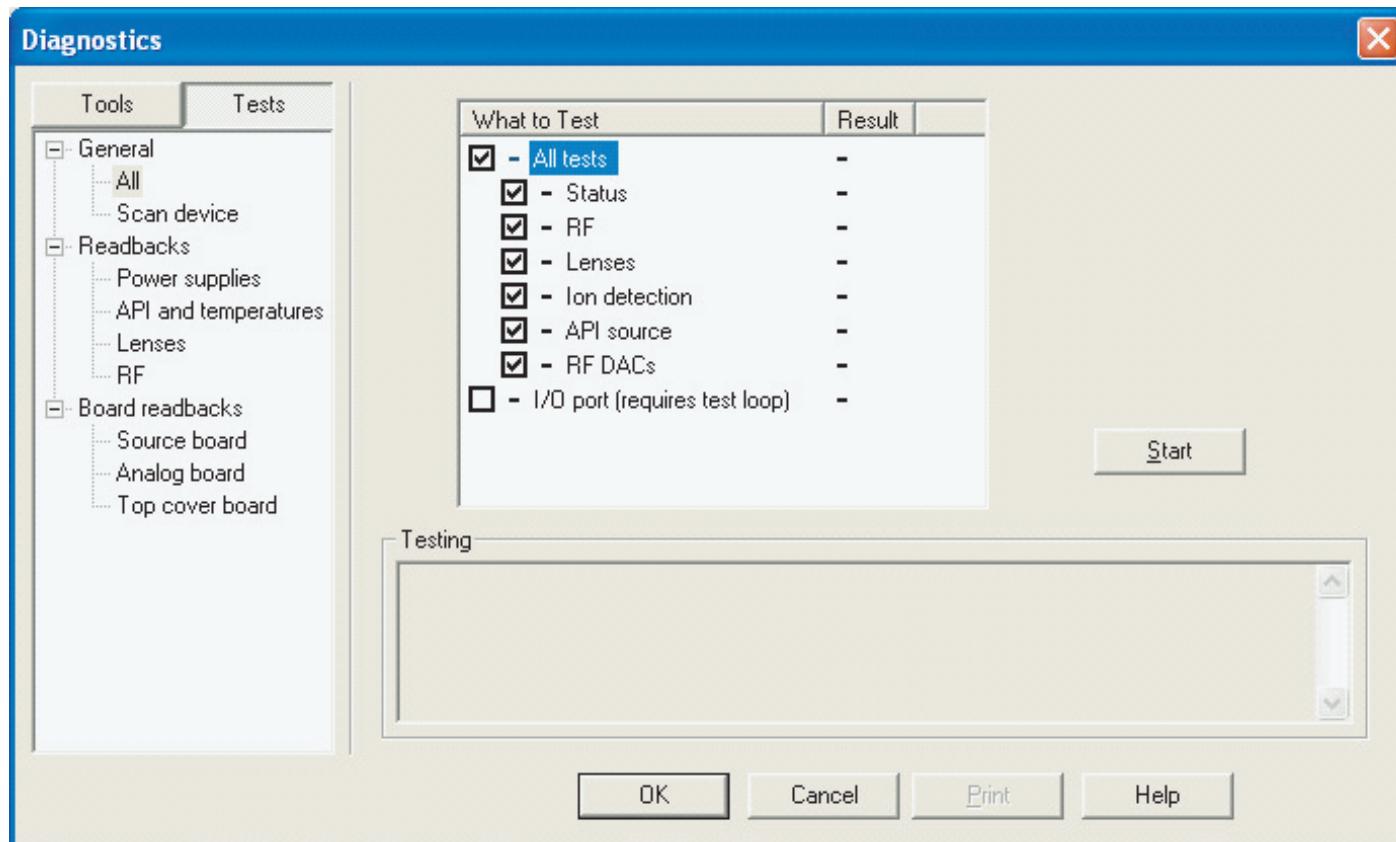
LXQ starts testing and displays a chronological log of all diagnostic tests in the Testing text box. Once testing for a specific subsystem is completed the LXQ displays for the subsystem either a Pass (green check mark) or a Fail (red X) in the Result group box. If the LXQ diagnostics indicate a problem, perform the maintenance procedure as instructed by one of the following: a) the LXQ diagnostics, b) Thermo Electron Technical Support, c) a Thermo Electron Customer Support Engineer. For more information on the LXQ diagnostics, refer to the LXQ online Help.



**Figure 53.** Diagnostics dialog box showing All Tests checked.

## 6 Diagnostics and PCB and Assembly Replacement

Running the LXQ Diagnostics



**Figure 54.** Diagnostics dialog box showing All Tests checked.

## Replacing a Fuse

Fuses protect the various circuits by opening the circuits whenever overcurrent occurs. On the MS detector the fuses are located on the Interlock PCB and Source PCB. The function and current rating of the various fuses are listed in [Table 5](#).

Check fuses when power is lost to a fused subsystem.



**CAUTION** Always shut down the system and disconnect the power cord before you replace fuses.

Use only the fuses specified in [Table 5](#). Never replace a fuse with a fuse of a different type, voltage, or current rating.

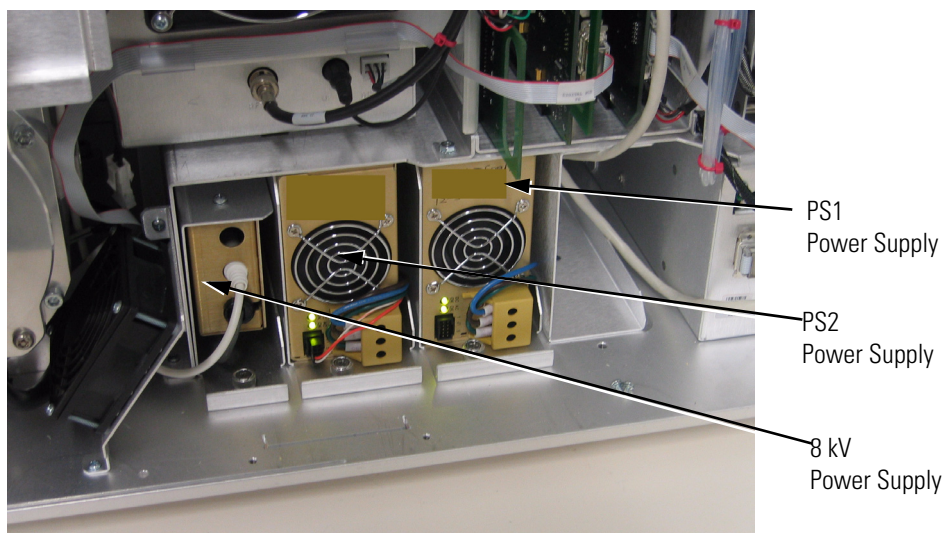
**Table 5.** MS detector fuses

Location	Fuse	Circuit	Description	P/N
Interlock PCB	F1, F3	APCI vaporizer heater	3.15 A, Type F, 5 x 20 mm, 250 V	00006-10510
Interlock PCB	F2, F4	220 Vac	6.3 A, 250 V	00006-11450
Source PCB	F3		4.0 A, 250 V	00006-11420

## Replacing Power Supplies

The following power supplies are used in the LXQ. They are easily accessed from the front of the LXQ if service or replacement is needed. See [Figure 55](#).

