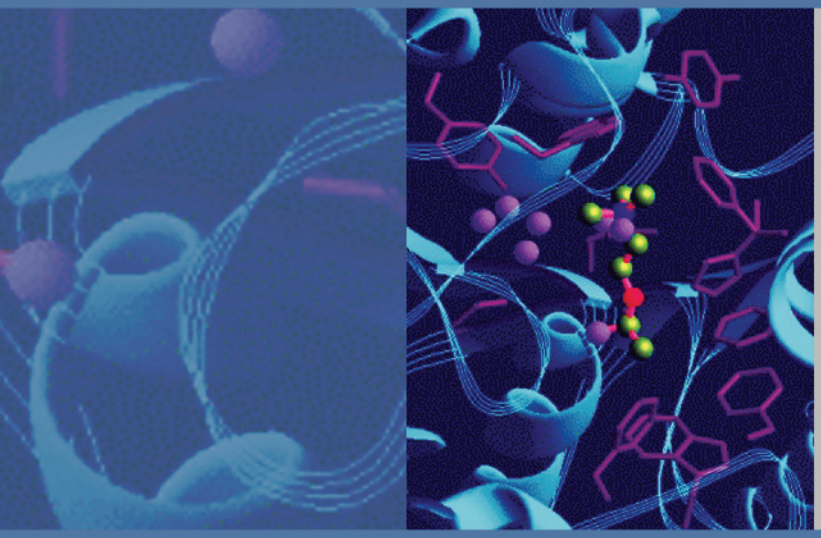

LTQ Series

Hardware Manual

97055-97072 Revision A April 2009

DOCUMENTATION SURVEY

Part of Thermo Fisher Scientific

Thermo SCIENTIFIC

Release history: Revision A released April 2009

Software Version: Xcalibur 2.1.0 or earlier, LTQ Series 2.6.0 or earlier

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

Regulatory Compliance

Thermo Fisher Scientific 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 in the next section or sections by product name.

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

Regulatory compliance results for the following Thermo Scientific products:

LXQ (February 2005)

EMC - Directives 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, A1: 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: 1995	EN 61000-4-5: 1995, A1: 2001
EN 61326-1: 1997	EN 61000-4-6: 1996, A1: 2001
EN 61000-4-2: 1995, A1: 1998, A2: 2001	EN 61000-4-11: 1994, A1: 2001
FCC Class A, CFR 47 Part 15, Subpart B: 2004	CISPR 11: 1999, A1: 1999, A2: 2002

Low Voltage Safety Compliance

Compliance with safety issues is declared under Thermo Fisher Scientific sole responsibility. This device complies with Low Voltage Directive 73/23/EEC and harmonized standard EN 61010-1:2001.

Thermo SCIENTIFIC

LTQ XL (September 2006)

EMC Directives 89/336/EEC

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

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

Low Voltage Safety Compliance

Compliance with safety issues is declared under Thermo Fisher Scientific sole responsibility. This device complies with Low Voltage Directive 73/23/EEC and harmonized standard EN 61010-1:2001.

LTQ XL/ETD System (January 2007)

EMC Directives 89/336/EEC

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

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

Low Voltage Safety Compliance

Compliance with safety issues is declared under Thermo Fisher Scientific sole responsibility. This device complies with Low Voltage Directive 73/23/EEC and harmonized standard EN 61010-1:2001.

MALDI LTQ XL System (August 2007)

EMC Directives 2004/108/EC

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

EN 55011: 1998, A1: 1999, A2: 2002
EN 61000-3-2: 2000
EN 61000-3-3: 1995, A1: 2001
EN 61326-1: 1998, A2: 2001, A3: 2003
EN 61000-4-2: 2001
FCC Class A, CFR 47 Part 15: 2006
EN 61000-4-3: 2002
EN 61000-4-4: 1995, A1: 2000, A2: 2001
EN 61000-4-5: 2001
EN 61000-4-6: 2003
EN 61000-4-11: 2001
CISPR 11: 1998, A1:1999, A2: 2002

Low Voltage Safety Compliance

Compliance with safety issues is declared under Thermo Fisher Scientific sole responsibility. This device complies with Low Voltage Directive 2006/95/EC and harmonized standard EN 61010-1:2001.

Safety of Laser Products

Compliance with safety of laser products is declared under Thermo Fisher Scientific sole responsibility. This device complies with the harmonized standard IEC/EN 60825-1/A2: 2001.

LTQ Velos (August 2008)

EMC Directives 2004/108/EEC

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

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

Low Voltage Safety Compliance

Compliance with safety issues is declared under Thermo Fisher Scientific sole responsibility. This device complies with Low Voltage Directive 2006/95/EEC and harmonized standard EN 61010-1:2001.

LTQ Velos/ETD System (November 2008)

EMC Directives 2004/108/EEC

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

EN 61326-1: 2006
EN 55011: 2007
EN 61000-3-2: 2006
EN 61000-3-3: 2005
EN 61000-4-2: 2001
EN 61000-4-3: 2006
EN 61000-4-4: 2004
EN 61000-4-5: 2005
EN 61000-4-6: 2007
EN 61000-4-11: 2004
FCC Part 15: 2007

Low Voltage Safety Compliance

Compliance with safety issues is declared under Thermo Fisher Scientific sole responsibility. This device complies with Low Voltage Directive 2006/95/EEC and harmonized standard EN 61010-1:2001.

FCC Compliance Statement

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

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.

Notice on Lifting and Handling of Thermo Scientific Instruments

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

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Notice on the Proper Use of Thermo Scientific Instruments

In compliance with international regulations: Use of this instrument in a manner not specified by Thermo Fisher Scientific could impair any protection provided by the instrument.

Notice on the Susceptibility to Electromagnetic Transmissions

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

For manufacturing location, see the label on the instrument.

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 Fisher Scientific has contracted with one or more recycling or disposal companies in each European Union (EU) Member State, and these companies should dispose of or recycle this product. See www.thermo.com/WEEERoHS for further information on Thermo Fisher Scientific's compliance with these Directives and the recyclers in your country.

WEEE Konformität

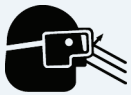
Dieses Produkt muss die EU Waste Electrical & Electronic Equipment (WEEE) Richtlinie 2002/96/EC erfüllen. Das Produkt ist durch folgendes Symbol gekennzeichnet:

Thermo Fisher Scientific hat Vereinbarungen mit Verwertungs-/Entsorgungsfirmen in allen EU-Mitgliedsstaaten getroffen, damit dieses Produkt durch diese Firmen wiederverwertet oder entsorgt werden kann. Mehr Information über die Einhaltung dieser Anweisungen durch Thermo Fisher Scientific, über die Verwerter, und weitere Hinweise, die nützlich sind, um die Produkte zu identifizieren, die unter diese RoHS Anweisung fallen, finden sie unter www.thermo.com/WEEERoHS.

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 Fisher Scientific 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 Fisher Scientific à ces directives, les recycleurs dans votre pays et les informations sur les produits Thermo Fisher Scientific qui peuvent aider la détection des substances sujettes à la directive RoHS sont disponibles sur www.thermo.com/WEEERoHS.

CAUTION Symbol	CAUTION	VORSICHT	ATTENTION	PRECAUCION	AVVERTENZA
	**Electric Shock:** This instrument uses high voltages that can cause personal injury. Before servicing, shut down the instrument and disconnect the instrument from line power. Keep the top cover on while operating the instrument. Do not remove protective covers from PCBs.	**Elektroschock:** 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.	**Choc électrique:** L'instrument utilise des tensions capables d'infliger des blessures corporelles. L'instrument doit être arrêté et débranché de la source de courant avant tout intervention. Ne pas utiliser l'instrument sans son couvercle. Ne pas enlever les étuis protecteurs des cartes de circuits imprimés.	**Descarga eléctrica:** Este instrumento utiliza altas tensiones, capaces de producir lesiones personales. Antes de dar servicio de mantenimiento al instrumento, éste debera apagarse y desconectarse de la línea de alimentacion eléctrica. No opere el instrumento sin sus cubiertas exteriores quitadas. No remueva las cubiertas protectoras de las tarjetas de circuito impreso.	**Shock da folgorazione.** L'apparecchio è alimentato da corrente ad alta tensione che puo 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).
	**Chemical:** This instrument might contain hazardous chemicals. Wear gloves when handling toxic, carcinogenic, mutagenic, or corrosive or irritant chemicals. Use approved containers and proper procedures to dispose waste oil.	**Chemikalien:** 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.	**Chimique:** Des produits chimiques dangereux peuvent se trouver dans l'instrument. Portez des gants pour manipuler tous produits chimiques toxiques, cancérigènes, mutagènes, ou corrosifs/irritants. Utiliser des récipients et des procédures homologuées pour se débarrasser des déchets d'huile.	**Química:** El instrumento puede contener productos quimicos peligrosos. Utilice guantes al manejar productos quimicos tóxicos, carcinogenos, mutagenos o corrosivos/irritantes. Utilice recipientes y procedimientos aprobados para deshacerse del aceite usado.	**Prodotti chimici.** 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.
	**Heat:** Before servicing the instrument, allow any heated components to cool.	**Hitze:** Warten Sie erhitzte Komponenten erst nachdem diese sich abgekühlt haben.	**Haute Temperature:** Permettre aux composants chauffés de refroidir avant tout intervention.	**Altas temperaturas:** Permita que lop componentes se enfríen, ante de efectuar servicio de mantenimiento.	**Calore.** Attendere che i componenti riscaldati si raffreddino prima di effetturare l'intervento di manutenzione.
	**Fire:** Use care when operating the system in the presence of flammable gases.	**Feuer:** Beachten Sie die einschlägigen VorsichtsmaBnahmen, wenn Sie das System in Gegenwart von entzündbaren Gasen betreiben.	**Incendie:** Agir avec précaution lors de l'utilisation du système en présence de gaz inflammables.	**Fuego:** Tenga cuidado al operar el sistema en presencia de gases inflamables.	**Incendio.** Adottare le dovute precauzioni quando si usa il sistema in presenza di gas infiammabili.
	**Eye Hazard:** Eye damage could occur from splattered chemicals or flying particles. Wear safety glasses when handling chemicals or servicing the instrument.	**Verletzungsgefahr der Augen:** Verspritzte Chemikalien oder kleine Partikel können Augenverletzungen verursachen. Tragen Sie beim Umgang mit Chemikalien oder bei der Wartung des Gerätes eine Schutzbrille.	**Danger pour les yeux:** 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.	**Peligro par los ojos:** Las salicaduras de productos químicos o particulas que salten bruscamente pueden causar lesiones en los ojos. Utilice anteojos protectores al mnipular productos químicos o al darle servicio de mantenimiento al instrumento.	**Pericolo per la vista.** 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.
	**General Hazard:** A hazard is present that is not included in the above categories. Also, this symbol appears on the instrument to refer the user to instructions in this manual.	**Allgemeine Gefahr:** Es besteht eine weitere Gefahr, die nicht in den vorstehenden Kategorien beschrieben ist. Dieses Symbol wird im Handbuch auBerdem dazu verwendet, um den Benutzer auf Anweisungen hinzuweisen.	**Danger général:** 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.	**Peligro general:** Significa que existe un peligro no incluido en las categorias anteriores. Este simbolo también se utiliza en el instrumento par referir al usuario a las instrucciones contenidas en este manual.	**Pericolo generico.** 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.
	When the safety of a procedure is questionable, contact your local Technical Support organization for Thermo Fisher Scientific San Jose Products.	Wenn Sie sich über die Sicherheit eines Verfahrens im unklaren sind, setzen Sie sich, bevor Sie fortfahren, mit Ihrer lokalen technischen Unterstützungsorganisation für Thermo Fisher Scientific San Jose Produkte in Verbindung.	Si la sûreté d'une procédure est incertaine, avant de continuer, contacter le plus proche Service Clientèle pour les produits de Thermo Fisher Scientific San Jose.	Cuando la certidumbre acerca de un procedimiento sea dudosa, antes de proseguir, pongase en contacto con la Oficina de Asistencia Tecnica local para los productos de Thermo Fisher Scientific San Jose.	Quando e 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 Fisher Scientific San Jose.

CAUTION Symbol	CAUTION	危険警告	危險警告
	**Electric Shock:** This instrument uses high voltages that can cause personal injury. Before servicing, shut down the instrument and disconnect the instrument from line power. Keep the top cover on while operating the instrument. Do not remove protective covers from PCBs.	**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、必ず操業を停止し、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 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。	電擊：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。
	**Chemical:** This instrument might contain hazardous chemicals. Wear gloves when handling toxic, carcinogenic, mutagenic, or corrosive or irritant chemicals. Use approved containers and proper procedures to dispose waste oil.	**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。	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。
	**Heat:** Before servicing the instrument, allow any heated components to cool.	**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。	高溫：請先等高溫零件冷卻之後再進行維修。
	**Fire:** Use care when operating the system in the presence of flammable gases.	**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。	火災：在有易燃氣體的場地操作該系統時，請務必小心謹慎。
	**Eye Hazard:** Eye damage could occur from splattered chemicals or flying particles. Wear safety glasses when handling chemicals or servicing the instrument.	**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。	眼睛傷害危險：飛濺的化學品或顆粒可能造成眼睛傷害。處理化學品或維修儀器設備時請佩戴安全眼鏡。
	**General Hazard:** A hazard is present that is not included in the above categories. Also, this symbol appears on the instrument to refer the user to instructions in this manual.	**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。	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。
	When the safety of a procedure is questionable, contact your local Technical Support organization for Thermo Fisher Scientific San Jose Products.	**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ールサポートセンターごご連絡ください。**	如对安全程序有疑问，请在操作之前与当地的菲尼根技术服务中心联系。

Contents

Preface

This manual describes the modes of operation, hardware components, cleaning, and maintenance of your LTQ Series mass spectrometer:

- LXQ™, a 2D linear ion trap mass spectrometer
- LTQ XL™, a 2D linear ion trap mass spectrometer
- LTQ Velos™, a dual cell linear ion trap mass spectrometer

Related Documentation

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

- A printed copy of the *Safety and Regulatory Guide*

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

- PDF files of the documents in Table 1 that you can access from the data system computer

Table 1. LTQ Series MS documentation

Model	Related documents
LXQ, LTQ XL, LTQ Velos	*LTQ Series Getting Started Guide*
LXQ, LTQ XL, LTQ Velos, LTQ XL/ETD system, LTQ Velos/ETD system, MALDI LTQ XL system	*LTQ Series Preinstallation Requirements Guide* *LTQ Series Getting Connected Guide*
ETD module	*ETD Module Getting Started Guide* *ETD Module Hardware Manual*
MALDI source	*MALDI Source Getting Started Guide* *MALDI Source Hardware Manual*

To access the manuals for the mass spectrometer, from the Microsoft™ Windows™ taskbar, choose **Start > All Programs > Thermo Instruments > LTQ > Manuals > *model*** and then click the PDF that you want to view.

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

The software also provides Help. To access the Help, choose **Help** from the menu bar or click the  button on the toolbar.

Safety and Special Notices

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

Safety and special notices include the following:

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

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

Note Highlights information of general interest.

Tip Highlights helpful information that can make a task easier.

Contacting Us

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

❖ **To contact Technical Support**

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

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

❖ To contact Customer Service for ordering information

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

❖ To copy manuals from the Internet

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

❖ To suggest changes to documentation or to Help

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

Introduction

The LTQ Series linear ion trap mass spectrometers are part of the Thermo Scientific family of mass spectrometers.

Contents

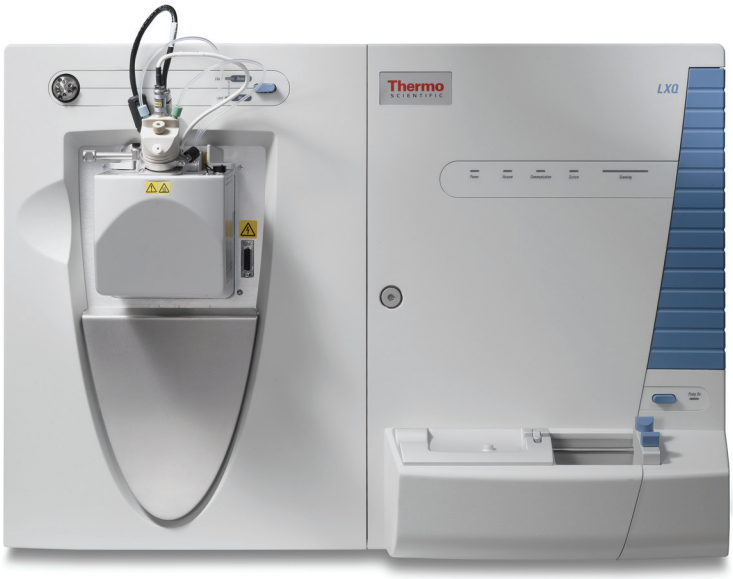
LTQ Series Mass Spectrometers

The LTQ Series mass spectrometers includes the following models:

LXQ

The LXQ is a 2D linear ion trap mass spectrometer that includes a syringe pump, a divert/inject valve, and an Ion Max-S ion source (Figure 1). The LXQ is described in Chapter 2, "Functional Description," on page 25.