- PS1 power supply (P/N 97055-60014S)
- PS2 power supply (P/N 97055-60015S)
- 8 kV power supply (P/N 97055-60033)



**Figure 55.** Power supplies

### To replace the power supplies

1. Shut down and vent the system as described in the topic [“Shutting Down the System Completely”](#) on [page 131](#).



**CAUTION** Make sure that the LXQ power cord is unplugged before you proceed.

2. Open the right front door of the MS detector by loosening the Allen screw on the right door.
3. If necessary, remove the left front cover as follows:
  - a. If necessary, remove the Ion Max ion source housing as described in the topic [“Removing the Ion Max Ion Source Housing”](#) on [page 93](#).



- b. Unscrew the two fasteners that secure the left front cover to the vertical beam.
  - c. Move the left front cover up by 0.2 in., and then pull it out enough to access the cables that connect to the back.
  - d. Disconnect the cables and remove the cover.
4. If necessary, remove the vertical beam.
5. The power supplies in the Power Supply Housing have bulkhead connectors on the back. To remove a power supply, loosen the fastener that holds it to the chassis and then carefully tug on the power supply to remove it as a module.
6. Unpack the new power supply. Retain the packing materials so that you can pack and ship the defective switching power supply assembly to the Thermo Electron Repair Center in San Jose. **Be sure to note the apparent problem or symptoms on the enclosed forms.**
7. Slide the new power supply into the space occupied by the old power supply. Push carefully on the power supply to seat the connectors in the rear.
8. Tighten the fastener that holds the power supply to the tower.
9. If necessary, reinstall the vertical beam if you removed it in [step 4](#).
10. If necessary, reinstall the left front cover if you removed it in [step 3](#), as follows:
  - a. While holding the left front cover next to the left side of the MS detector, reconnect the cables to the back of the cover.
  - b. Reinstall the left front cover on the MS detector and tighten the two fasteners that secure the left front cover to the vertical beam.
  - c. If necessary, reinstall the Ion Max ion source as described in [“Removing the Ion Max Ion Source Housing”](#) on [page 104](#).
11. Close the right front door of the MS detector. Tighten the Allen screw on the on the right front door.
12. Restart the system as described in [“Starting the System after a Complete Shutdown”](#) on [page 133](#).
13. Run the LXQ diagnostics to verify that the system is operational.

## Replacing PCBs in the MS Detector

The LXQ electronic assemblies are close-packed to minimize the size of the system. Due to the complexity of removing and reinstalling many of the LXQ PCBs, we recommend that a Thermo Electron Field Service Engineer replace the electronic assemblies.

PCBs and assemblies in the MS detector are shown in [Figure 56](#).

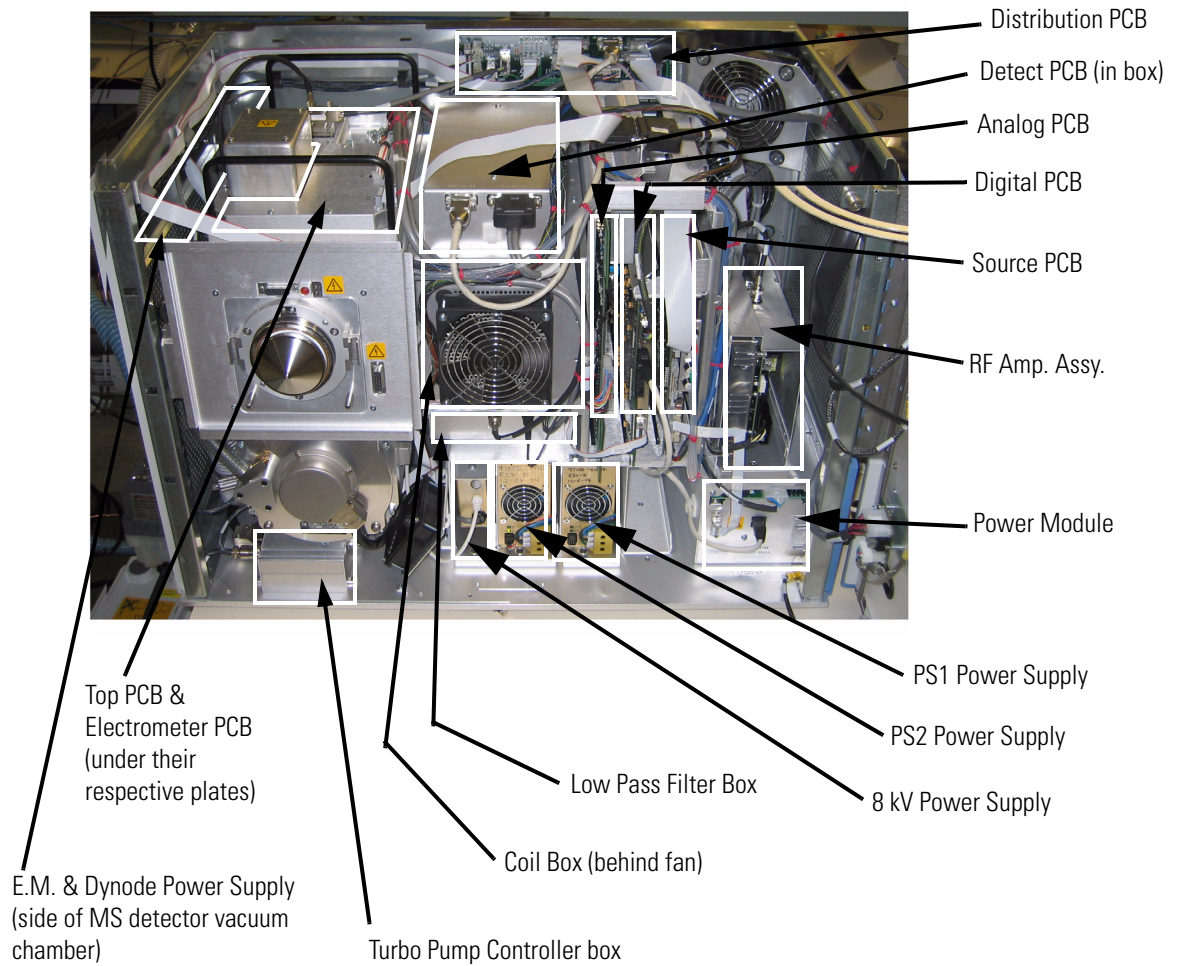


**CAUTION** Shutdown the system and unplug the power cord before you access PCBs and electronic assemblies.



**CAUTION** To prevent damage to the electronics due to electrostatic discharge, attach an electrostatic discharge (ESD) strap to your wrist before handling PCBs.





**Figure 56.** LXQ PCBs, power supplies, and electronic modules



## Chapter 7 Replaceable Parts

This chapter contains part numbers for replaceable and consumable parts for the mass spectrometer, data system, and kits. To ensure proper results in servicing the LXQ system, order only the parts listed or their equivalent.

**Note** Not all parts are available for purchase separately. Some parts may be only available for purchase as part of a kit or assembly.

Some parts are also available as exchange parts. An exchange part is a refurbished part that can be purchased at a discounted price. Exchange parts are specified by placing *EX* in front of the part number. For example, EX70111-60002S

This chapter contains part numbers for the following:

- [MS Detector](#)
- [Manuals](#)
- [Accessory Kit](#)
- [Metal Needle Kits](#)
- [Fittings, Ferrules, Sample Loops, and Tubing](#)
- [Chemicals Kit](#)

## MS Detector

Replaceable parts are available for the following:

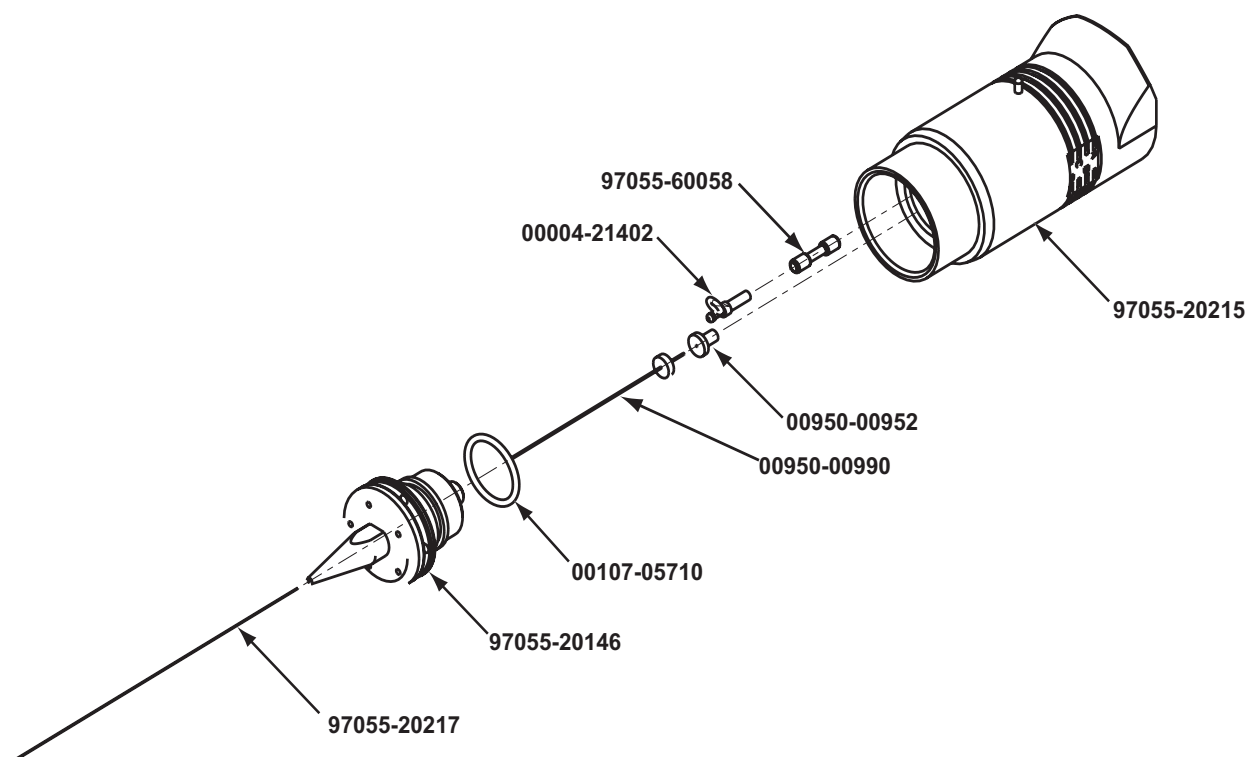
- ESI source
- APCI source
- Ion source interface
- Ion guides
- Mass analyzer
- Divert/inject valve
- Syringe pump
- Turbomolecular pump
- Forepump
- Pressure gauges
- Vacuum system assemblies
- Vacuum manifold O-rings
- Vent valve
- Power supplies
- Printed circuit boards (PCBs)
- RF control / detection assemblies
- Cables
- Fans

## ESI Source

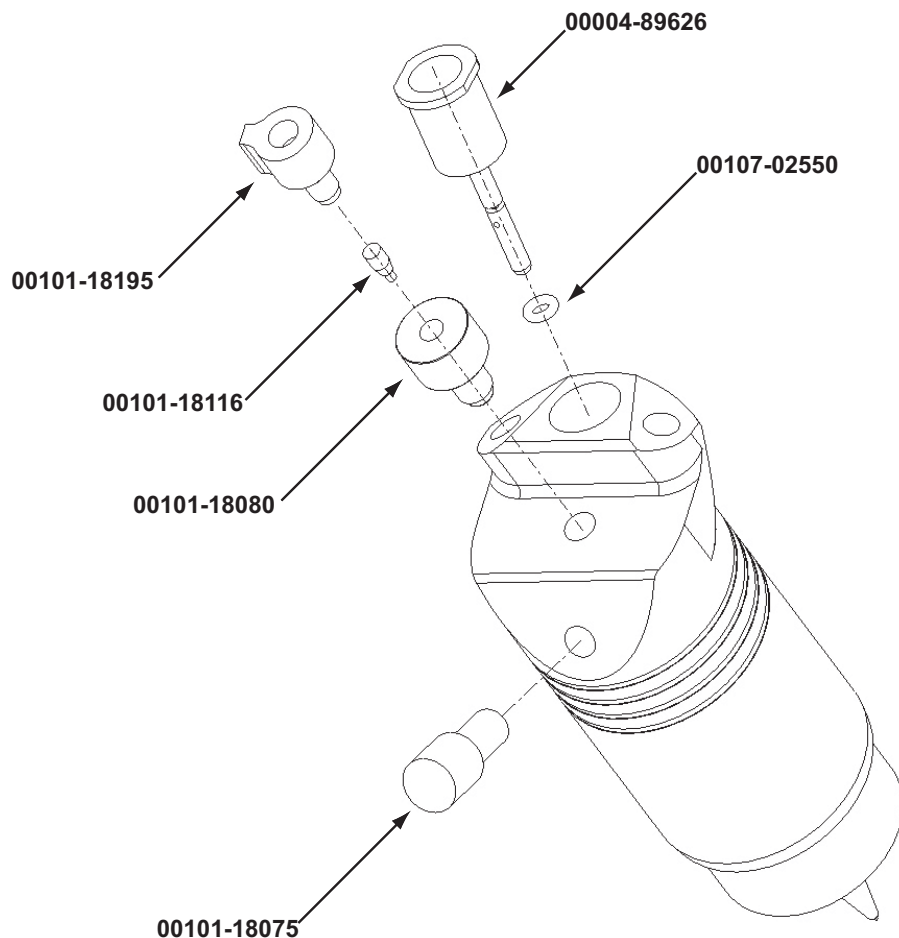
Please note that not all parts are available for purchase separately, some parts may only be available for purchase as part of a kit or assembly.

<b>ESI Probe .....</b>	<b>OPTON-20011</b>
Body-probe manifold, .....	97055-20215
Nozzle-ESI probe 3-port, .....	97055-20146
Fitting, union, ZDV, 1/4-28, PEEK, black,.....	00109-00304
Needle, metal, 32 gauge, ESI,.....	97055-20217
Contact, Battery, BECU, 0.598 mml, 0.02 ohm@4A,..	00004-21402
Seal STD needle 5000 series,.....	00950-00952
Needle, D PNT 26 gauge, 2""L, .24D washer,.....	00950-00990
O-ring 00.438ID 1/16 in. Viton,.....	00107-05575

Connector receptacle, high voltage, shielded, .....	00004-89626
Ferrule .012ID KEL-F HPLC, .....	00101-18116
Fitting, Fingertight 2 Upchurch, .....	00101-18195
Fitting, plug 1/4-28 TEFZEL HPLC, .....	00101-18075
O-ring 0.676 ID 1/16 TH VI, .....	00107-05710
O-ring 00.125ID 1/16TH VI, .....	00107-02550
Assembly-resistor contact-ESI probe,.....	97055-60058
Sleeve-resistor, .....	97055-20147
Resistor FXD CC 1/4W 22M 5%,.....	00015-27820
Fitting HPLC adptr 10-32 × 1/4-28KEL,.....	00101-18080
Tubing fused-silica .10 ID × .19, .....	00106-10499
Ferrule .008 ID KEL-F HPLC, .....	00101-18114
<b>Safety Sleeve Kit .....</b>	<b>70005-62015</b>
Ferrule .27 ID PEEK HPLC, .....	00101-18119
Tube .009IDx. 024 OD × 10" natural PEEK,.....	00301-22806
Instructions safety sleeve,.....	70005-97009
FTG Fingertight 2 Upchurch, .....	00101-18195
FTG, nut, finger, HPLC, 10-32, PEEK, .....	00101-18081
<b>Stainless steel needle kit, 32 gauge,.....</b>	<b>OPTON-20014</b>
<b>Stainless steel needle kit, 34 gauge,.....</b>	<b>OPTON-20015</b>