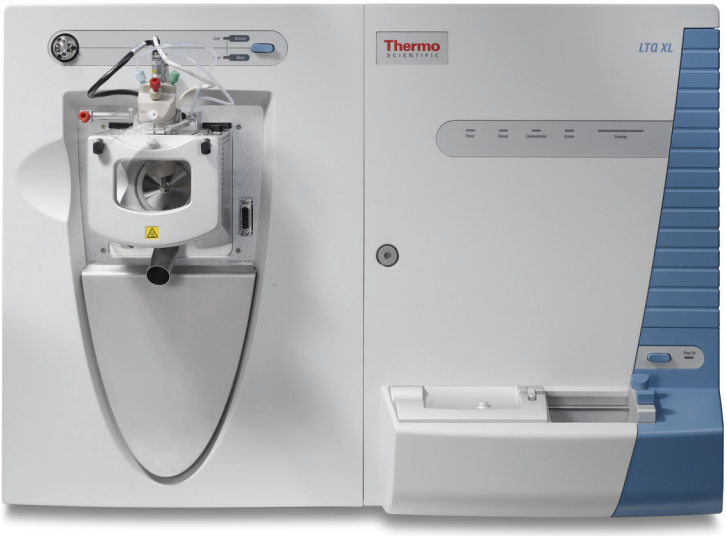
Figure 1. LXQ mass spectrometer



LTQ XL

The LTQ XL is a 2D linear ion trap mass spectrometer that includes a syringe pump, a divert/inject valve, and an Ion Max ion source (Figure 2). The LTQ XL is described in Chapter 2, "Functional Description," on page 25.

Figure 2. LTQ XL mass spectrometer



LTQ Velos

The LTQ Velos is a dual cell linear ion trap mass spectrometer that includes a syringe pump, a divert/inject valve, and an Ion Max ion source (Figure 3). The LTQ Velos is described in Chapter 2, "Functional Description," on page 25.

Figure 3. LTQ Velos mass spectrometer

Overview of an LC/MS Analysis

In a typical LC/MS analysis, the liquid chromatograph (LC) portion of the system separates a mixture into its chemical components. The LC pump produces a solvent stream (the mobile phase) that passes through an LC column (containing the stationary phase) under high pressure. An autosampler introduces a measured quantity of sample into this solvent stream. As the solvent stream passes through the LC column, the sample separates into its chemical components. The rate at which the components of the sample elute from the column depends on their relative affinities to the mobile phase and the solid particles that make up the column packing.

As the separated chemical components exit the LC column, they pass through a transfer line and enter the MS detector where they are ionized and analyzed. As the MS detector analyzes the ionized components and determines their mass-to-charge (*m/z)* ratios, it sends a data stream to the data system computer. In addition to supplying information about the mass-to-charge ratios of ionized compounds, the LTQ Series mass spectrometer can also supply structural and quantitative information by performing MS^n experiments.

Because the LTQ Series mass spectrometer has a built-in syringe pump and divert/inject valve, it provides four additional ways to introduce a sample into the MS detector, described in Table 1 on page 4.

Table 1. Introducing samples into the MS detector

Method to introduce sample	Description
Infusion	Connect the built-in syringe pump directly to the atmospheric pressure ionization (API) source of the mass spectrometer.
High-flow infusion	Use a union tee to combine the flow from the syringe pump with the flow from an LC pump.
Manual loop injection	Connect a sample loop, a needle port fitting, and an LC pump to the divert/inject valve. After you fill the sample loop with sample, switch the position of the divert/inject valve, which places the contents of the sample loop in the path of the solvent flow produced by the LC pump.
Automated loop injection	Connect a sample loop, an LC pump, and the syringe pump to the divert/inject valve. After you connect the plumbing, specify the flow rate at which the syringe pump fills the sample loop. After the loop is filled, the data system triggers an injection.

The LTQ Series mass spectrometer consists of an atmospheric pressure ionization (API) source, ion optics, a mass analyzer, and an ion detection system. The ion optics, mass analyzer, and 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 ion optics transmit the ions produced in the API source 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 set up data acquisition methods for the LTQ Series mass spectrometer to analyze positively or negatively charged ions or to switch between these polarity modes during a single run.

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. An automatic gain control (AGC) process controls the function of these lenses and sets them to transmit the optimum number of ions to the mass analyzer.

The mass analyzer measures the mass-to-charge ratios of the ions produced in the API source. Selected ions are ejected from the mass analyzer and reach the ion detection system where they produce a signal. The detection system electronics then amplify this signal for analysis by the data system.

The data system serves as the user interface to the mass spectrometer, autosampler, LC, and syringe pump. Refer to the Help provided with the data system for more information on the LTQ Series 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 LTQ Series mass spectrometer 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, provides you with greater flexibility in the instrumentation for solving complex analytical problems.

Ion Polarity Modes

The LTQ Series mass spectrometer can operate in either positive or negative ion polarity modes. The MS detector controls 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. The spectral characteristics for these two polarity modes are described in the next section, "Ionization Techniques." The ability to obtain both positive-ion and negative-ion mass spectra during a single run reduces the time required to obtain a complete qualitative analysis of your sample.

Ionization Techniques

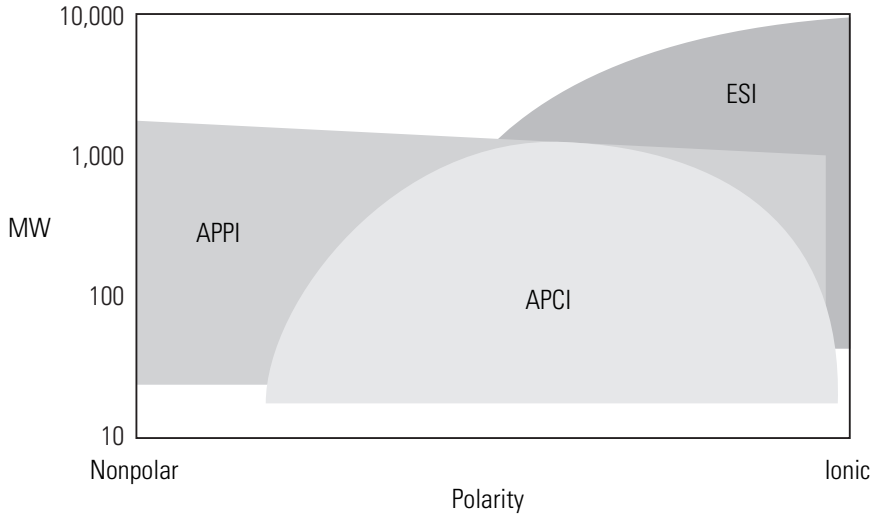
You can operate the LTQ Series mass spectrometer using any of the following four ionization techniques:

- "Electrospray Ionization," next section
- "Atmospheric Pressure Chemical Ionization" on page 8
- "Atmospheric Pressure Photoionization" on page 11
- "Nanospray Ionization" on page 13

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

Figure 4 on page 6 shows the ranges of applicability (molecular weight as a function of polarity) of three of the ionization techniques: atmospheric pressure photoionization (APPI), atmospheric pressure chemical ionization (APCI), and electrospray ionization (ESI).

Figure 4. Molecular weight ranges of ionization techniques



Electrospray Ionization

The ESI technique transforms ions in solution into ions in the gas phase[1]. This means that you must consider the solution chemistry when using the ESI technique, but because proton transfer can occur in the gas phase, the types and relative intensities of the gas phase ions can differ from the solution phase. You can use ESI to analyze many samples that previously were not suitable for mass analysis (for example, heat-labile compounds or high molecular weight compounds). ESI is also useful for analyzing any polar compound that makes a preformed ion in solution. The term *preformed ion* can include adduct ions. For example, you can analyze polyethylene glycols from a solution containing ammonium acetate, because of the adduct formation between the NH_4^+ ions in the solution and oxygen atoms in the polymer. With ESI, the range of molecular masses that the LTQ Series mass spectrometer can analyze is greater than 100000 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 in solution are transferred into the gas phase as follows:

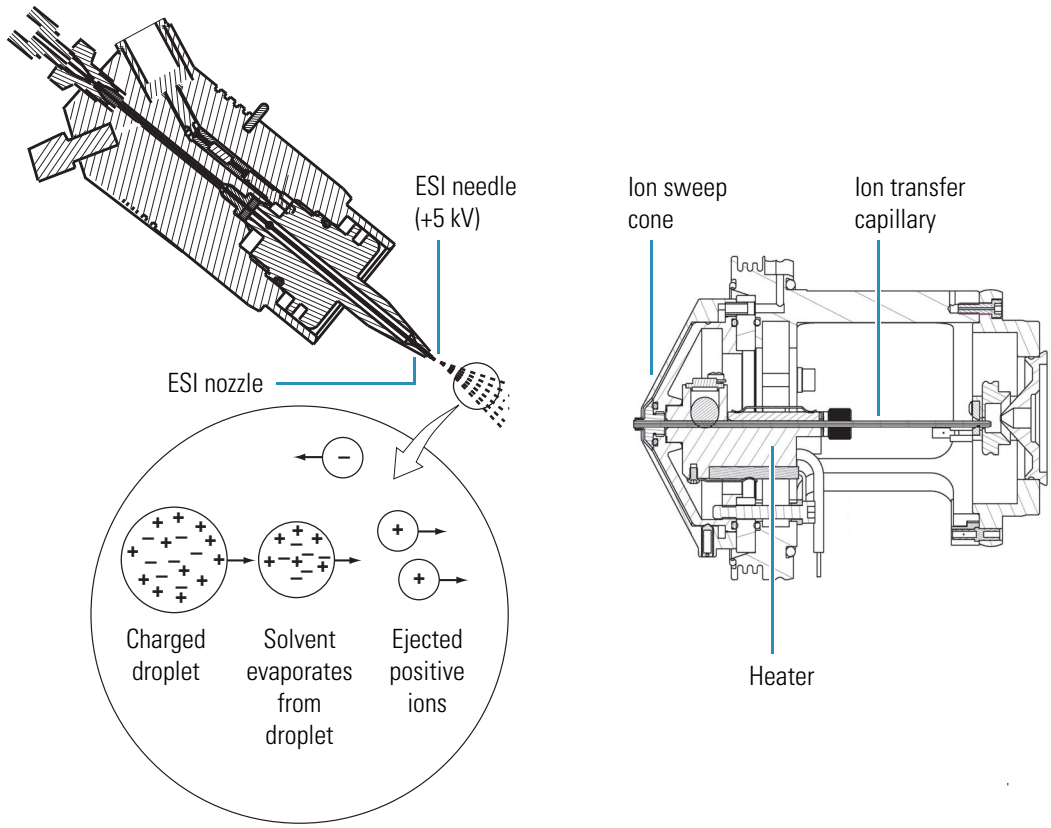
1. The sample solution enters the ESI needle, to which a high voltage is applied.
2. The ESI needle sprays the sample solution into a fine mist of droplets that are electrically charged at their surface.

[1] 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; Ikonomou, M. G.; Blades, A. T.; Kebarle, P. *Anal. Chem.* **1991**, *63*, 1989.

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. The electrostatic repulsion between the sample ions in these very small, highly-charged droplets causes the sample ions to be ejected into the gas phase.
6. The sample ions pass through an ion transfer capillary and enter the MS detector for analysis.

In the LTQ Series mass spectrometer, the ESI needle is 60 degrees to the axis of the ion transfer capillary that carries ions into 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 5 shows the steps in the formation of ions from highly-charged droplets and the relationship between the ESI probe and the ion transfer capillary.

Figure 5. ESI process in the positive ion polarity mode



You can use the ESI probe in either positive or negative ion polarity mode. The polarity of the preformed ions in solution determines the ion polarity mode of choice; 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. You use a positively charged needle to analyze positive ions and a negatively charged needle to analyze negative ions.

Sample ions can carry a single charge or multiple charges. The number of charges that the sample ions carry depends on the structure of the analyte of interest and the carrier solvent. (In ESI, because the buffer and the buffer strength both have a noticeable effect on sensitivity, you must 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 (CH_3OH), acetonitrile CH_3CN), and isopropyl alcohol [$(CH_3)_2CHOH$], 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 (TEA), 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. Use APCI 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 and enter the MS detector for analysis.

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.

Because APCI is a gas phase ionization technique, 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 the following:

Primary ion formation

$e^- + N_2 \rightarrow N_2^{+\cdot} + 2e^-$

Secondary ion formation

$N_2^{+\cdot} + H_2O \rightarrow N_2 + H_2O^{+\cdot}$

$H_2O^{+\cdot} + H_2O \rightarrow H_3O^+ + HO\cdot$

Proton transfer

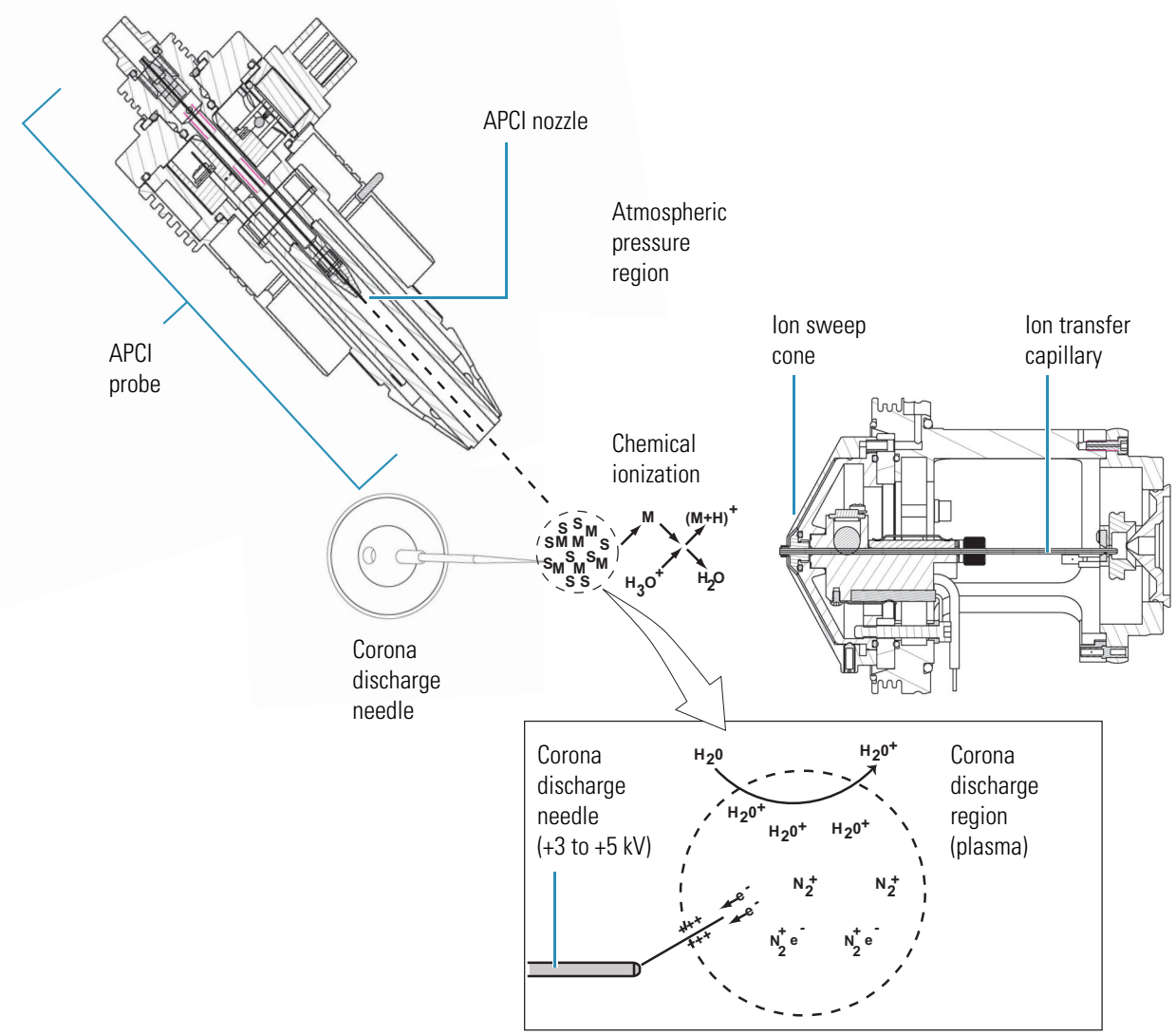
$H_3O^+ + M \rightarrow (M+H)^+ + H_2O$

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

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

Figure 6 on page 10 shows the APCI process in the positive-ion polarity mode.

Figure 6. APCI process in the positive ion polarity mode



You can use APCI in the 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, APCI produces fewer negative ions are produced than positive ions, negative ion polarity is sometimes more selective than positive ion polarity because it generates less chemical noise than the positive ion polarity 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.

APPI produces and analyzes ions 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 hν:

   $M + h\nu \rightarrow M^{+\cdot} + e^-$

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

   $M^+ + S \rightarrow MH^+ + S[-H]$

5. The analyte ions pass through the ion transfer capillary and enter the MS detector for analysis.

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 7 and Figure 8 on page 12.

Figure 7. Energetics of photoionization

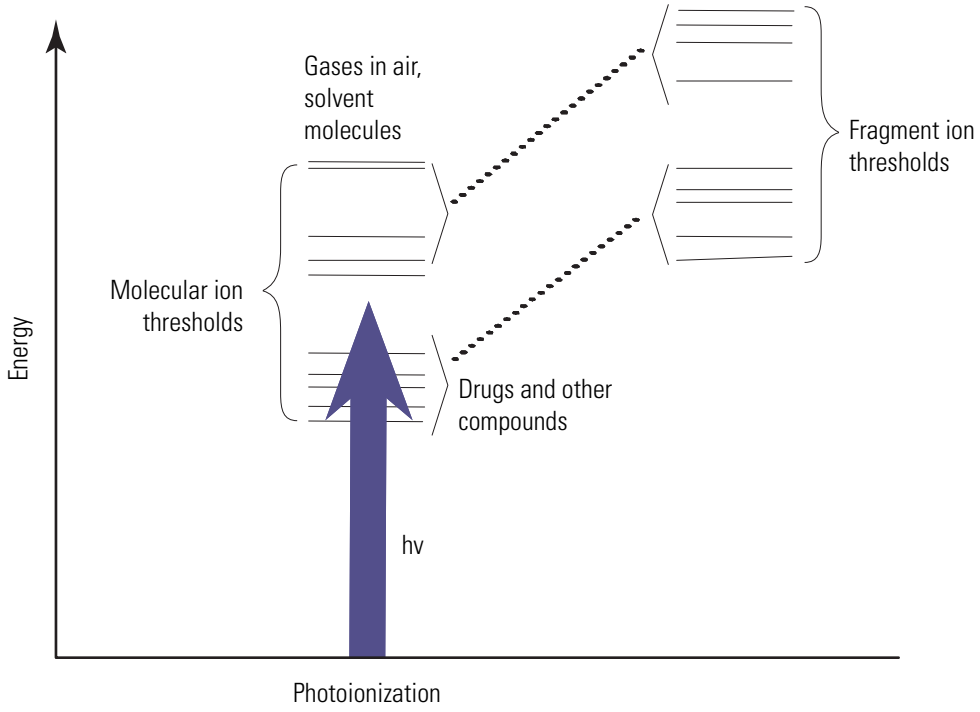
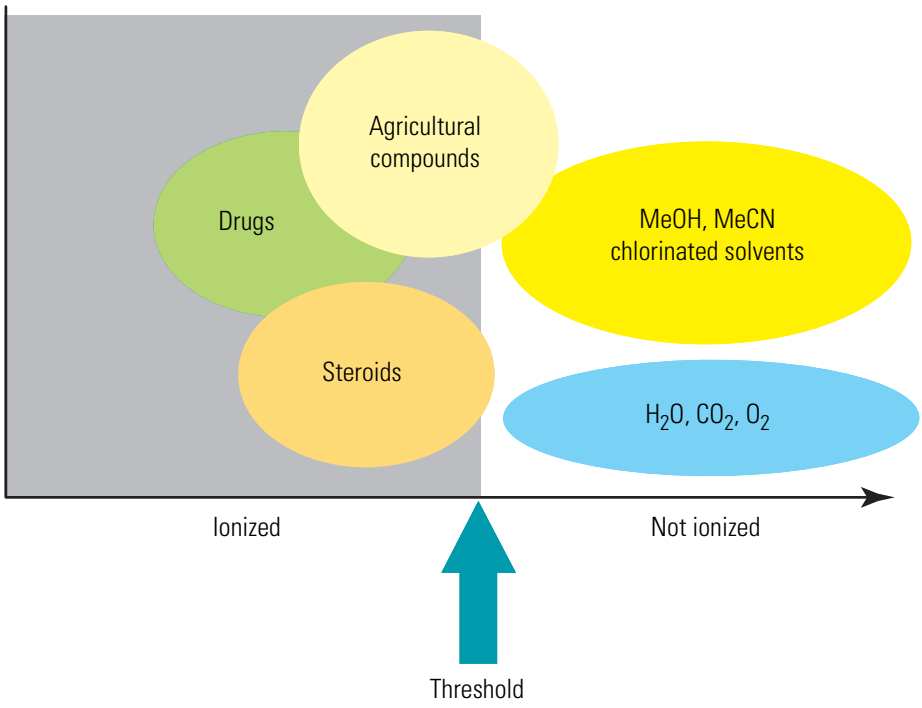


Figure 8. Selective photoionization



The light source is a krypton lamp that 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. The ionization potentials of typical compounds and solvents are listed in Table 2. Compounds and solvents with an ionization potential below 10 eV appear in red.

Table 2. Compound and solvent ionization potentials

Compound ionization potentials (IP)		Solvent ionization potentials (IP)	
Anthracene	7.4 eV	Toluene	8.82 eV
Fluoranthene	7.8 eV	Acetone	9.7- eV
Caffeine	8.0 eV		
4-Nitrotoluene	9.5 eV		
10 eV -			
		Methanol	10.85 eV
		Acetonitrile	12.19 eV
		Water	12.51 eV

Nanospray Ionization

Nanospray ionization (NSI) is a technique for performing electrospray ionization on amounts of liquid as small as 1 µL for time periods of greater than 30 minutes. Using NSI, you can obtain stable mass spectra 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*. To produce a mass spectrum, the mass analyzer varies its dc and rf voltages to sequentially eject ions from the trap based on their *m/z* values. Or, by varying the rf voltages of the mass analyzer, the LTQ Series mass spectrometer can first eject all ions, except for several selected parent ions, and then collide these ions with the helium that is present in the mass analyzer. This helium is known as *buffer gas*. The collisions can cause the selected parent ions, or precursor ions, to fragment into product ions. These product ions can then be sequentially ejected from the trap based on their *m/z* values to produce a mass spectrum.

The number of stages of mass analysis is represented as MS^n where n is the scan power. Each stage of mass analysis where $n>1$, includes an ion selection step. The LTQ Series mass spectrometer supports scan powers of $n = 1$ to $n = 10$. As you raise the scan power, you can obtain more structural information about the analyte.

The LTQ Series mass spectrometer in its standard configurations supports these scan powers:

- "MS Scan Mode," next section
- "MS/MS Scan Mode" on page 14
- "MS^n Scan Mode" on page 14

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 16).

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 LTQ Series mass spectrometer in the following scan types:

- "Full Scan," next section
- "Selected Ion Monitoring" on page 16
- "Selected Reaction Monitoring" on page 16
- "Consecutive Reaction Monitoring" on page 17
- "ZoomScan" on page 17

Full Scan

A full scan provides a full mass spectrum of the analyte during a particular scan time. With a 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 provides more information about an analyte than does selected ion monitoring (SIM) or selected reaction monitoring (SRM). But because a full scan scans an entire mass range during a particular scan time, it does not provide the sensitivity that the other scan types can achieve.

The full scan type includes the following:

- "Single-Stage Full Scan (ms^1)," next section
- "Two-Stage Full Scan ($m2^1$)" on page 15

Single-Stage Full Scan (ms^1)

The single-stage full scan has one stage of mass analysis (where n = 1 scan power). With the single-stage full scan, the mass analyzer stores ions formed in the ion source. These ions are then sequentially scanned out of the mass analyzer to produce a full mass spectrum (a mass spectrum of the observable ions in the specified mass range at a specific time point in the analysis).

Single-stage full-scan analysis is a useful tool for qualitative analysis. 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.

After you determine the molecular weight of a compound of interest, you can use the SIM or SRM scan type to perform routine quantitative analyses of the compound (see "Selected Ion Monitoring" on page 16 and "Selected Reaction Monitoring" on page 16)

Two-Stage Full Scan ($m2^1$)

The two-stage full scan has two stages of mass analysis (where n = 2 scan power). In the first stage, the ions mass analyzer stores ions formed in the ion source. 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 mass analyzer stores the product ions. Then they are sequentially scanned out of the mass analyzer to produce a full product ion mass spectrum.

A two-stage full scan gives you more information about a sample than does SRM but at a lower speed than SRM does.

To use the SRM scan you must know which parent and product reaction ions 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 where you monitor a particular ion or set of ions. In a SIM scan, the mass analyzer stores ions formed in the ion source. 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 you know the mass spectrum of the target compound. SIM is useful in trace analysis and in the rapid screening of a large number of samples for a target compound.

Because a SIM scan monitors only a few ions, 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 it only monitors a few ions of interest while ignoring regions of the spectrum that are empty or have no ions of interest.

SIM can improve the detection limit and decrease analysis time, but it can also reduce target compound specificity. SIM analysis decreases the analysis time because it only monitors particular ions. SIM analysis reduces specificity because any compound that produces the ion or ions being monitored would appear to be the target compound. To avoid false positive results when using SIM for routine analyses, first verify that the ions being monitored with SIM are from the target compound and nothing else.

Selected Reaction Monitoring

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

In the first stage of mass analysis, the mass analyzer stores the ions formed in the ion source. 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 then 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 mass analyzer stores the product ions. 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 an SRM product ion mass spectrum.

Like SIM, SRM provides 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. You are very unlikely to get a false positive result with SRM. To get a false positive result, the interfering compound must form a parent ion of the same mass-to-charge ratio as the selected parent ion from the target compound. The compound 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), that monitors a multistep reaction path. 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 then 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 mass analyzer stores the product ions. 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 mass analyzer stores the new product ions. This process is repeated up to seven more times until the final product ions of interest are produced.

In the nth stage of mass analysis, the mass analyzer stores the final product ions. 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 many fragmentation pathways are available to the ion.

ZoomScan

Determining of the mass of an ion from its mass-to-charge ratio can be complicated if the charge state of the ion is unknown. ZoomScan™ is a high resolution MS scan in which the LTQ Series mass spectrometers perform a high resolution scan to determine the charge state and molecular mass of an ion. The MS detectors conduct a high resolution scan of 10 u width and evaluates the ^{12}C /^{13}C isotopic separation of a specified ion or ions. If the isotopic peaks are 1 u apart, the ion has a charge state of ±1. If the isotopic peaks are 0.5 u apart, the ion has

a charge state of ±2. If the isotopic peaks are 0.33 u apart, the ion has a charge state of ±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

With the LTQ Series mass spectrometer you can acquire and display mass spectral data (intensity versus mass-to-charge ratio) in one of two data types:

- "Profile Data," next section
- "Centroid Data" on page 18

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 12 (for LTQ Velos) or 15 (for LXQ and LTQ XL) sampling intervals. The intensity of the ion current is determined at each sampling interval. The intensity at each sampling interval is displayed with the intensities connected by a continuous line. In general, use the profile scan data type when you tune and calibrate the mass spectrometer so that you can easily see and measure mass resolution.

Centroid Data

Centroid data displays the mass spectrum as a bar graph. In this scan data type, the intensities of each set of sampling intervals are summed. This sum is displayed versus the integral center of mass of the 12 (for LTQ Velos) or 15 (for LXQ and LTQ XL) 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

You can perform several types of experiments with an LTQ Series mass spectrometer. The experiments are grouped into the following categories:

- "General MS or MS^n Experiments," next section
- "Data Dependent Experiments" on page 19
- "Ion Mapping Experiments" on page 21
- "Ion Tree Experiments" on page 22

Specify which type of experiment you want to perform in the Xcalibur 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. For more information, refer to the Help provided with the data system.

General MS or MS^n Experiments

A General MS or MS^n 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 that you can get started with a General MS or MS^n experiment.

In a General MS quantitation experiment, you must specify the mass range of your analyte or analytes of interest, a parent (precursor) ion that fragments into distinctive product ions, or the mass-to-charge ratios of all the parent ions of interest. The LTQ Series mass spectrometer can then collect data on the ions in the range or on the product ions of the parent ions that you specify.

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

The LTQ Series mass spectrometer can generate reproducible, product-specific spectra, even from laboratory to laboratory. Consequently, you can use reference spectra that are generated with one LTQ Series mass spectrometer to confirm structures of compounds generated with another LTQ Series mass spectrometer.

Data Dependent Experiments

Use Data Dependent™ experiments for the qualitative analysis of unknown compounds for structure elucidation or confirmation. The LTQ Series mass spectrometer 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 LTQ Series mass spectrometers automatically select the ions for fragmentation. The LTQ Series mass spectrometers 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 about how the experiment should best proceed, as long as you specify that one or more scan events of an experiment segment are to be run as Data Dependent. The MS detector then collects MS/MS or MS^n 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 MS detector determines which parent ion to isolate, the charge state of the parent ion, and the molecular mass 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 a type of Data Dependent experiment that provides methods for automatically interpreting MS^n 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, 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 MS detector generates product spectra. Decide later if the information is useful. Parameters might include threshold values for the intensity of the MS or MS^n 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 LTQ Series mass spectrometers then collect full scan MS data, pick the most intense parent ion in the spectrum, and fragment 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 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 MS detector determines a charge state equal to two, 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 and including *m/z* 1000 (or 2 × 500).

Use a Data Dependent experiment to do the following:

- Identify low-level impurities in high-purity compounds (Data Dependent MS/MS).

  For example in the quality assurance process for aspirin, the LTQ Series mass spectrometers can identify impurities of 0.1%.

- Identify metabolites in a complex mixture (chromatographic separation with Data Dependent MS/MS).

  For example characteristic masses along the metabolic pathways of a drug can produce MS/MS spectra that are specific to the structure of the drug. These spectra are essential to metabolite identification.

- Build a custom library of composite MS^n spectra (Ion Tree).

  A Data Dependent experiment can produce a composite spectrum of, for example, MS/MS, MS^3, and MS^4 data. The LTQ Series mass spectrometers 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 LTQ Series mass spectrometers include the following Ion Mapping templates:

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

These experiments 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 Map 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 and to 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 Map experiment collects scans for masses that have lost neutral fragments. As with a full-scan Ion Map, 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 Map 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 Map 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* 250, a Parent Ion Map includes all the parent ions that yielded the specified product ion, *m/z* 250.

A Data Dependent Zoom Map is an Ion Map 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.

You can view the results of any of the Ion Map experiments in the Xcalibur Qual Browser window.

Ion Tree Experiments

In an Ion Tree experiment, the LTQ Series mass spectrometers can collect MS^n data automatically. You can specify a particular parent ion for fragmentation or let the MS detector find the parent ions automatically and fragment them to any level between MS/MS and MS^{10}. The LTQ Series mass spectrometers automate 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 to prioritize how the MS detector gathers information, Depth Focus or Breadth Focus.

- Depth Focus characterizes an ion by performing a series of MS^n-level fragmentations (for example, MS/MS, MS^3, MS^4, and so on) for a particular parent ion before characterizing the next most intense parent 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 three and a Maximum Breadth of two in an Ion Tree experiment, the following occurs:

1. With either Depth or Breadth Focus, the MS detector 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 choose the Depth Focus, after the most intense ion of the MS spectrum is fragmented—producing an MS/MS spectrum—the LTQ Series mass spectrometers select and fragment 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 MS detector 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 choose the Breadth Focus, after the most intense ion of the MS spectrum is fragmented—producing an MS/MS spectrum—the LTQ Series mass spectrometers select and fragment 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,

two). After the two most intense peaks on the MS level are fragmented, the MS detector 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.

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

Functional Description

This chapter describes the principal components of the LTQ Series mass spectrometers and their functions.

Contents

Overview of the LTQ Series System

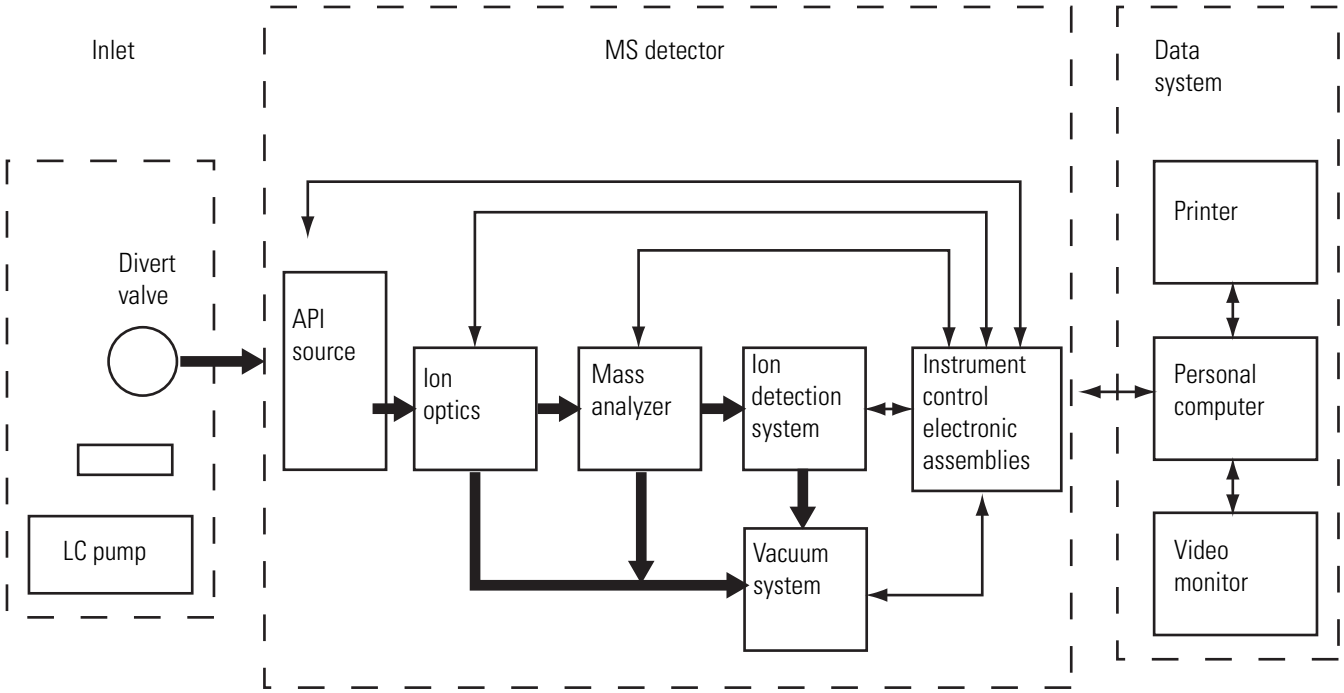
Figure 9 on page 26 shows a functional block diagram of an LTQ Series system that uses either a liquid chromatograph with an autosampler or the syringe pump as the inlet. A sample transfer line connects the LC to the MS detector. The autosampler and LC are usually installed to the left of the MS detector. The divert/inject valve is integrated into the front panel of the MS detector.

In a typical 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 for analysis.

Upon entering the atmospheric pressure ionization (API) source, sample molecules are ionized and desolvated into the gas phase by any of these methods (described in "Ionization Techniques" on page 5: electrospray ionization (ESI), heated-electrospray ionization (H-ESI), atmospheric pressure chemical ionization (APCI), atmospheric pressure photoionization (APPI), or nanospray ionization (NSI). The ion optics focus and accelerate the resulting gas phase sample ions into the mass analyzer, where they are isolated and then ejected according to their mass-to-charge ratios. As the mass analyzer ejects the sample ions, they are detected by

one or two ion detection systems that produce a signal proportional to the number of ions detected. The system electronics receive and amplify the ion current signal from the ion detection systems. The signal is then passed on to the data system for further processing, storage, and display. The data system provides the primary LTQ Series user interface.