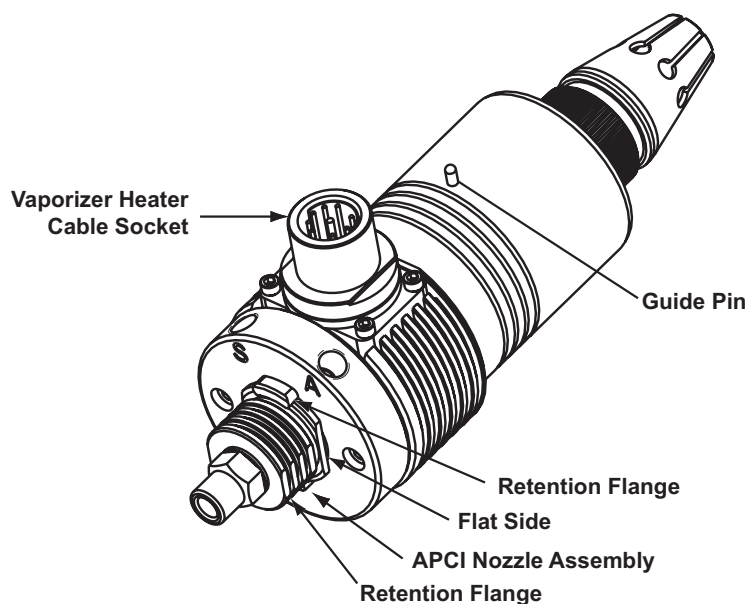
**Figure 57.** Exploded view of the ESI probe



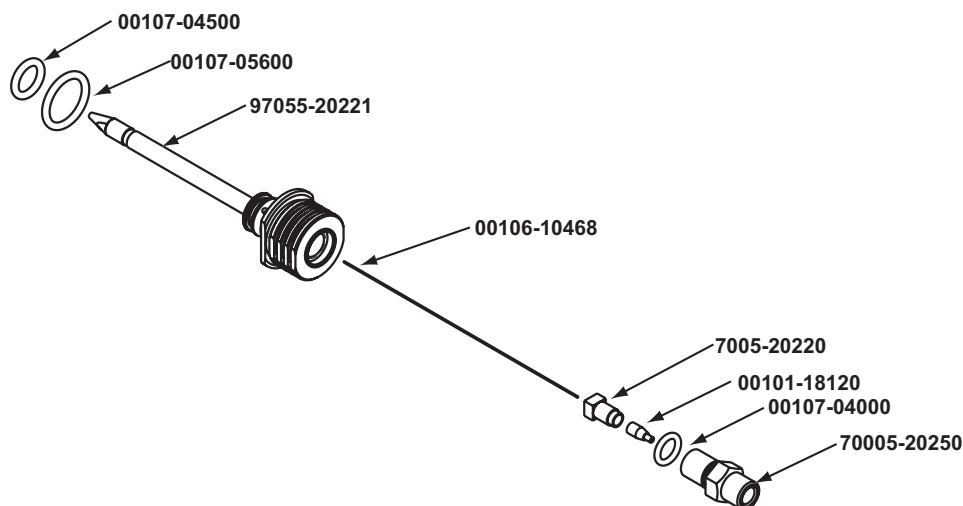
**Figure 58.** Replaceable parts for the ESI probe

## APCI Source

APCI probe, .....	OPTON-20012
APCI probe nozzle assembly, .....	97055-60089
Ferrule, .016ID PEEK HPLC, .....	00101-18120
Tubing, fused silica 150U X 390U, .....	00106-10498
O-ring, .239 1/16th Viton, .....	00107-04000
O-ring, 00.312 ID=5/16 1/16, .....	00107-04500
O-ring, 00.500 ID 1/16TH VI, .....	00107-05600
Fitting, 10-32 male nut PEEK, .....	70005-20220
Fitting, APCI flange, .....	70005-20250
Nozzle, APCI probe, .....	97055-20221



**Figure 59.** APCI Probe Assembly (OPTON-20012)



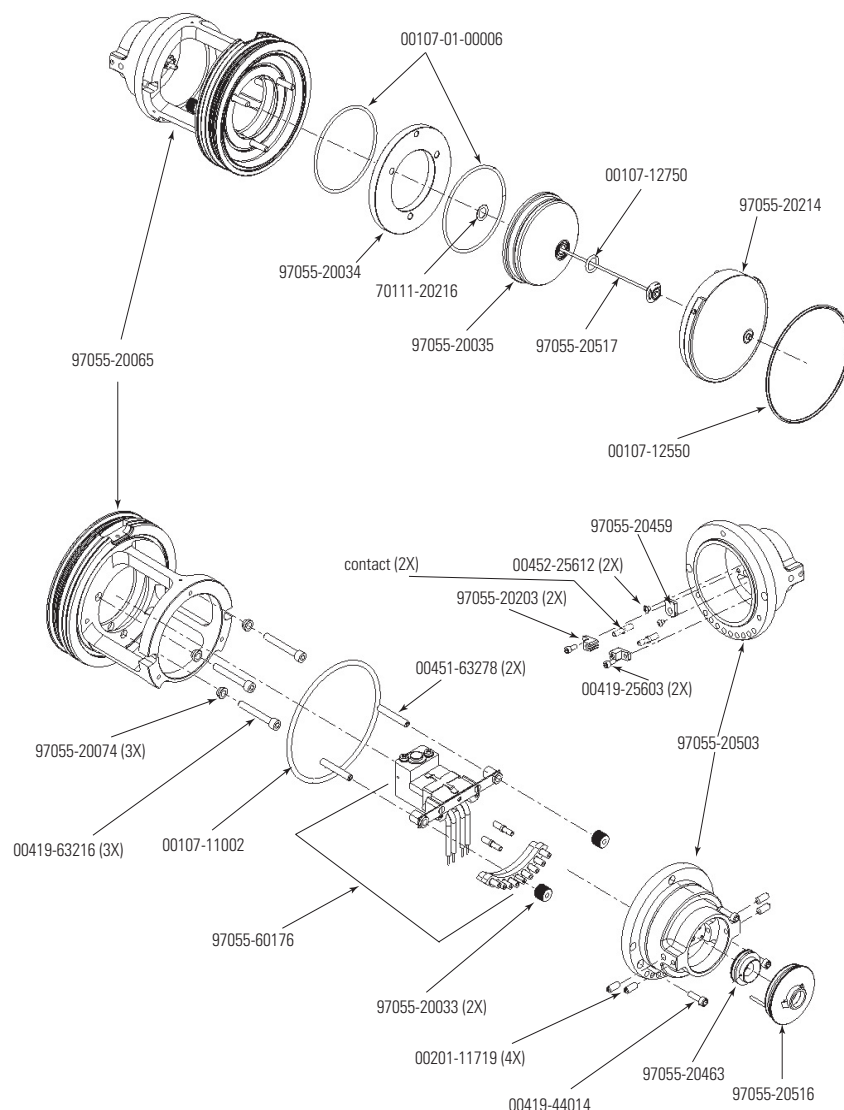
**Figure 60.** APCI probe nozzle assembly (P/N 97055-60089)