Figure 9. LTQ Series system with a liquid chromatograph inlet (functional block diagram)



Liquid Chromatograph

A liquid chromatograph consists of an LC pump and an LC column. 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 can control a selection of LC pumps manufactured by Thermo Scientific, Agilent™, and Waters™ from the Xcalibur data system. For information on how to connect an LC to the LTQ Series mass spectrometer, refer to the *LTQ Series Getting Connected Guide*. If the Xcalibur data system controls your LC pump, you can access additional information by choosing **Start > All Programs > Xcalibur > Manuals > LC Devices >** [*Brand name*].

Autosampler

Use an autosampler to inject samples automatically into the LC inlet. You can control a selection of autosamplers manufactured by Thermo Fisher Scientific, Agilent, Waters, and CTC Analytics™.

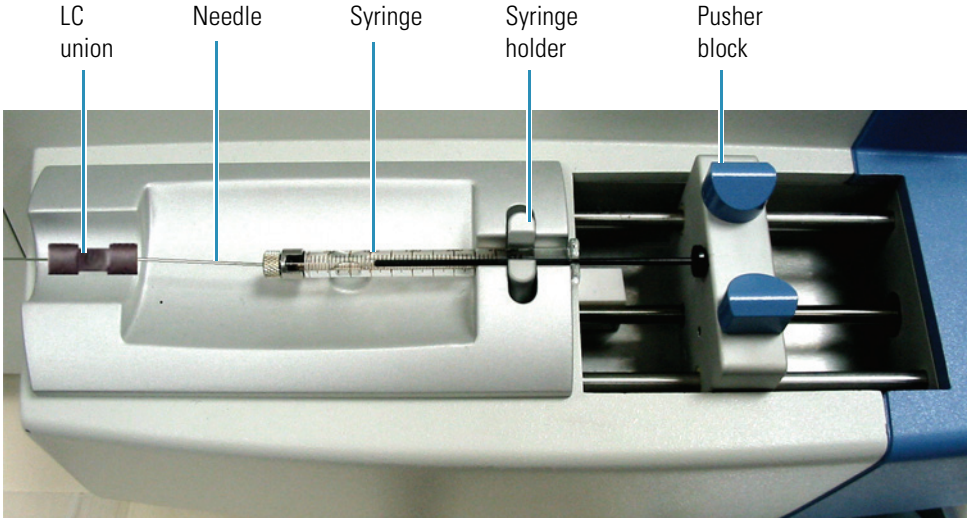
For information on how to connect an autosampler to the LTQ Series mass spectrometer, refer to the *LTQ Series Getting Connected Guide*. If the Xcalibur data system controls your LC pump, you can access additional information by choosing **Start > All Programs > Xcalibur > Manuals > LC Devices >** [*Brand name*]

Note For other autosamplers, the LTQ Series mass spectrometer provides contact closure Start and Stop signals. Refer to the *LTQ Series Getting Connected Guide* for information on connecting an autosampler to the LTQ Series mass spectrometer by contact closure Start and Stop signals.

Syringe Pump

The LTQ Series mass spectrometer includes an electronically controlled, integrated, syringe pump (Figure 10). The syringe pump delivers sample solution from the syringe into the API source.

Figure 10. Syringe pump



When the syringe pump is operating, a motor drives a pusher block that depresses the plunger of the syringe at a user selectable rate. 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. For instructions on setting up the syringe pump, refer to the *LTQ Series Getting Started Guide*.

On/Off Button

The blue button located on the front panel above the syringe pump (Figure 11) turns the syringe pump on and off. The motor has two speeds, normal and fast. The normal speed is the speed required to produce the flow rate specified in the data system. Pressing and releasing the button turns on the syringe pump and sets the motor speed to the normal speed. Pressing the button in and holding it in that position causes the motor to move the pusher block at the fast speed. The motor maintains the fast speed until you release the button or the pusher block reaches the end of its travel. When you release the button, the pusher block slows to normal speed. Pushing the button a second time turns the syringe pump off.

Figure 11. Syringe pump on/off button

Syringe Pump LED

A light-emitting diode (LED) to the right of the button indicates whether the pump is on or off. Table 3 lists the states of the syringe pump LED.

Table 3. Syringe pump LED states

State	Meaning
Not illuminated	The syringe pump is off.
Steady green	The syringe pump is on. The pusher block is moving at a speed that produces the flow rate specified in the data system. The allowable flow rate setting depends on the syringe size.
Flashing green	The syringe pump is on and the pusher block is moving at the fast speed.

Divert/Inject Valve

The divert/inject valve is located on the front of the LTQ Series mass spectrometer to the left of the API source.

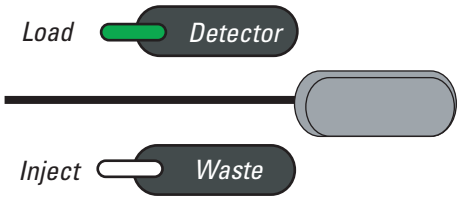
You can configure (plumb) the divert/inject valve in one of two ways: as a divert valve for direct infusion, high-flow infusion, or LC/MS experiments; or as a loop injector for flow-injection analysis. Procedures for plumbing the valve in the loop injector or divert valve configuration are provided in the *LTQ Series Getting Started*.

You can use the divert/inject valve button or the data system to control the divert/inject valve. Refer to Help for instructions on operating the divert/inject valve from the data system.

Divert/Inject Valve LEDs and Button

The button located on the front panel above the divert/inject valve switches the position of the two-position valve. Light-emitting diodes (LEDs) to the left of the button indicate the position of the valve as shown in Figure 12.

Figure 12. Divert/inject valve button and LEDs



When the divert/inject valve is set up for loop injections (flow injection analysis, FIA), pressing the divert/inject valve button switches the valve between the load and inject modes. The Load and Inject LEDs indicate the position of the valve.

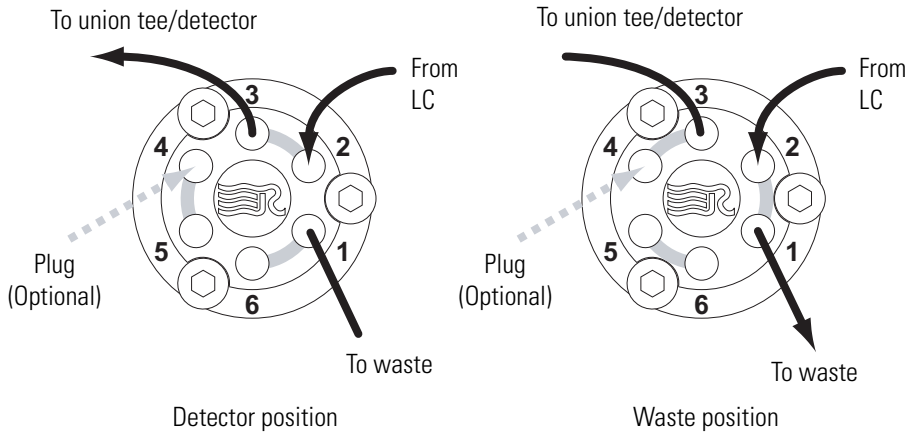
When the divert/inject valve is set up for divert valve operation, pressing the divert/inject valve button switches the LC flow between the MS detector and the waste container. The Detector and Waste LEDs indicate the position of the valve.

Divert Valve Positions

Use the divert/inject valve to divert the solvent flow between the MS detector and waste (Figure 13). The valve has two positions:

- Detector position—Solvent flow from the LC pump enters the valve through port 2 and exits the valve through port 3.
- Waste position—Solvent flow from the LC pump enters the valve through port 2 and exits the valve through port 1 to waste.

Figure 13. Divert valve positions

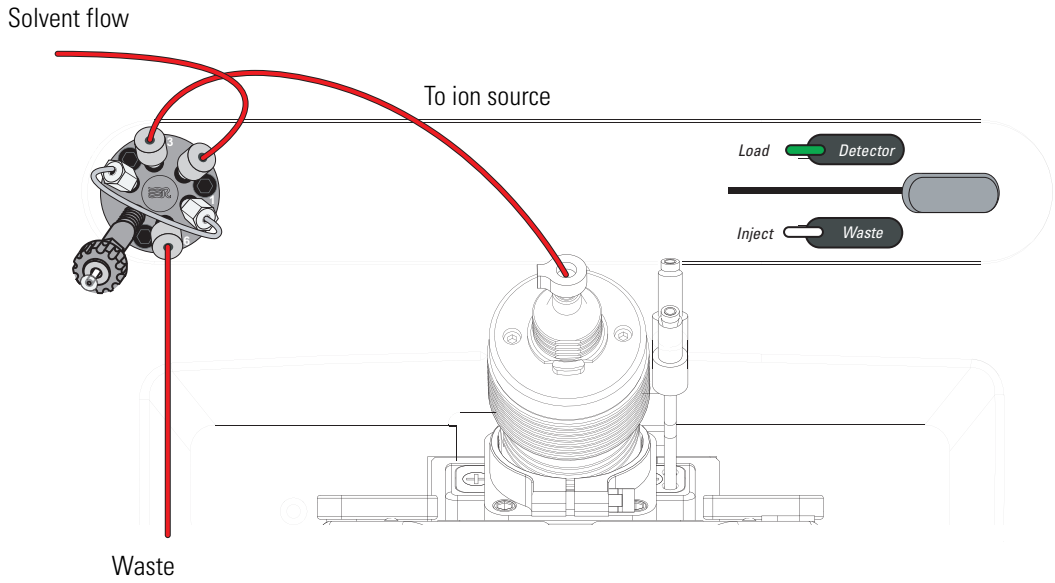


Injection Valve Operation

In the loop injection configuration (Figure 14), use the divert/inject valve button to switch between load and inject modes. The valve has two positions:

- Load position—Inject the sample solution through port 5. The injected sample enters and exits the sample loop through ports 4 and 1, respectively. As you overfill the sample loop, the sample solution exits the valve through port 6. Solvent flow from the LC pump enters and exits the valve through ports 2 and 3, respectively.
- Inject position—After you fill the sample loop, press the blue button above the injection valve or use the controls available in Tune Plus. Solvent flow from the LC pump backflushes sample out of the sample loop and then out of the valve through port 3 toward the detector.

Figure 14. Load/Inject positions



Mass Spectrometer

The mass spectrometer provides sample ionization and mass analysis of injected samples or samples eluted from a liquid chromatograph. The LTQ Series mass spectrometer uses a linear ion trap mass analyzer with an ion source external to the mass analyzer.

The LTQ Series mass spectrometer includes the following components:

- "LEDs," next section
- "Power Panel" on page 33
- "API Source" on page 34
- "Ion Optics" on page 40

- "Mass Analyzer" on page 42
- "Ion Detection Systems" on page 46
- "Vacuum System" on page 47
- "Inlet Gases Hardware" on page 51
- "Cooling Fans" on page 52

LEDs

The LEDs on the front panel of the LTQ Series mass spectrometer are shown in Figure 15 and described in Table 4.

Figure 15. LTQ Series front panel LEDs

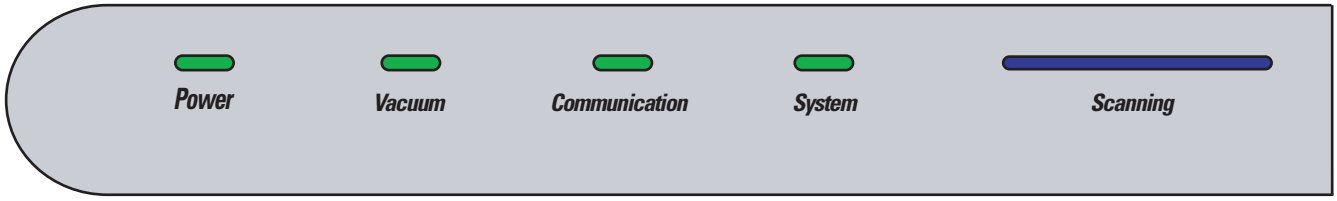


Table 4. LTQ Series front panel LEDs (Sheet 1 of 2)

LED	State	Meaning
Power	Green	Power is being supplied to the mass spectrometer. (The electronics service switch is in the Electronics Normal position.)
	Off	Power is not being supplied to the mass spectrometer. (The electronics service switch is in the Service mode position.)
Vacuum	Yellow	The vacuum is not within the allowable operating range.
	Green	The vacuum is within the allowable operating range.
Communication	Yellow	The mass spectrometer and data system are trying to establish a communication link.
	Green	The mass spectrometer and data system are communicating.
System	Yellow	The mass spectrometer is in Standby mode.
	Green	The mass spectrometer is on.
	Off	The mass spectrometer is off.

Table 4. LTQ Series front panel LEDs (Sheet 2 of 2)

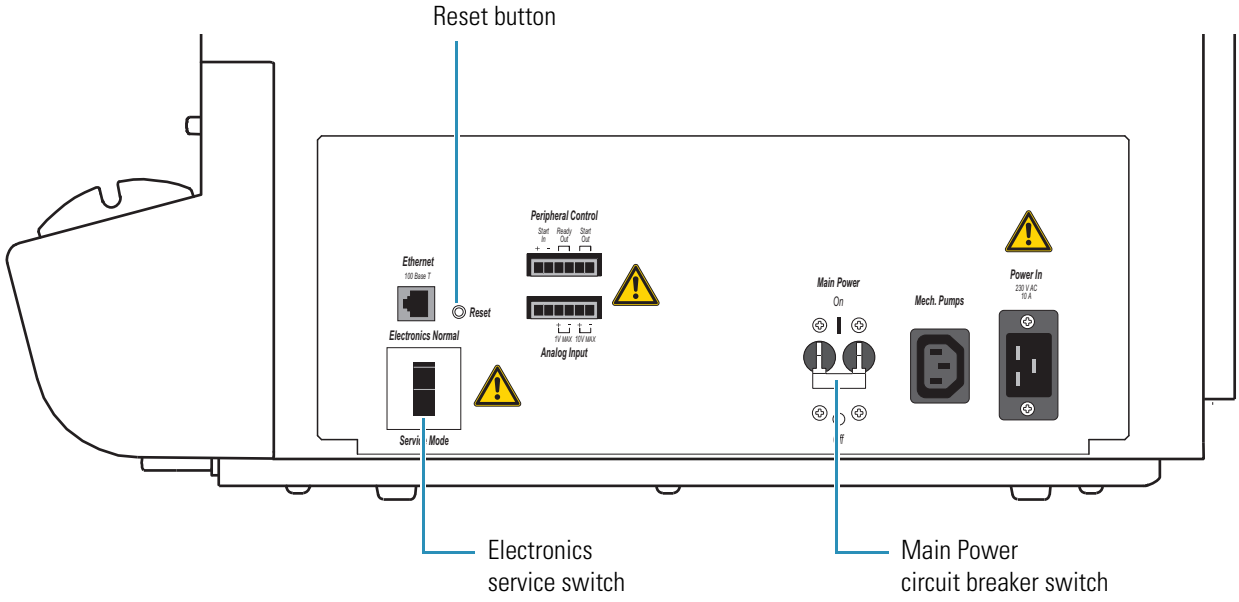
LED	State	Meaning
Scanning	Flashing blue	The mass spectrometer is on and is scanning ions.
	Off	The mass spectrometer is not scanning ions.

Power Panel

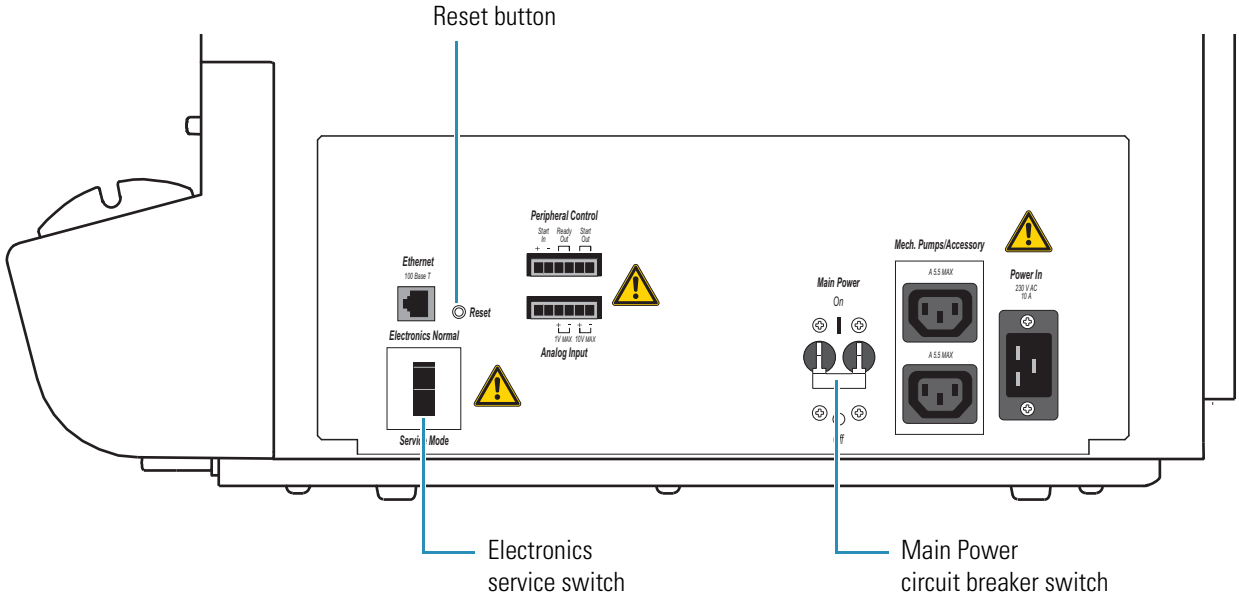
The power panel is located on the lower portion of the right side of the mass spectrometer. Figure 16 shows the power panels for the LXQ, LTQ XL, and LTQ Velos mass spectrometers.