## Ion Source Interface

<b>Ion Source Interface Assembly .....</b>	<b>97055-60181</b>
Contact socket for 0.048 x 0.064D pin, .....	00107-12550
O-ring, 2-033 Viton V884 (2 x 1/16), .....	00107-01-00006
O-ring, 2.625ID x 3/32, AS-146, Viton, .....	00107-11002
O-ring, 2-74 x 0.063, 2-039 Viton, .....	00107-12550
O-ring, 0.30ID x 0.054, Kalrez, CMPD, 4079, .....	00107-12750
Plunger ball, 6-40 x 0.31, 1lb, .....	00201-11719

Screw, socket, 2-56 x 3/16, ss, .....	00419-25603
Screw, 4-40 x 3/8, SHCS, vented, stainless steel, .....	00419-44014
Screw, socket, 6-32 x 1, ss, .....	00419-63216
Screw, set, socket, 6-32 x 7/8, alloy, A574, .....	00451-63278
Screw, 2-56 x 3/32, socket head, stainless steel, .....	00452-25612
Seal, graphite source heater, .....	70111-20216
Thumbnut, knurled 6-32in., .....	97055-20033
Seal, API cone, .....	97055-20034
Cone, API source (sweep cone), .....	97055-20035
Ring, contact, support, .....	97055-20503
Capillary heater assembly, .....	97055-60176
Bushing, nose cone insulator, .....	97055-20074
Cage, capillary heater mount, .....	97055-20065
Ion transfer capillary, 500 micron, .....	97055-20517
Clamp socket, .....	97055-20203
Ion sweep cone, .....	97055-20214
Tube lens, .....	97055-20463
Skimmer, .....	97055-20516

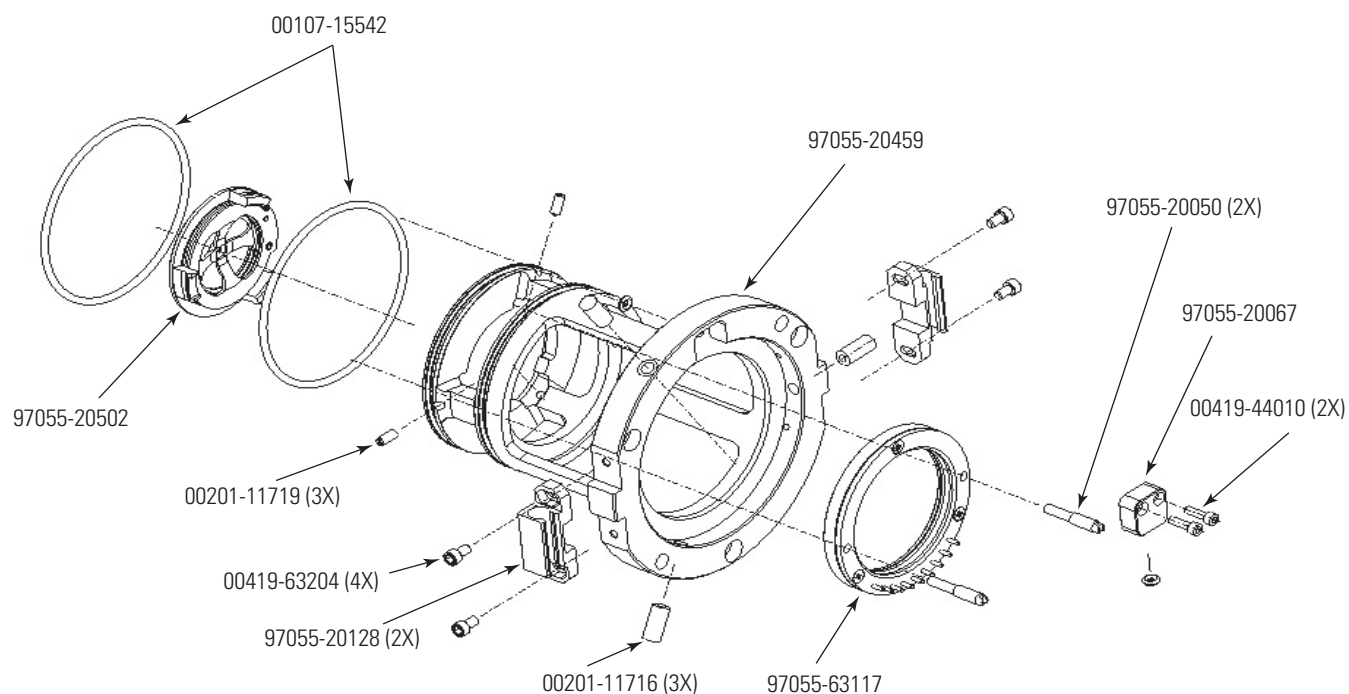




**Figure 61.** Ion source interface part numbers

<b>Q00 RF Lens</b>	<b>Q00 Device Assembly</b>	<b>97055-60180</b>
	O-ring, 0.101ID x 0.070, Viton, .....	00107-02456
	O-ring, 2-148, Viton 884, .....	00107-15542
	Plunger ball, ¼-20 x 0.53, 4lb, .....	00201-11716
	Plunger ball, 6-40 x 0.31, 1lb, .....	00201-11719
	Screw, socket HD, CAP, 4-40 x 3/8, ss, .....	00419-44010
	Screw, socket, 6-32 x ¼, ss, .....	00419-63204
	Rod, threaded guide, .....	97055-20050

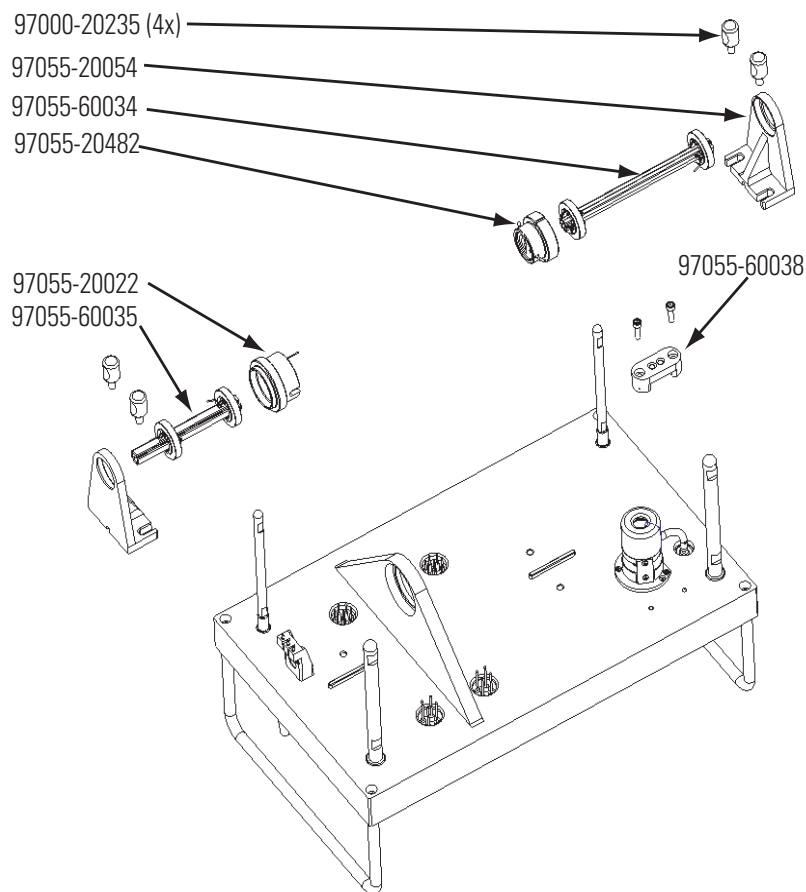
Cage, outer contact support, .....	97055-20459
Manifold, API gas inlet, .....	20504
Latch block, probe housing, .....	97055-20128
Cage Contact Ring Assembly, .....	97055-63117
Device, Combo Q00/L0, .....	97055-20502