Figure 16. Power panels

LXQ



LTQ XL and LTQ Velos



Line power at 230 V ac ± 10%, 15 A (for the LTQ XL and LTQ Velos) or 10 A (for the LXQ), 50/60 Hz, single phase, enters the mass spectrometer through the power panel (see Figure 16 on page 33) on the right side of the mass spectrometer. The power panel provides system power control, a contact closure interface, an Ethernet 100Base-T connection from the mass spectrometer to the data system PC, and a system Reset button. The power panel accepts line power, filters it, and provides it to various components of the mass spectrometer.

Main Power Circuit Breaker Switch

In the Off position, the Main Power circuit breaker switch removes all power to the MS detector, including the external forepump or forepumps. In the On position, power is supplied to the mass spectrometer. In the standard operational mode, the circuit breaker is kept in the On position.

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

Electronics Service Switch

The electronics service switch is a circuit breaker. In the Service Mode position, the switch removes power to all components of the mass spectrometer other than the fans and vacuum system. This setting allows you to service nonvacuum system components of the mass spectrometer with the vacuum system still operating. In the Electronics Normal position, power is supplied to all components of the mass spectrometer.

Reset Button

When you briefly press the reset button, the system software is reloaded from the data system. See "Resetting the Mass Spectrometer" on page 60 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 mass spectrometer. You can operate the API source in the electrospray ionization (ESI), heated electrospray ionization (H-ESI), nanospray ionization (NSI), atmospheric pressure photo ionization (APPI), or atmospheric pressure chemical ionization (APCI) mode. The ionization techniques are described in "Ionization Techniques" on page 5. For more information about the API source, see Chapter 4, "Removing or Installing the Ion Source Housing."

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).

LXQ and LTQ XL

The ion source interface in the LXQ and LTQ XL includes an ion transfer capillary, two cartridge heaters, a heater block, a sensor, a vent prevent ball, an ion sweep cone, a tube lens, and a skimmer (Figure 17, and Figure 18 on page 36).

Figure 17. LXQ ion source interface (cross section)

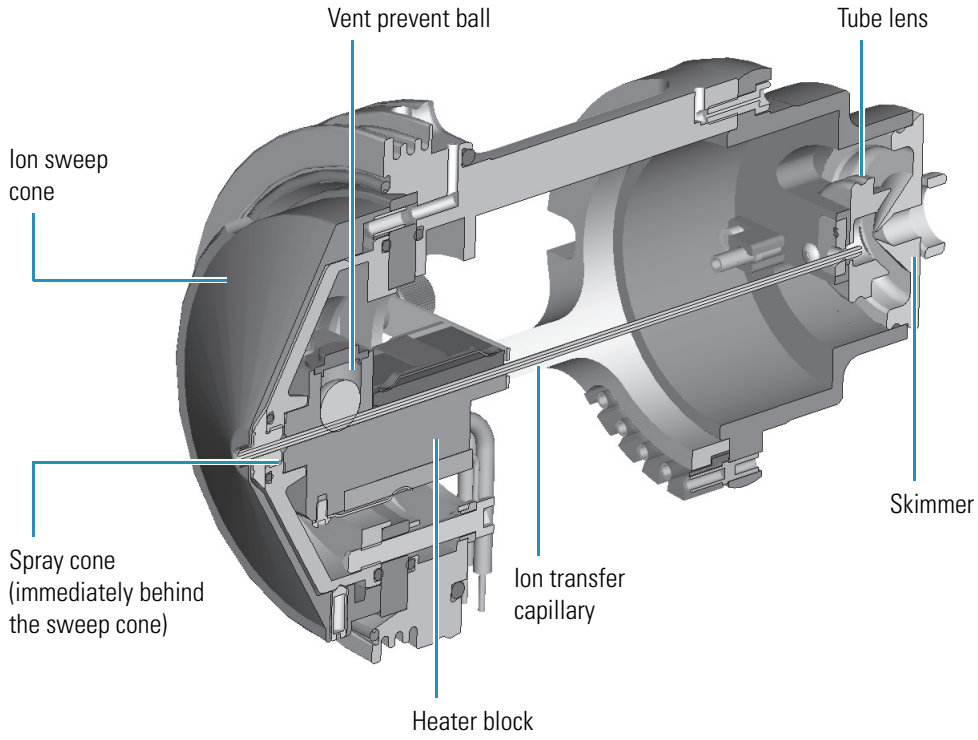
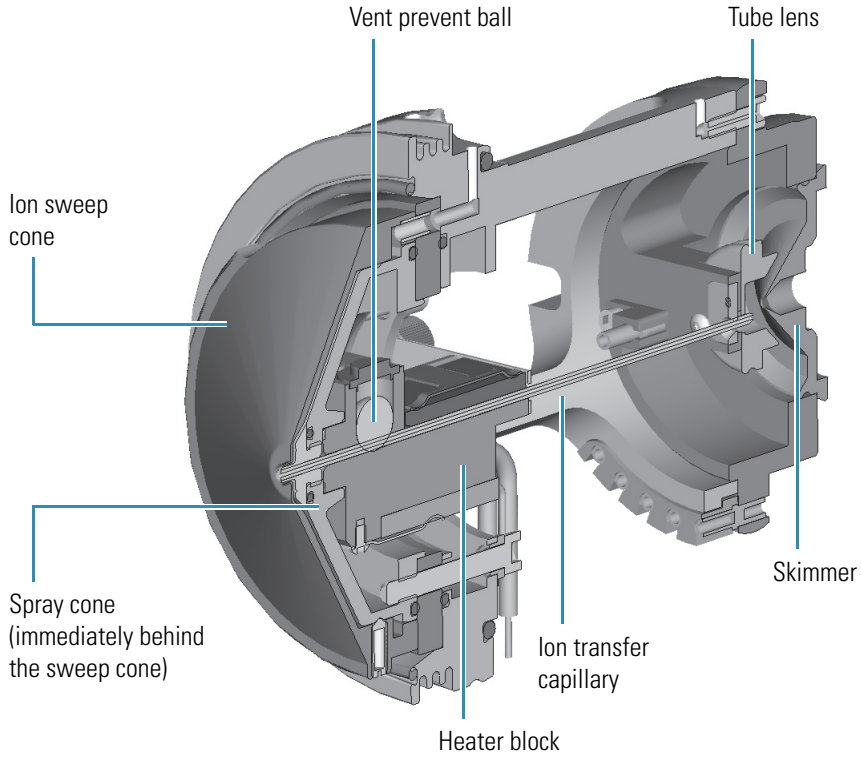


Figure 18. LTQ XL ion source interface (cross section)



The ion transfer capillary assists in desolvating ions that are produced by the API probe. The capillary is an elongated cylindrical tube made of metal. 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 probe sensor measures the temperature of the heater block. A decreasing pressure gradient draws ions into the ion transfer capillary in the atmospheric pressure region and transports them to the ion transfer capillary-skimmer region of the vacuum manifold. The vent prevent ball prevents air from entering the vacuum manifold when the capillary is removed and so that you can remove the ion transfer capillary for cleaning without venting the system.

The ion sweep cone is a metal cone over the capillary. The ion sweep cone acts as a physical barrier that protects the entrance of the capillary and increases source robustness.

Ions from the ion transfer capillary enter the tube lens. The tube lens has a potential applied to it to focus the ions toward the opening of the skimmer. When you tune the LXQ or LTQ XL mass spectrometer, adjust the tube lens potential to maximize sensitivity by balancing desolvation with fragmentation.

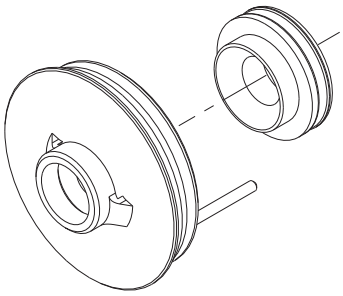
Ions from the tube lens pass through the skimmer and move toward the Q00 rf lens. The skimmer acts as a vacuum baffle between the higher pressure ion source interface region and the lower pressure Q00 rf lens region of the vacuum manifold.

The ion source interface is enclosed in a vacuum chamber the rotary vane pumps evacuate.

On the LXQ and LTQ XL, ions from the ion transfer tube enter the tube lens (Figure 19). The tube lens has a mass-dependent potential applied to it to focus the ions toward the opening of the skimmer. An additional potential, called the tube lens offset voltage, can be applied to the tube lens. This accelerates the ions into background gas that is present in the ion transfer tube-skimmer region. Collisions with the background gas aid in the desolvation of the ions and increase sensitivity. If the tube lens offset voltage is too high, however, collisions with the background gas can be energetic enough to cause ion fragmentation. This fragmentation, called ion source collision-induced dissociation (CID), decreases sensitivity. When you tune the LXQ or LTQ XL mass spectrometer, adjust the tube lens offset voltage to maximize sensitivity by balancing desolvation with fragmentation.

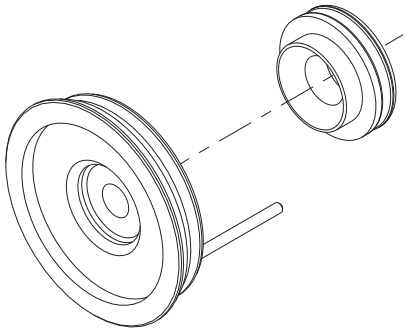
Figure 19. Tube lens and skimmer (front view)

LXQ



Front

LTQ XL

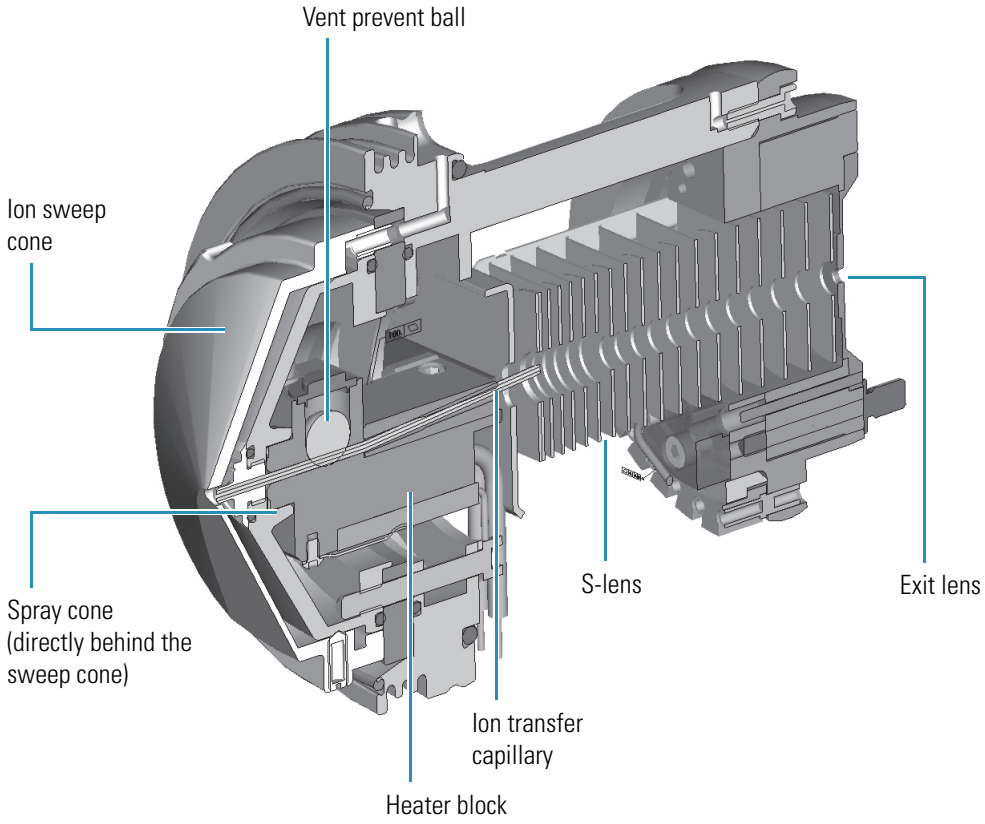


Front

LTQ Velos

The ion source interface in the LTQ Velos (Figure 20) includes an ion transfer capillary, two cartridge heaters, a heater block, a sensor, a vent prevent ball, an ion sweep cone, an S-lens, and an exit lens.

Figure 20. LTQ Velos ion source interface (cross section)



The ion transfer capillary assists in desolvating ions that are produced by the API probe. The capillary is an elongated cylindrical tube made of metal. 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 probe sensor measures the temperature of the heater block. A decreasing pressure gradient draws ions into the ion transfer capillary in the atmospheric pressure region and transports them to the ion transfer capillary-skimmer region of the vacuum manifold. The vent prevent ball prevents air from entering the vacuum manifold when the capillary is removed so that you can remove the ion transfer capillary for cleaning without venting the system.

The ion sweep cone, also made of metal, fits over the capillary. The ion sweep cone acts as a physical barrier that protects the entrance of the capillary and increases source robustness.

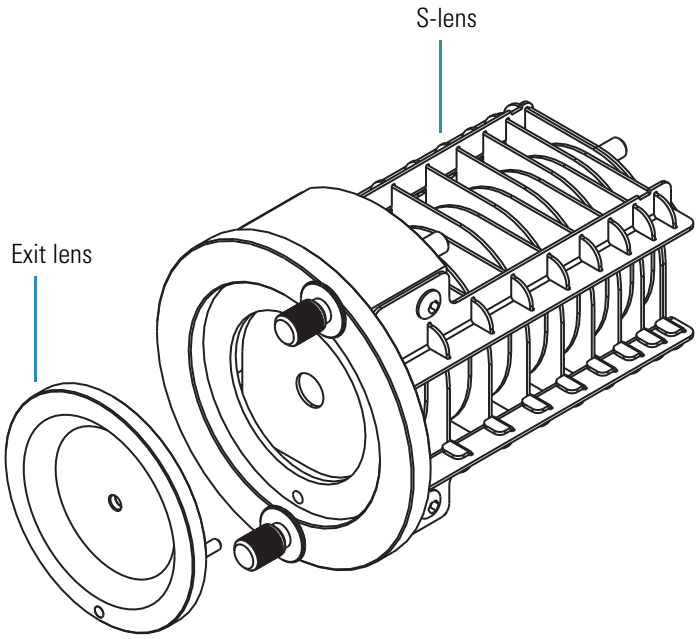
Ions from the ion transfer capillary enter the S-lens. Rf is applied to the S-lens to focus the ions toward the opening of the exit lens. When you tune the LTQ Velos mass spectrometer, adjust the S-lens rf to maximize sensitivity.

Ions from the S-lens pass through the exit lens and move toward the Q00 rf lens. The exit lens acts as a vacuum baffle between the higher pressure ion source interface region and the lower pressure Q00 rf lens region of the vacuum manifold.

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

The LTQ Velos uses an S-lens and exit lens rather than a tube lens and skimmer. The S-lens is an ion transmission device consisting of progressively-spaced, stainless-steel electrodes (Figure 21). An rf voltage is applied to the electrodes, and adjacent electrodes have voltages of opposite phase. As the rf amplitude increases, ions of progressively higher mass-to-charge ratios pass through to the exit lens. During the tune procedure, the LTQ Velos determines the mass-dependent rf amplitudes for optimum transmission of ions through the lens.

Figure 21. LTQ Velos exit lens and S-lens (back view)



Ions from the S-lens pass through the exit lens and move toward the Q00 rf lens. In the LXQ and LTQ XL, the tube lens and skimmer act as a vacuum baffle between the higher pressure ion source interface region and the lower pressure Q00 ion optics region of the vacuum manifold. In the LTQ Velos, the S-lens and exit lens perform the same function. The tube lens and skimmer (LXQ and LTQ XL), or the S-lens and exit lens (LTQ Velos) mount to the ion source interface cage.

Ion Optics

The following ion optics focus the ions produced in the API source and transmit them to the mass analyzer:

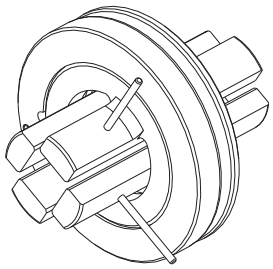
- "Q00 Ion Optics," next section
- "Q0 Ion Optics" on page 40
- "Q1 Ion Optics" on page 41

Q00 Ion Optics

The Q00 ion optics are the optics located closest to the API source. The Q00 ion optics include the Q00 rf lens and the lens L0.

The Q00 rf lens is a square array of thin metal elements that act as an ion focusing device (Figure 22). An rf voltage that is applied to the elements gives rise to an electric field that focuses the ions along the axis of the lens. A dc voltage offset from ground applied to Q00 (called the Q00 offset voltage) increases the translational kinetic energy of ions emerging from the skimmer or exit lens. During ion focusing, the offset voltage is negative for positive ions and positive for negative ions. Increasing the offset voltage increases the translational kinetic energy of the ions.

Figure 22. Q00 rf lens



The lens L0 is a metal plate with a small hole in one end through which the ion beam can pass. A potential is applied to lens L0 to aid in ion transmission. Lens L0 also acts as a vacuum baffle between the Q00 and Q0 ion optics chambers.

Q0 Ion Optics

The Q0 ion optics transmit ions from the Q00 ion optics to the mass analyzer. The Q0 ion optics include the Q0 quadrupole, the lens L1, and the gate lens or split gate lens.

The Q0 quadrupole is a square array of square-profile rods that act as an ion transmission device (Figure 23 and Figure 24 on page 41). An rf voltage applied to the rods gives rise to 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 Q00.

Figure 23. LXQ and LTQ XL Q0 quadrupole

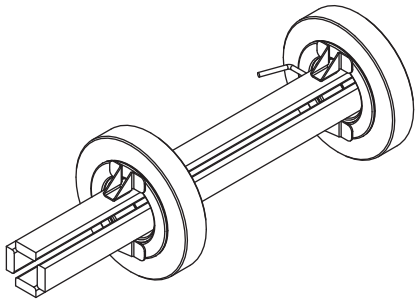
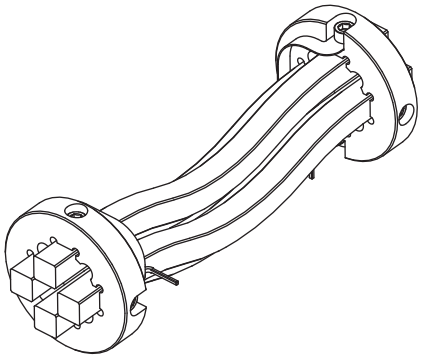


Figure 24. LTQ Velos Q0 quadrupole



The lens L1 is a metal plate with a circular hole in the center through which the ion beam can pass. An electrical potential applied to the lens accelerates (or decelerates) ions as they approach the lens. This electrical potential focuses the ion beam as it passes through the lens. Lens L1 also acts as a vacuum baffle between the Q0 ion optics chamber and the mass analyzer chamber. A gate lens or split gate lens starts and stops the injection of ions into the mass analyzer.

Q1 Ion Optics

The Q1 ion optics transmit ions from the Q0 ion guide to the mass analyzer. The Q1 ion optics include the Q1 octapole and the gate lens (Figure 25 and Figure 26 on page 42). The Q1 octapole is an octagonal array of round-profile rods that acts as an ion transmission device similar to Q0. An rf voltage 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.

Figure 25. LXQ and LTQ XL Q1 ion optics

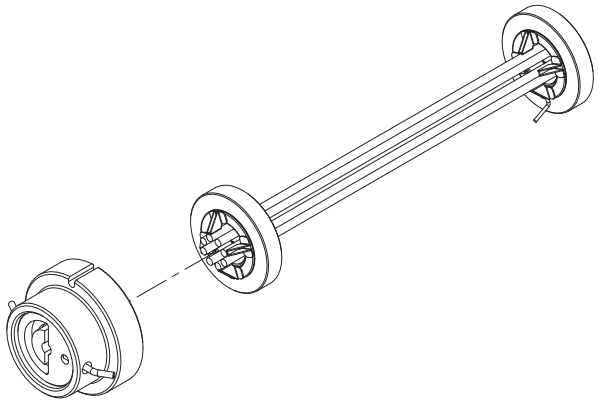
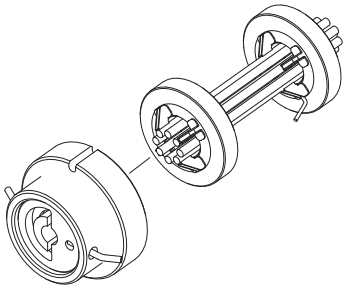


Figure 26. LTQ Velos Q1 ion optics



Mass Analyzer

The mass analyzer is the site of mass analysis that includes ion storage, ion isolation, collision-induced dissociation, and ion ejection. 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 operating the mass analyzer during mass analysis.

Components of the Mass Analyzer

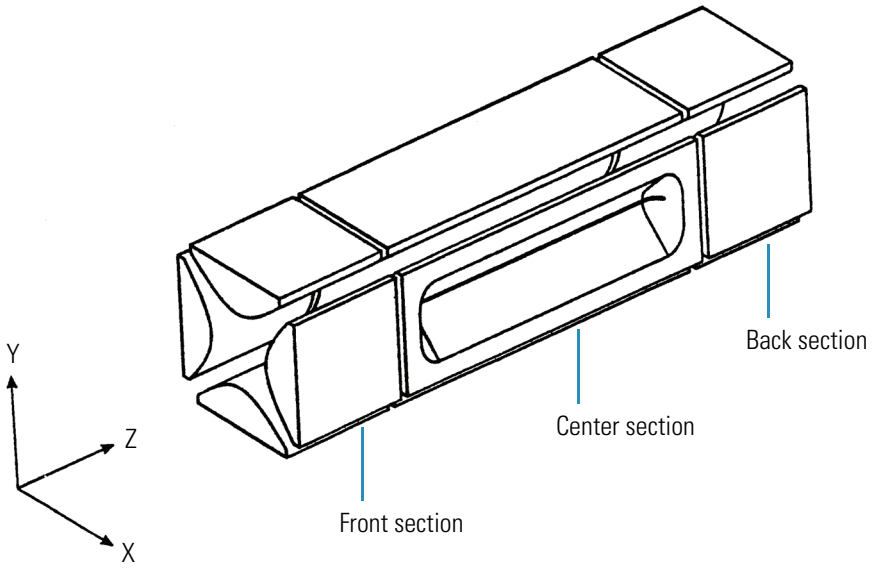
The LXQ and LTQ XL mass spectrometers contain a single two-dimensional linear ion trap. The LTQ Velos contains a dual cell two-dimensional linear ion traps

LXQ and LTQ XL

The mass analyzer in the LXQ and LTQ XL mass spectrometers consists of a front lens, linear ion trap, and back lens. The front and back lenses are metal plates with a circular hole in the center through which the ion beam can pass. The front and back lenses provide conductance limits.

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 27. The LXQ rods have one section and the LTQ XL rods have three sections. The exit rods have a slot through which the ions are ejected during scan out. In each trap, rods opposite each other in the array are connected electrically. You can then consider the four rods of each section to be two pairs of two rods each.

Figure 27. LTQ XL linear ion trap quadupole rod assembly



LTQ Velos

The mass analyzer in the LTQ Velos consists of a front lens, a linear ion trap, a center lens, another linear ion trap, and a back lens. The front, center, and back lenses are metal plates with a circular hole in the center through which the ion beam can pass. The front, center, and back lenses provide conductance limits.

The linear ion trap is a square array of precision-machined and precision-aligned hyperbolic rods. The LTQ Velos rods have three sections. All rods have a slot. Ions are ejected only through the x-rods during scan out. In each trap, rods opposite each other in the array are connected electrically. You can then consider the four rods of each section to be two pairs of two rods each.

Axial Trapping Voltages

The LXQ mass analyzer uses three dc axial trapping voltages, one for each lens and one for the trap. These voltages establish axial trapping by creating a potential well. These dc axial trapping voltages allow the mass analyzer to perform its storage and scan out functions.

The LTQ XL also uses three dc axial trapping voltages, one for each rod section.

The LTQ Velos uses six dc axial trapping voltages, one for each rod section on both traps. These voltages establish axial trapping by creating potential wells.

Types of AC Voltages 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 exit rods to stimulate motion of the ions in the direction of the ion detection system. When the ac frequency applied to the 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 (X direction).

The ion isolation waveform voltage acts during the ion isolation step of SIM, SRM, CRM, or MS^n ($n > 1$) 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.

During the collision induced dissociation step of SRM, CRM, or MS^n ($n > 1$) full-scan applications, the resonance excitation ac voltage is applied to the exit rods to fragment parent ions into product ions. Ion motion 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 during the ramp of the main rf voltage. Only when the mass analyzer is about to eject an ion is about to be ejected from the mass analyzer cavity by the main rf voltage is the ion in resonance with the resonance ejection ac voltage. When an ion approaches resonance, it moves farther away from the center of the mass analyzer and is ejected.

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 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, which results in damping the amplitude of their oscillations. The ions are then focused to the axis of the cavity rather than 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^n ($n > 1$) full-scan analysis, the resonance excitation ac voltage applied to the exit 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:

1. Ion storage
2. Ion isolation (SIM, SRM, CRM, or MS^n ($n > 1$) full scan only)
3. Collision-induced dissociation (SRM, CRM, or MS^n ($n > 1$) full scan only)
4. Ion scan out (the ion detection step)

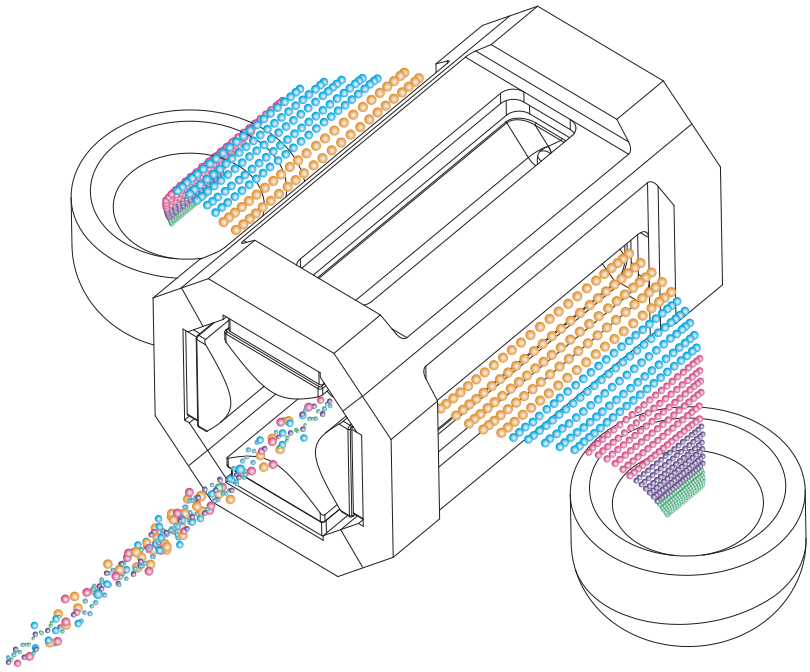
For SRM and MS/MS full-scan applications, the mass analyzer performs the ion isolation and collision induced dissociation steps are once. For CRM and MS^n ($n > 1$) full-scan applications the ion isolation and collision induced dissociation steps are performed n-1 times.

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.

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 a mass-to-charge ratio of less than the minimum storage mass-to-charge ratio are stored.

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. Most of these ions are focused toward the ion detection system where they are detected. Figure 28 on page 46 illustrates this process.

Figure 28. Visual representation of mass analyzer operation



The LTQ Velos operates in a slightly different manner. The LXQ and LTQ XL perform all four steps in one trap, but the LTQ Velos does not. In the LTQ Velos, the scan out step can only occur in the trap with the detectors.

Ion Detection Systems

The LTQ Series mass spectrometers have high-sensitivity, off-axis ion detection systems. The LXQ has one system and the LTQ XL and LTQ Velos mass spectrometers have two systems. These ion detection systems produce a high signal-to-noise ratio and enable voltage polarity switching between positive ion and negative ion modes of operation. Each ion detection system includes a conversion dynode and an electron multiplier. The ion detection systems are located on opposite sides of the mass analyzer.

The conversion dynode is a concave metal surface located at a right angle to the ion beam. A positive potential for negative ion detection and a negative potential for positive ion detection are applied to the conversion dynode. An ion striking the surface of the conversion dynode produces one or more secondary particles. The curved surface of the conversion dynode focuses these secondary particles and the voltage gradient accelerates them into the electron multiplier. The conversion dynode shields the vacuum manifold from the electric field that the conversion dynode produces.

The electron multiplier is mounted on the top cover plate of the vacuum manifold next to the mass analyzer. The electron multiplier includes a cathode and an anode. The cathode of the electron multiplier is a funnel-like resistor. At the exit end of the cathode is an anode. The anode collects the electrons that the cathode produces.

Secondary particles from the conversion dynode strike the inner walls of the electron multiplier cathode with sufficient energy to eject electrons. The ejected electrons strike the inner surface of the cathode further up, which creates a cascade of even more ejected electrons. The final result is a measurable current at the anode. The current collected by the anode is proportional to the number of secondary particles striking the cathode.

The current that leaves the electron multiplier via the anode is recorded by the data system.

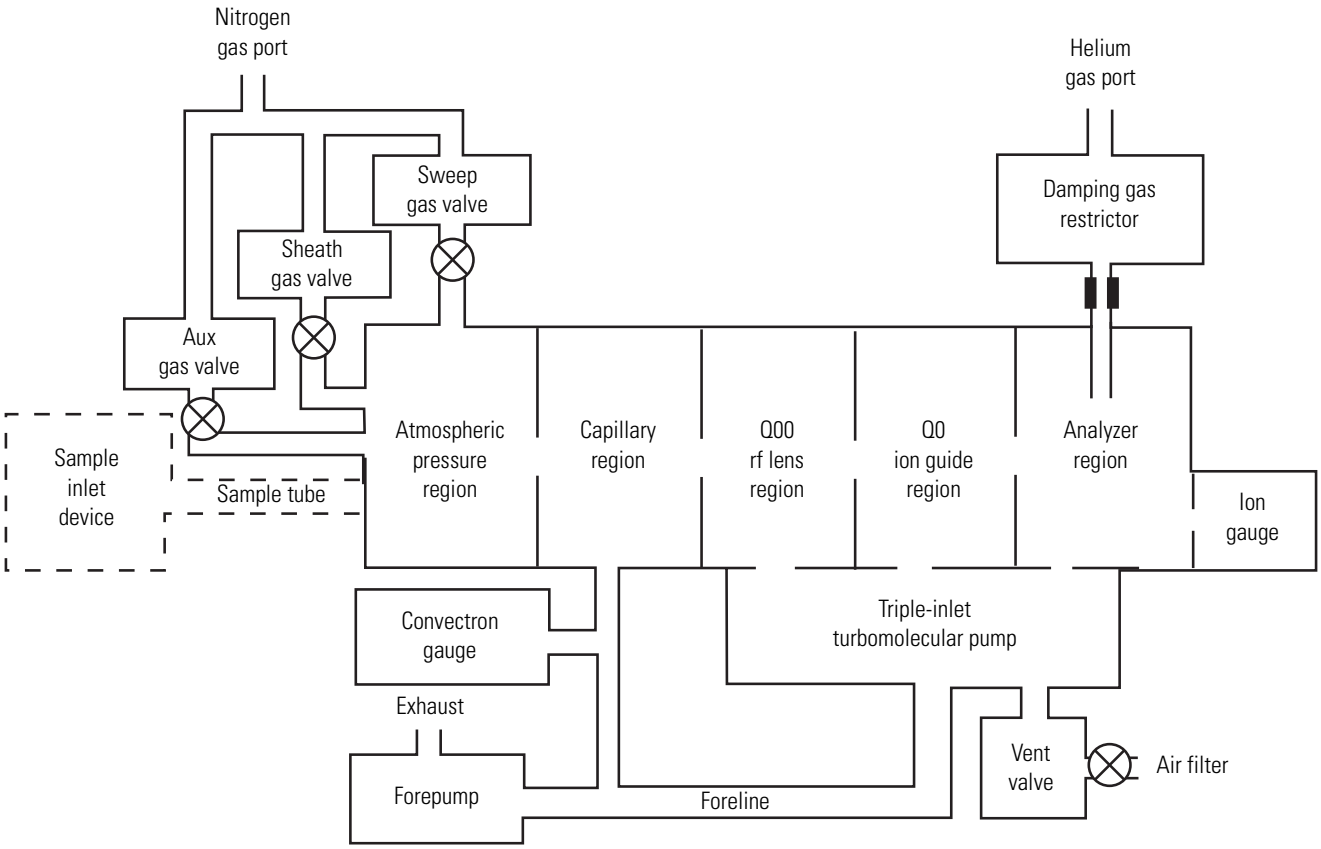
Because of the off-axis orientation of the ion detection system relative to the mass analyzer, neutral molecules from the mass analyzer tend not to strike the conversion dynode or electron multiplier. As a result, the noise from neutral molecules is reduced.

Vacuum System

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 (Figure 29 on page 48):

- "Vacuum Manifold," next section
- "Turbomolecular Pump" on page 49
- "Forepumps" on page 50
- "Convectron Gauge" on page 51
- "Ion Gauge" on page 51

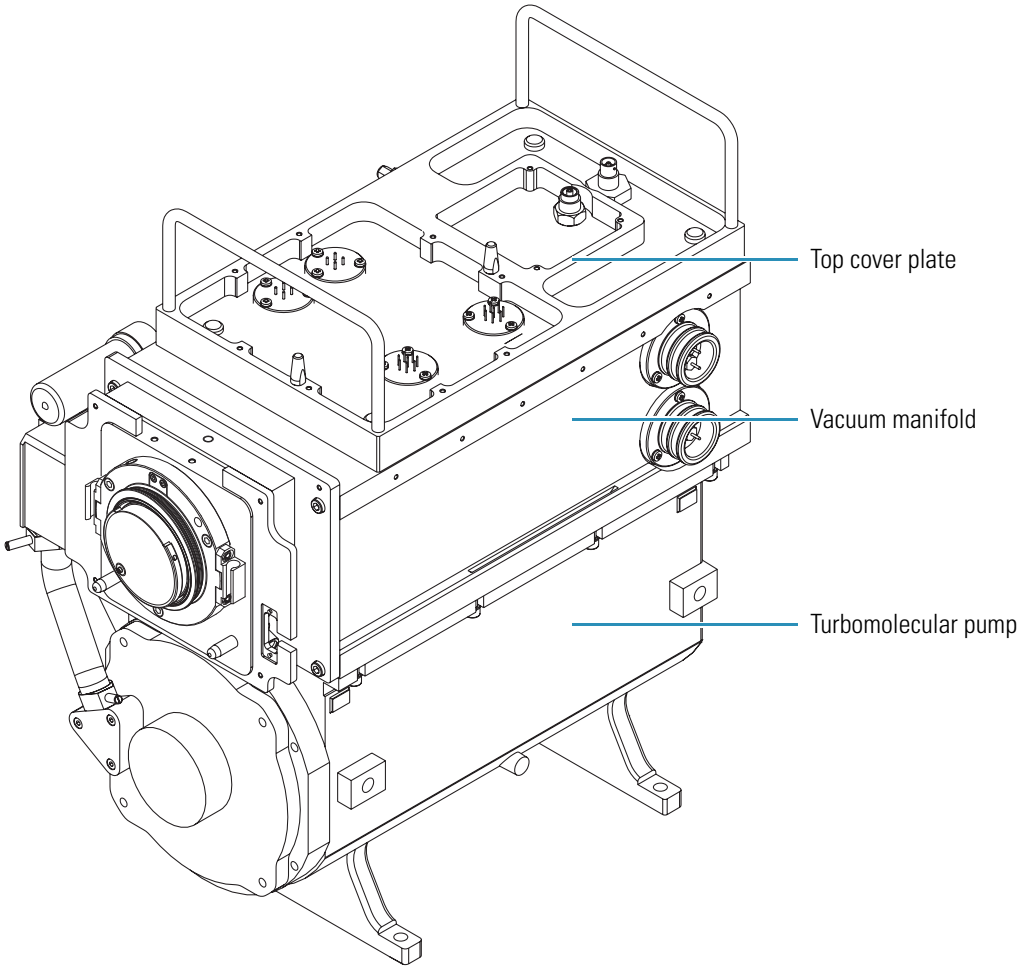
Figure 29. Vacuum system functional block diagram



Vacuum Manifold

The vacuum manifold (Figure 30) 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.