**Figure 62.** Q00 Device (RF Lens) part numbers

## Q0 and Q1 Ion Guides

Thumb screws, 10-32,.....	97000-20235
Lens L1, .....	97055-20022
Gate lens, .....	97055-20482
Multipole bracket,.....	97055-20054
Q1 octapole, .....	97055-60034
Q0 quadrupole,.....	97055-60035



**Figure 63.** Q0 and Q1 ion guides part numbers

<b>Mass Analyzer</b>	Mass analyzer assembly, linear ion trap, ..... 97055-60169
<b>Electron Multiplier</b>	Electron multiplier assembly, ..... 96000-60036
<b>Coil Module</b>	RF coil and PCB Assembly, ..... 97055-60171
<b>Divert/Inject Valve</b>	Divert/inject valve (Rheodyne MM501, 2 position, 6 port), ..... 00110-03-00001 .....
<b>Syringe Pump</b>	Syringe pump, ..... 97055-98006

## **Turbomolecular Pump**

Turbomolecular pump insert (Leybold TW 220/150/15),  
..... EX00108-01-00004  
Turbomolecular pump controller (Leybold TDS),..... 00108-10012

## **Forepump**

**Forepump Kit,..... 70111-62014**  
Forepump (mechanical pump), E2M30, 650 L<sup>3</sup>/min, 220V AC,  
..... 00108-02655  
Vacuum hardware clamp, KF-20/25,..... 00102-10020  
Pump hardware centering ring, ..... 00108-02011  
Mist Filter, ..... 00108-02-00002  
Hose clamp, band, ..... 00201-03810  
PVC vacuum hose reinforced, 1.5-in ID, ..... 00301-24163  
Tool, extraction, minifit, ..... 00725-00050  
Drain oil return kit,..... 00960-01-00007  
Adapter, pump roughing line, ..... 70111-20210

## **Pressure Gauges**

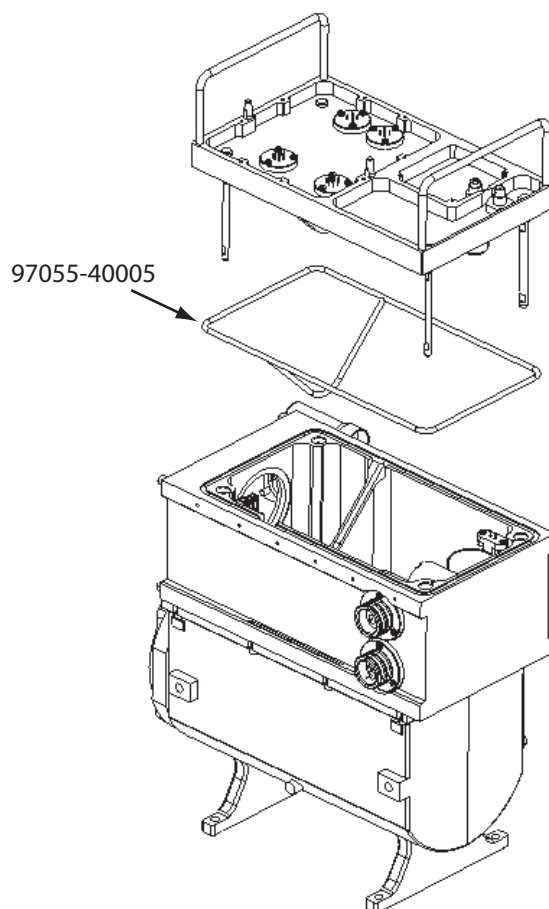
Convectron gauge, ..... 00105-00501  
Ion gauge, ..... 97055-62001

## **Vacuum Accessories**

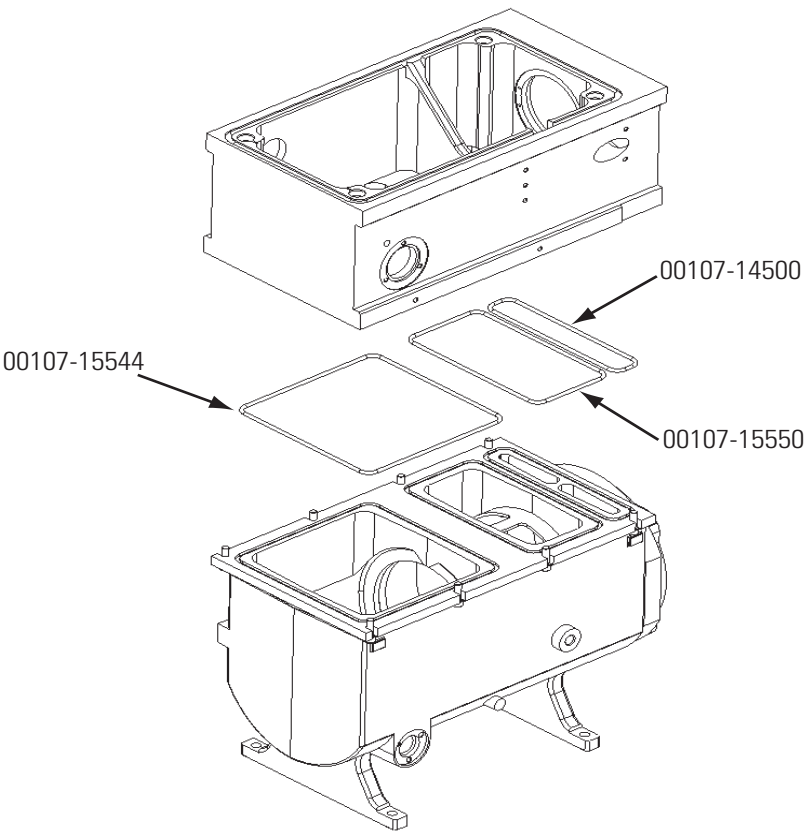
**Hose and Accessories Kit,..... 97055-62007**  
PVC vacuum hose reinforced, 1.5-in. ID, ..... 00301-24163  
Manifold, 3-port, 1.5-in.,..... 97055-20222  
Flange, NW40, long,..... 00108-02-00003  
Clamp, NW32/40, swing, ..... 00108-02-00004  
Ring, centering,..... 00108-02-00005  
Adaptor, pump roughing line, ..... 70111-20210  
Hose clamp, band, ..... 00201-03810  
Pump hardware centering ring, ..... 00108-02011  
Vacuum hardware clamp KF-20/25,..... 00102-10020

## **Vacuum Manifold O-Rings**

O-ring, 0.31-in. ID × 1/16,..... 00107-05000  
O-ring, 4.5-in. ID × 1/8, Viton,..... 00107-14500  
O-ring, 6.48-in. ID × 1/8, Viton,..... 00107-15270  
O-ring, 7.734-in. ID × 1/8, Viton,..... 00107-15544  
O-ring, 5.86-in. ID × 1/8, Viton,..... 00107-15550  
O-ring, split chamber, ..... 97055-40005



**Figure 64.** Vacuum manifold O-rings part numbers



**Figure 65.** Vacuum manifold O-rings part numbers

**Vent Valve** Vent valve assembly, ..... 97055-60084

**Power Supplies** PS1, +60 V (6 A), +5 V (35 A), ±15 V (14 A), ..... 97055-60014S  
PS2, +36 V (10 A), ±24 V (8.5 A), +28 V (6.7 A), ..... 97055-60015S  
8 kV Power Supply, ..... 97055-60033  
15 kV dual Electron Multiplier/Conversion Dynode power supply, .....  
..... 97055-98041  
Power module (available as exchange), ..... EX97055-60133

**Printed Circuit Boards (PCBs)** Source PCB (available as exchange), ..... 70111-61053S  
Interlock PCB, ..... 70111-61060S  
Digital PCB (available as exchange), ..... 97055-61011  
Distribution PCB, ..... 97055-61025  
Analog PCB (available as exchange), ..... 97055-61033

Top Cover PCB (available as exchange), .....	97055-61040S
I/O PCB, .....	97055-61070S
Front Panel PCB, .....	97055-61110S
Electrometer PCB, .....	97055-61190S
Low Pass Filter/Balun PCB (available as exchange), .....	97055-61420
Divert/Inject Valve PCB, .....	97055-61140S
RF Amplifier PCB, .....	97055-61180S

## Cables

Ethernet (Power Module) to Digital PCB, .....	00012-70064
Power Module wire set, .....	97055-63003
Interlock PCB to Power Module bulkhead, .....	97055-63004
Interlock PCB 220 Vac In, .....	97055-63006
I/O PCB to Power Module Elcon adapter, .....	97055-63008
Power module, +36/-28 Volt RF Amp Inhibit, .....	97055-63010
Convectron gauge to Power/Signal Distribution PCB, .....	97055-63016
Status Display/ Front Panel, .....	97055-63018
Divert Valve PCB to Divert Valve, .....	97055-63020
Manifold Flange to Power/Signal Distribution PCB, .....	97055-63022
RF Detect Sport to Power/Signal Distribution PCB, .....	97055-63024
RF Amplifier Control to Power/Signal Distribution PCB, .....	97055-63026
RF Amplifier Power to Power/Signal Distribution PCB, .....	97055-63028
Source & Top Cover SPI to Power/Signal Distribution PCB, .....	97055-63030
Vent, Turbo & Fans to Power/Signal Distribution PCB, .....	97055-63032
Daisy, Cooling Fans (3), .....	97055-63033
Dual Dynode / Electron Multiplier Supply to Power/Signal Distribution PCB, .....	97055-63041
Elcon, Power to Power/Signal Distribution PCB, .....	97055-63038
Elcon, System Signals to Power/Signal Distribution PCB, .....	97055-63040
PS2 to Elcon Connector, Sled, .....	97055-63042
PS1 to Elcon Connector, Sled, .....	97055-63044
Coax, WFM RF Signal, Analog to LPF, .....	97055-63046
Analog PCB to Top Cover PCB, .....	97055-63048
Interlock (AC Power Module) to Source PCB, .....	97055-63050
Turbomolecular pump RS485 to Digital PCB, .....	97055-63052
Analyzer Electrometer to Digital PCB, .....	97055-63056
Coaxial, LPF to RF Amplifier, .....	97055-63060
RF Amp Modulation to RF Detector, .....	97055-63062

## Fans

Fan, 100 CFM, 24V dc, located on fan housing assembly and on the coil box, .....	00013-00243
Fan, 21 CFM, 24V dc, located adjacent to the turbomolecular pump, .....	97055-63083
Fan filter, .....	97055-20254

<b>Manuals</b>	Finnigan LXQ Preinstallation Requirements Guide, .....	97055-97040
	Finnigan LXQ Getting Connected, .....	97055-97041
	Finnigan LXQ Getting Started, .....	97055-97042
	Finnigan LXQ Hardware Manual, .....	97055-97043



## Accessory Kit

<b>Accessory Kit, .....</b>	<b>97055-62038</b>
Adapter union, probe, ground, .....	97055-20230
Air duct, flexible, 1.0-in. ID, .....	00301-08301
Capillary, 500µm, length=4.87 inches, .....	97055-20517
Cable, serial, .....	00012-51086
Cable shield, 22 gauge, 24 ft., .....	00302-01800
Connector, receptical, 6 p, .....	00004-06-00008
Connector, receptical, 8 p, .....	00004-21507
Connector, acc., cable housing, 8 p, .....	00004-21509
Corona needle, APCI (5 each), .....	70005-98033
Drain, Ion Max 2, LTQ, .....	97055-20488
Fuse, 3.15 A, 250 V (Interlock PCB fuses F1 and F3), (4 each), .....	00006-10510
Fuse, 4 A, 250 V (Source PCB fuse F3), (4 each), .....	00006-11420
Fuse, 6.3 A, 250 V (Interlock PCB fuses F2 and F4), (4 each), .....	00006-11450
Ferrule, 0.008 in. ID, KEL-F, HPLC (4 each), .....	00101-18114
Ferrule, 0.016 in. ID, PEEK, HPLC (4 each), .....	00101-18120
Ferrule, Fingertight 2, Upchurch (3 each), .....	00101-18196
Ferrule, Tefzel, electrospray, 1/16-in., .....	00102-10148
Ferrule, tube, 1/16-in. (6 each), .....	2522-3830
Fitting, Swagelok, Adapt-M, 1/8 x 1/4-in., .....	00101-01740
Fitting, ferrule, HPLC, reducer, 1/8 x 16-in., .....	00101-02-00002
Fitting, Swagelok, bulkhead, 1/8 in., .....	00101-02102
Fitting, ferrule, Swagelok, Back, 1/8 in. (2 each), .....	00101-02500
Fitting, ferrule, Swagelok, Back, 1/4 in. (2 each), .....	00101-04000
Fitting, tube, bulkhead, 1/8 in., .....	00101-04-00001
Fitting, comp., elbow, 1/8 in., .....	00101-04-00002
Fitting, ferrule, Swagelok, Front, 1/8 in. (2 each), .....	00101-08500
Fitting, ferrule, Swagelok, Front, 1/4 in. (2 each), .....	00101-10000
Fitting, Swagelok, Nut, 1/4 in., brass, .....	00101-12500
Fitting, Swagelok, O-seal, 1/4 in., .....	00101-13510
Fitting, Swagelok, Nut, 1/8 in., brass (2 each), .....	00101-15500
Fitting, nut, HPLC, flangeless (2 each), .....	00101-18084
Fitting, Fingertight 2, Upchurch, .....	00101-18195
Fitting, flangeless, 1/8 in. Upchurch, .....	00101-18198
Fitting, ferrule, 1/8 in. Tefzel, .....	00101-18199
Fitting, flangeless, 1/8 in. Blue Delrin, .....	00101-18200
Fitting, HPLC Union, 0.010 orifice, PEEK, .....	00101-18202
Fitting, HPLC, Tee, 0.020 orifice, PEEK, .....	00101-18204
Fitting, ferrule, 1/8 in. Tefzel, short, .....	00101-18223
Fitting, union, tube, bulkhead, 1/4-in., .....	00103-01-00001
Fitting, tube, straight, 1/8-in. x 10-32, .....	00103-10990
Fitting, Tee, barbed, 1.0-in., .....	00102-10120
Fitting, HPLC, nut, flangeless, 1/4-in.-28, .....	00109-02-00002
Fitting, bushing, Rheodyne (6 each), .....	2522-0066