Figure 30. LXQ vacuum manifold with top cover plate and turbomolecular pump

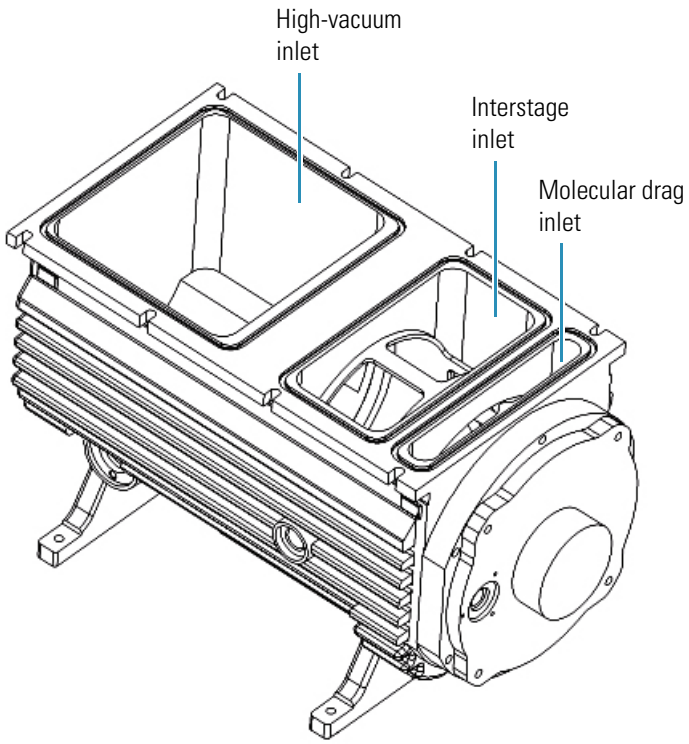


The vacuum manifold is divided into four chambers by three baffles.

Turbomolecular Pump

A triple-inlet turbomolecular pump (Figure 31 on page 50) provides the vacuum for the Q00 rf lens, Q0 ion guide, and analyzer regions of the vacuum manifold. The turbomolecular pump mounts onto the bottom of the vacuum manifold.

Figure 31. Turbomolecular pump



The main power circuit breaker switch turns off the turbomolecular pump. The electronics service switch has no effect on this pump. Power to the turbomolecular pump automatically shuts off if the turbomolecular temperature becomes too high.

The turbomolecular pump sends status information, such as its temperature or rotational speed, to the data system computer.

Forepumps

The LXQ mass spectrometer has one forepump and the LTQ XL and LTQ Velos mass spectrometers have two forepumps. Forepumps, also known as mechanical or rotary vane pumps, create the vacuum necessary for the proper operation of the turbomolecular pump. The forepumps also evacuate the ion transfer capillary region of the vacuum manifold.

The power cords of the forepumps are plugged into the outlet labeled *Mech. Pumps* on the power panel (Figure 16 on page 33). The main power circuit breaker switch controls this outlet and not the electronics service switch.

CAUTION Always plug the forepump power cords into the outlet labeled *Mech. Pumps* on the right side of the mass spectrometer. Never plug them into a wall outlet.

Convectron Gauge

A 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. The source PCB monitors the pressure measured by the vacuum gauge.

Ion Gauge

An ion gauge measures the pressure in the analyzer region of the vacuum manifold and is also used in vacuum protection.

Inlet Gases Hardware

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

- "Vent Valve," next section
- "Damping Gas Inlet Assembly" on page 51
- "Sheath Gas, Auxiliary Gas, and Sweep Gas Valves" on page 52

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, a solenoid-operated valve, is closed when the solenoid is energized.

The vacuum manifold is vented when external power is removed from the mass spectrometer. Power is removed from the mass spectrometer by a power failure or by placing the main power circuit breaker in the Off position. Power is briefly provided to the vent valve after the external power is removed to protect against the accidental loss of power. When power to the vent valve solenoid is shut off for more than a very brief period of time, the vent valve opens and the manifold is vented to filtered air.

Damping Gas Inlet Assembly

The damping gas inlet assembly controls the flow of helium into the mass analyzer cavity. Helium (40 ±10 psig [275 ±70 kPa], 99.999% [ultra high-purity]) enters the MS detector through a 1/8 in. port on the back of the MS detector. The MS detector regulates the flow of helium and delivers it to the mass analyzer.

Helium in the mass analyzer cavity dampens ionic motion and improves the performance of the mass spectrometer. See "Helium Damping Gas in the Mass Analyzer Cavity" on page 44.

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 the inner coaxial nitrogen gas of the API probe that sprays (nebulizes) the sample solution into a fine mist as it exits the sample tube. Auxiliary gas is the outer coaxial nitrogen gas that assists the sheath gas in the nebulization and evaporation of sample solutions. Sweep gas flows out from behind the sweep cone in the ion source interface. Sweep gas aids in solvent declustering and adduct reduction.

Dry nitrogen (100 ±20 psig [690 ±140 kPa], 99% purity) enters the MS detector through a 1/4 in. port in the back of the MS detector. Valves that are controlled by the data system regulate the nitrogen pressure. You can set the flow rates from the Tune Plus window.

Cooling Fans

Five fans provide cooling for the MS detector. One 100 $ft.^3$/min. fan cools the rf voltage coil. One 21 $ft.^3$/min. fan cools the turbomolecular pump. Three 100 $ft.^3$/min. fans cool the electronics in the tower. Air is drawn in from the back of the mass spectrometer. The exhaust air is expelled from the vent slots on the sides of the mass spectrometer.

CAUTION To ensure safety and proper cooling, always operate the mass spectrometer with its covers in place. This is also necessary to comply with product safety laws and electromagnetic interference regulations.

System Shutdown, Startup, and Reset

Many maintenance procedures for the LTQ Series mass spectrometer require that the system be shut down completely. If the system is not to be used for 12 hours or more, you can place the LTQ Series mass spectrometer in Standby mode.

Contents

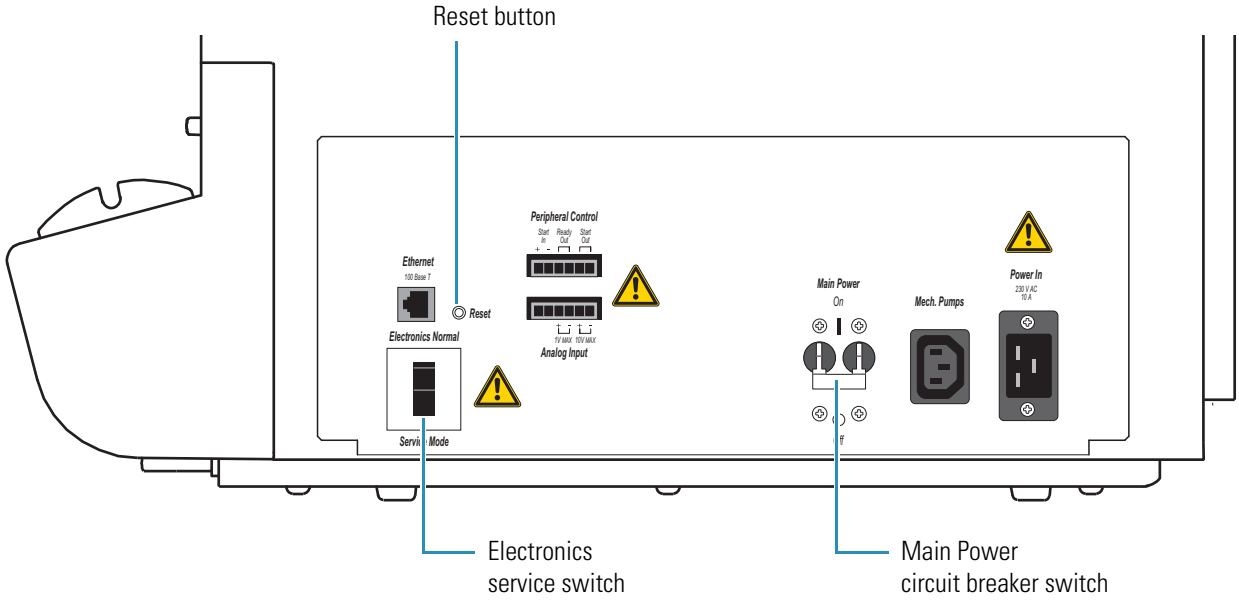
Shutting Down the System in an Emergency

CAUTION If you need to turn off the mass spectrometer in an emergency, place the main power circuit breaker switch, located on the power panel on the right side panel of the mass spectrometer (Figure 32 on page 54), in the Off position. This turns off all power to the mass spectrometer, including the vacuum pumps. Although removing power abruptly does no harm to components within the system, this is not the recommended shutdown procedure to follow. (See "Shutting Down the Mass Spectrometer Completely" on page 57.)

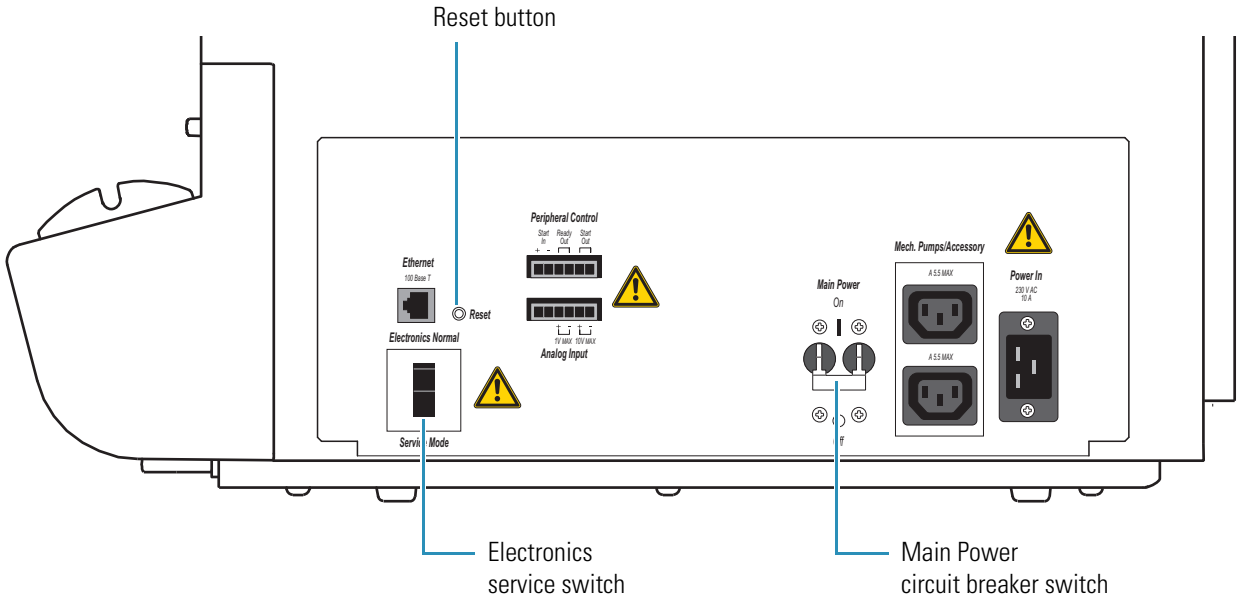
To turn off the LC, autosampler, and computer in an emergency, use the on/off switches on the LC, autosampler, and computer, respectively.

Figure 32. Power panels

LXQ



LTQ XL and LTQ Velos



Placing the Mass Spectrometer in Standby Mode

You do not need to shut down the LTQ Series mass spectrometer completely if you are not going to use it for 12 hours or more. Instead, place the mass spectrometer in Standby mode.

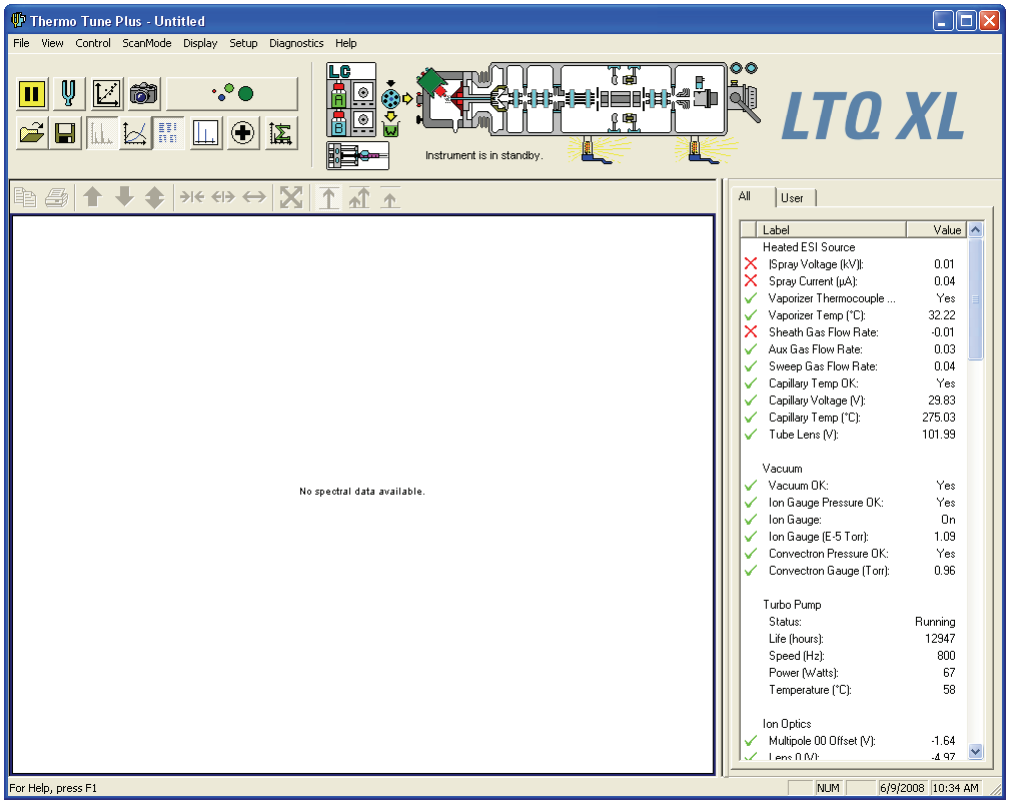
❖ To place the LTQ Series mass spectrometer in Standby mode

1. Wait until data acquisition, if any, is complete.
2. On the Windows taskbar, choose **Start > All Programs > Thermo Instruments > LTQ > *model* Tune.**

   Note For LTQ version 2.5.0 or earlier, the path is **Start > All Programs > Xcalibur > *model* Tune**.

   The Tune Plus window opens with the status view on the right side of the window (Figure 33).

   Figure 33. Tune Plus window for the LTQ XL mass spectrometer



3. Turn off the flow of sample solution from the LC to the API source:

   a. Choose **Setup > Inlet Direct Control**.

      The Inlet Direct Control dialog box opens.

   b. Click the tab for the LC pump.

The LC page opens.

c. Click the **Pump Off** or **Stop Pump** button 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.

On 

Standby 

4. On the Control/Scan Mode toolbar, click the **On/Off/Standby** button to place the mass spectrometer in Standby mode.

   The LTQ Series mass spectrometer turns off the electron multipliers, conversion dynodes, 8 kV power to the API source, main rf voltage, and ion optic rf voltages. The mass spectrometer also turns off the auxiliary and sheath gas flows. See Table 5 on page 63 for the On/Off status of mass spectrometer components when the mass spectrometer is in Standby mode. The System LED on the front panel of the mass spectrometer turns yellow when the system is in Standby mode.

Turning the Mass Spectrometer On

Before you can use the mass spectrometer, ensure that the system is on.

❖ **To turn the mass spectrometer on**

1. On the Windows taskbar, choose **Start > All Programs > Thermo Instruments > LTQ > *model* Tune.**

   Note For LTQ version 2.5.0 or earlier, the path is **Start > All Programs > Xcalibur > *model* Tune**.

   The Tune Plus window opens (Figure 33 on page 55).

On 

Off 

Standby 

   You can determine the state of the system by observing the state of the On/Off/Standby button on the Control/Scan Mode toolbar. The three different states of the On/Off/Standby button are shown at the left.

2. Click the **On/Off/Standby** button to turn the LTQ Series mass spectrometer on.

   The System LED on the front panel of the mass spectrometer turns green. The high voltage to the electron multipliers turns on.

Shutting Down the Mass Spectrometer Completely

Shut down the LTQ Series mass spectrometer completely only if it is not in use for an extended period of time or if it must be shut down for maintenance or service. You do not need to shut down the system completely if you are not going to use it for a short period of time, such as overnight or over weekends. Instead, put the system in Standby mode as described in "Placing the Mass Spectrometer in Standby Mode" on page 55.

❖ To shut down the LTQ Series mass spectrometer 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 was shipped with the LC.

2. On the Windows taskbar, choose **Start > All Programs > Thermo Instruments > LTQ > *model* Tune**.

   Note For LTQ version 2.5.0 or earlier, the path is **Start > All Programs > Xcalibur > *model* Tune**.

   The Tune Plus window opens (Figure 33 on page 55).