Hose, poly, spiral, PVC, superflex, 1.5 ft., .....	00301-24168
Ion transfer capillary, insert, replaceable, .....	97055-20198
Kit, Chemicals, .....	97000-62042
Needle, D Point, 26 gauge, 2 in. long, 0.24D washer, .	00950-00990
Nut, flangeless, electrospray, 1/16-in., .....	00102-10146
O-ring, 0.101 ID, Viton (6 each), .....	00107-02456
O-ring, 0.125 ID, Viton (2 each), .....	00107-02550
O-ring, 0.174 ID, Viton , .....	00107-02464
O-ring, 3/16-in. (6 each), .....	00107-01-00009
O-ring, 0.218-in., Viton (2 each), .....	00107-01-00004
O-ring, 0.239 ID, Viton (3 each), .....	00107-04000
O-ring, 0.30 ID, Kalrez, .....	00107-12750
O-ring, 0.312 ID, .....	00107-05000
O-ring, 0.375 ID, .....	00107-07000
O-ring, 0.468 ID, Viton, .....	00107-07600
O-ring, 0.5 ID, Viton, .....	00107-08000
O-ring, 0.737 ID, Viton (2 each), .....	00107-10056
O-ring, 0.739 ID, Viton, .....	00107-10100
O-ring, 0.926-in., Viton, .....	00107-01-00013
O-ring, 1.37 ID, 0.103 thickness, Viton, .....	00107-10400
O-ring, 1.375 ID, 1/16th thickness, Viton, .....	00107-05904
O-ring, 2.033-in., Viton, .....	00107-01-00006
O-ring, 2.5-in., Viton, .....	00107-01-00002
Oil, vacuum pump, 1 L, .....	00301-15101
Sample loop, 2 µL, PEEK, .....	00110-16012
Sample loop, 20 µL, stainless steel, .....	00110-22014
Sample loop, 5 µL, stainless steel, .....	00110-22026
Seal, STD, Needle, 5000 Series, .....	00950-00952
Seal, API source heater, graphite, .....	70111-20216
Syringe, 10 µL, Rheodyne, .....	00301-19008
Syringe, 250 µL, Gas Tight, Removable needle, .....	00301-19015
Syringe, 500 µL, Gas Tight, Removable needle, .....	00301-19016
Tool, ion transfer capillary removal, .....	70111-20258
Troubleshooting guide, HPLC, .....	00920-05914
Tubing, Teflon, 0.125 mm OD × 0.03 w (2 each), .....	00101-50000
Tubing, PFA, 0.25 mm OD × 0.062 w (2 each), .....	00101-50100
Tubing, fused silica, 0.150 mm × 0.390 mm, .....	00106-10498
Tubing, fused silica, 0.10 mm ID × 0.19 mm OD, .....	00106-10499
Tubing, fused silica, 0.05 mm ID × 0.19 mm OD, deactivated, .....	00106-10502
Tubing, fused silica, 0.11 mm ID × 0.4 mm OD, deactivated, .....	00106-10504
Tubing, Cu, refrigeration, 1/8-in. OD 16.5 ft. long, ...	00301-22701
Tubing, PVC, unreinforced 0.005 ID × 1/16 in. OD, 10 ft. long, .....	00301-22895
Tubing, Teflon, 0.030 in. ID × 1/16 in. OD, .....	00301-22915

Tubing, PEEK, 0.005 ID × 1/16 in. OD, Red, 5 ft. (1.5 m long),  
..... 00301-22912  
Wrench, Allen/hex, 1/4 inch BP/W-handle, ..... 00725-00022

## Metal Needle Kits

### **High Flow Needle Kit, ..... OPTON-20004** **(Recommended for LC flow rates between 5 and 400 $\mu$ L/min)**

Ferrule, 0.012 in. ID, Kel-F, .....	00101-18114
Ferrule, 0.012 in. ID, Kel-, F .....	00101-18116
Fitting, Fingertight 2, Upchurch, .....	00101-18195
Union, zero dead volume, 1/4-28, Upchurch, .....	70111-20233
Blunt-tip, 32-gauge, 50 $\mu$ m ID, stainless steel needle, ..	70111-20287

### **Low Flow Metal Needle Kit, ..... OPTON-20005** **(Recommended for LC flow rates between 500 nL/min and 10 $\mu$ L/min)**

Ferrule, 0.012 in. ID, Kel-F, .....	00101-18114
Ferrule, 0.012 in. ID, Kel-F, .....	00101-18116
Fitting, Fingertight 2, Upchurch, .....	00101-18195
Union, zero dead volume, 1/4-28, Upchurch, .....	70111-20233
Blunt-tip, 34-gauge, 30 $\mu$ m ID, stainless steel needle, .	70111-20288

# Fittings, Ferrules, Sample Loops, and Tubing

Ferrule, Fingertight 2, Upchurch. (for: PEEK tubing and Teflon tube), .....	00101-18196
Ferrule, 0.016 in. ID, PEEK, Upchurch (for: Fused-silica capillary infusion line), .....	00101-18120
Ferrule, 0.012 in. ID, Kel-F, Upchurch (for: High flow metal needle and low flow metal needle), .....	00101-18114
Ferrule, 0.008 in. ID, Kel-F, Upchurch (for: Fused-silica capillary sample line), .....	00101-18116
Ferrule, LC, 1/16 in., stainless steel, Rheodyne, .....	2522-3830
Fitting, Fingertight, Upchurch, .....	00101-18195
Fitting, Fingertight, Upchurch, .....	00101-18081
Fitting, adapter, Kel-F, 10-32 × 1/4-28, Upchurch (connects directly to ESI probe inlet), .....	00101-18080
Nut, LC, 1/16 in., stainless steel, Rheodyne, .....	2522-0066
Fitting, LC union, 0.010 in. orifice, PEEK, .....	00101-18202
Fitting, LC TEE union, 0.020 in. orifice, PEEK, .....	00101-18204
Fitting, adapter union, PEEK, Upchurch, .....	00101-18206
5 µL sample loop, stainless steel, .....	00110-22010
10 µL sample loop, stainless steel, .....	00110-22012
20 µL sample loop, stainless steel, .....	00110-22014
50 µL sample loop, stainless steel, .....	00110-22016
100 µL sample loop, stainless steel, .....	00110-22018
500 µL sample loop, stainless steel, .....	00110-22020
1 mL sample loop, stainless steel, .....	00110-22022
Tubing, 0.15 mm ID × 0.39 mm OD fused-silica capillary (APCI sample tube), .....	00106-10498
Tubing, 0.10 mm ID × 0.19 mm OD fused-silica capillary (ESI sample tube), .....	00106-10499
Tubing, 0.05 mm ID × 0.19 mm OD fused-silica capillary (low flow ESI < 200 µL/min), .....	00106-10502
Tubing, 0.1 mm ID × 0.363 mm OD fused-silica capillary (infusion line), .....	00106-10504
Tubing, 0.075 mm ID × 0.3193 mm OD fused-silica capillary (low flow ESI),.....	00106-10511
Teflon tube (syringe adapter assembly), .....	00301-22915

## Chemicals Kit

<b>Chemicals Kit, .....</b>	<b>97000-62042</b>
Met-Arg-Phe-Ala, 20 mg, .....	00301-07709
Ultramark 1621, .....	00301-12200
Caffeine, 1 mg/mL, .....	00301-12310
Reserpine, 1 g, .....	00301-12901



**CAUTION** Store and handle all chemicals in accordance with standard safety procedures. The Material Safety Data Sheets (MSDS) describing the chemicals being used are to be freely available to lab personnel for them to examine at any time.

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