On 
Standby 

3. On the Control/Scan Mode toolbar, click the **On/Off/Standby** button to put the mass spectrometer in Standby mode.

   When you place the mass spectrometer in Standby mode, the electron multiplier, conversion dynode, 8 kV power to the API source, main rf voltage, and ion optic rf voltage, sheath, and auxiliary gasses are turned off.

4. Place the electronics service switch in the Service position. This switch is located on the power panel (see Figure 32 on page 54). Power to the nonvacuum system electronics is turned off when you place the electronics service switch in the Service position.

5. Place the main power circuit breaker in the Off position. This switch is located on the power panel (see Figure 32 on page 54). When you place the main power circuit breaker switch in the Off position, the following occurs:

   - All power to the mass spectrometer, including the turbomolecular pump and rotary vane pump, is turned off. (All LEDs on the front panel of the mass spectrometer are off.)
   - After 5 seconds, 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 2 minutes, the vacuum manifold is at atmospheric pressure.

6. Unplug the power cord for the mass spectrometer.

CAUTION Allow heated components to cool before servicing them.

Note If you are planning to perform routine or preventive system maintenance on the mass spectrometer only, you do not need to turn off the LC, data system, and autosampler. In this case, the shutdown procedure is complete. However, if you do not plan to operate your system for an extended period of time, Thermo Fisher Scientific recommends that you turn off the LC, data system, and autosampler as described in steps 7 through 12 (below0.

7. Turn off the LC if one is connected to your system. Follow the procedure described in the manual that was shipped with the LC.
8. Turn off the helium damping gas supply at the tank.
9. Turn off the nitrogen supply at the tank.
10. Turn off the data system as follows:
    a. On the Windows taskbar, choose **Start > Shut Down**.

       The Shut Down Windows dialog box opens.

    b. Select **Shut Down** and then click **OK**.
    c. When the Windows shutdown procedure tells you it is safe to turn off the computer, turn off the monitor and computer using the On/Off switches.
11. If a printer is a part of the system, turn it off using its On/Off switch.
12. If an autosampler is a part of the system, turn it off by using its main power On/Off switch.

Starting the System after a Complete Shutdown

To start up the LTQ Series mass spectrometer after it has been shut down completely, do the following:

- "Starting the LC," next (if this a part of the system)
- "Starting the Data System" on page 59
- "Starting the Mass Spectrometer" on page 59
- "Starting Up the Autosampler" on page 60 (if this is a part of the system)

Starting the LC

To start up the LC, follow the startup procedure described in the manual that was shipped with the LC. If necessary, configure the LC as described in the *LTQ Series Getting Connected Guide*. Do not turn on the liquid flow to the mass spectrometer at this point in the procedure.

Starting the Data System

❖ **To start the data system**

1. Turn on the monitor, computer, and printer.
2. Follow the Windows startup procedure on the monitor.

Starting the Mass Spectrometer

❖ **To start the mass spectrometer**

Note Make sure the data system is running before you start the mass spectrometer. The mass spectrometer will not operate it receives a instructions 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 position and the electronics service switch is in the Service position.
3. Plug in the power cord for the mass spectrometer.
4. Place the main power circuit breaker switch in the On position. The rotary vane pumps and the turbomolecular pump now start. All LEDs on the mass spectrometer front panel are off.
5. Allow the LTQ Series mass spectrometer to pump down for 5 minutes.
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 mass spectrometer front panel turns green to indicate that power is provided to the mass spectrometer electronics. (The electron multiplier, conversion dynode, 8 kV power to the API source, main rf voltage, and ion optic rf voltage remain off.)
   - The embedded computer boots. After several seconds the Communication LED on the front panel turns yellow to indicate that the data system and the mass spectrometer have started to establish a communication link.
   - After several more seconds, the Communication LED turns green to indicate that the data system and the mass spectrometer have established a communication link. Ensure that the instrument console window is active. The data system transfers operational software to the mass spectrometer.

- After three minutes, the System LED turns yellow to indicate that the software transfer from the data system to the mass spectrometer is complete and that the mass spectrometer is in Standby mode. Or, the System LED turns green to indicate that the mass spectrometer is functional and the high voltages are on.

> **Note** The Vacuum LED on the front panel of the mass spectrometer is illuminated green only if the pressure in the vacuum manifold is below the maximum allowable pressure (5×10^{-4} Torr in the analyzer region, and 2 Torr in the capillary-skimmer region).

If you have an autosampler, see "Starting Up the Autosampler," next.

Starting Up the Autosampler

Start up the autosampler by placing 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, and so forth, refer to the manual supplied with the autosampler. The *LTQ Series Getting Connected Guide* provides autosampler connection procedures.

Resetting the Mass Spectrometer

If communication between the mass spectrometer and data system computer is lost, it may be necessary to reset the mass spectrometer using the reset button on the power panel. See Figure 32 on page 54 for the location of the reset button.

The following procedure assumes that the mass spectrometer and data system computer are both powered on and operational. If the mass spectrometer, data system computer, or both are off, see "Starting the System after a Complete Shutdown" on page 58.

❖ To reset the mass spectrometer

1. Ensure that the Communication LED is off.
2. Press the reset button on the power panel (Figure 16 on page 33).

   When you press the Reset button the following occurs:

   - The embedded computer reboots. All LEDs on the front panel of the mass spectrometer turn off except the Power LED.
   - After several seconds, the Communication LED turns yellow to indicate that the data system and the mass spectrometer are starting to establish a communication link.
   - After several more seconds, the Communication LED turns green to indicate that the data system and the mass spectrometer have established a communication link. The data system transfers operational software to the mass spectrometer.

- After three minutes, the System LED turns yellow to indicate that the software transfer from the data system to the mass spectrometer is complete and that the mass spectrometer is in Standby mode. Or, the System LED turns green to indicate that the mass spectrometer is functional and the high voltages are on.

Resetting the Tune and Calibration Parameters to their Default Values

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

❖ **To reset the 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 (such as spray voltage, sheath and auxiliary gas flow, ion transfer capillary temperature) before you reset the system parameters to their default values.

1. In the Tune Plus window, choose one of the following:
   - **File > Restore Factory Calibration** to restore the default calibration parameters.
   - **File > Restore Factory Tune Method** to restore the default tune parameters.
2. To calibrate or tune the LTQ Series mass spectrometer, perform the calibration procedures described in the *LTQ Series Getting Started Guide*.

Resetting the Data System

There are two ways to reset the data system:

- "Resetting the Data System Using Windows," next section
- "Resetting the Data System Using the Reset Button on the Personal Computer" on page 62

Resetting the Data System Using Windows

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

❖ **To reset the data system using Windows**

1. On the Windows taskbar, choose **Start > Shut Down**.

   The Shut Down Windows dialog box opens.

2. Select **Restart**, and then click **OK** to start the Windows shutdown and restart procedure.

3. Follow the Windows shutdown and restart procedure on the monitor.

Note The communications link between the data system and the mass spectrometer should be automatically reestablished after you reset the data system. When this occurs the Communication LED on the front panel of the mass spectrometer 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 mass spectrometer for three seconds.

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

❖ **To reset the data system using the reset button**

1. Press the reset button on the data system computer.
2. Observe the Windows shutdown and restart procedure on the monitor.
3. When the shutdown and restart procedure has completed, choose **Start > Programs > Xcalibur > LTQ Tune** to open the Tune Plus window.

Note The communications link between the data system and the mass spectrometer should be automatically reestablished after you reset the data system. When this occurs, the Communication LED on the front panel of the mass spectrometer 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 mass spectrometer for three seconds.

Turning Off Selected Mass Spectrometer Components

There are five ways that you can turn off some or all of the mass spectrometer components:

- Turn off individual mass spectrometer components from the Tune Plus window. Turning off individual mass spectrometer components might be necessary when you are troubleshooting a problem or when you are running certain diagnostic procedures.
- Place the mass spectrometer in Standby mode. Standby mode is the normal condition to leave the mass spectrometer in when it is not in use. Choose **Control > Standby** or on the Control/Scan Mode toolbar click the **On/Standby** button.
- Turn the mass spectrometer Off. Off is similar to Standby, except all high-voltage components of the mass spectrometer are turned off. Choose **Control > Off** in the Tune Plus window to turn the mass spectrometer off.
- Turn the electronics service switch to Service. In the service position, you can perform maintenance procedures involving nonvacuum system components of the mass spectrometer.
- Place the main power circuit breaker switch in the Off position. Placing the main power circuit breaker switch in the Off position removes all power to the mass spectrometer, including the vacuum system.

Table 5 summarizes the On/Off status of mass spectrometer components, voltages, and gas flows.

Table 5. On/off status of MS detector components, voltages, and gas flows (Sheet 1 of 2)

MS detector component	Standby	Off	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
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	Off	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 (5 sec)
Turbomolecular pump	On	On	On	Off
Rotary vane pump	On	On	On	Off
Turbomolecular Pump Controller	On	On	On	Off
Power supply, electron multipliers/conversion dynodes	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
Power supply, +300 V dc	On	Off	Off	Off
Fan, turbomolecular pump	On	On	On	Off

Table 5. On/off status of MS detector components, voltages, and gas flows (Sheet 2 of 2)

MS detector component	Standby 	Off 	Electronics service switch in Service position	Main power circuit breaker switch in Off (O) position
Fan, rf coil	On	On	Off	Off
Fans, electronics tower	On	On	On	Off
Convectron gauge	On	On	Off	Off
Ion gauge	On	On	Off	Off

Removing or Installing the Ion Source Housing

The Ion Max or Ion Max-S API source housing holds the ESI, HESI-II, or APCI probe. The Ion Max has two features that the Ion Max-S does not have: an adjustable probe port and a front door with a window. Aside from these two features, these two source housings have the same functionality and mount to the mass spectrometer in the same way.

Follow these procedure to install or remove the source housing:

- "Removing the Ion Max or Ion Max-S API Source Housing," next section
- "Installing the Ion Max or Ion Max-S API Source Housing" on page 66
- "Ion Source Drain Assembly" on page 68

Removing the Ion Max or Ion Max-S API Source Housing

You must remove the API source housing to access the APCI corona needle or the ion source interface.

❖ **To remove the API source housing**

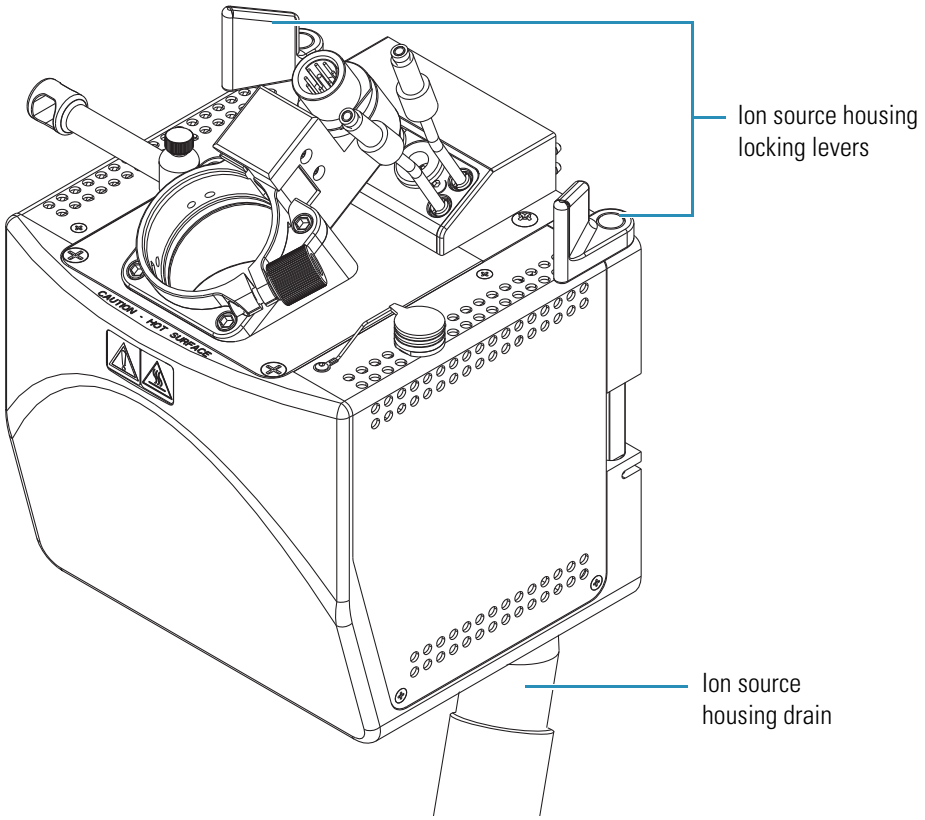
1. If the mass spectrometer was recently in operation, allow the ion source housing to cool to room temperature before you touch its external metal surface.

CAUTION **Avoid burns**. During operation of the mass spectrometer, the external surface of the ion source housing can become hot. Allow the ion source housing to cool to room temperature (approximately 20 minutes) before touching or removing it from the mass spectrometer.

2. If a probe is connected to the source housing, disconnect the external liquid lines before removing the source housing from the mass spectrometer.
3. Remove the drain tube from the ion source housing drain (Figure 34 on page 66).

Note Figure 34 on page 66 shows the Ion Max-S source housing whose locking levers and drain are the same as those for the Ion Max source housing.

Figure 34. Ion Max-S source housing locking levers and drain



4. Rotate the ion source housing locking levers 90 degrees away from the housing to release the ion source housing from the ion source mount assembly (Figure 34).
5. Remove the ion source housing by pulling it straight off of the ion source mount assembly. Place the housing in a safe location for temporary storage.

Installing the Ion Max or Ion Max-S API Source Housing

❖ **To install the API source housing**

1. Carefully align the two guide pin holes on the back of the ion source housing with the ion source housing guide pins on the mass spectrometer. Carefully press the housing onto the ion source mount (Figure 35 and Figure 36 on page 67).

Note From the back view, the Ion Max looks the same as the Ion Max-S.

Figure 35. Ion Max-S API source housing (back view)

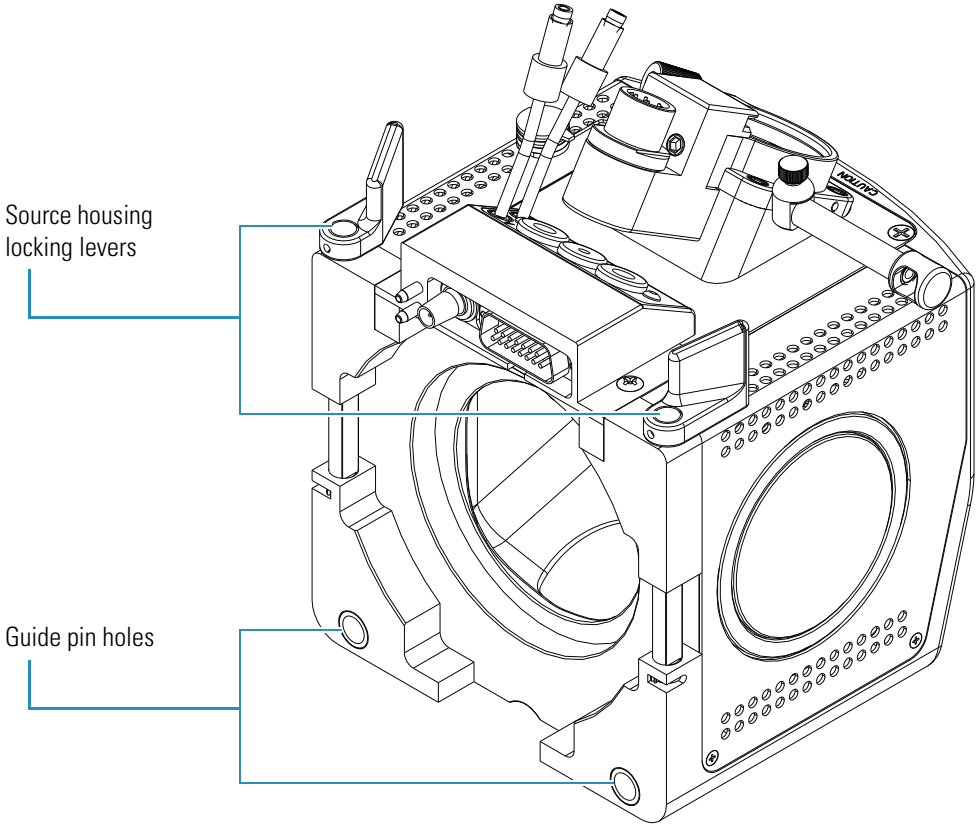
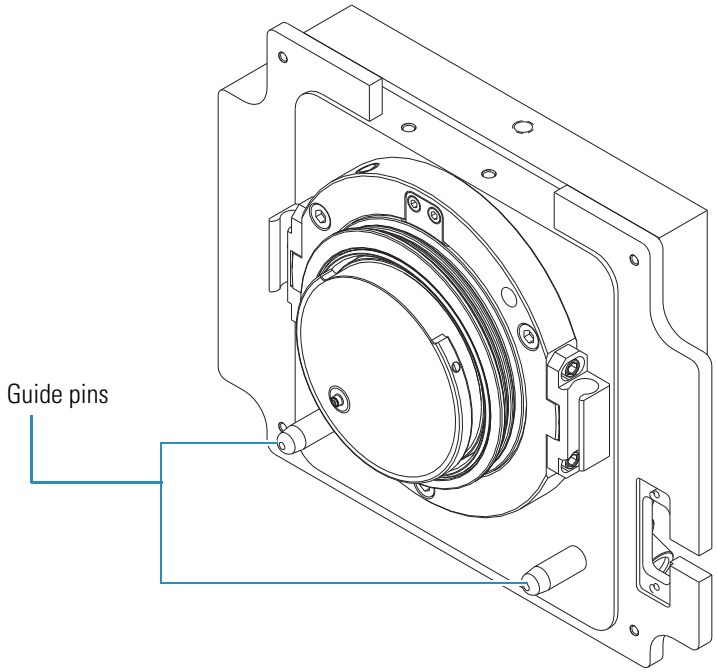


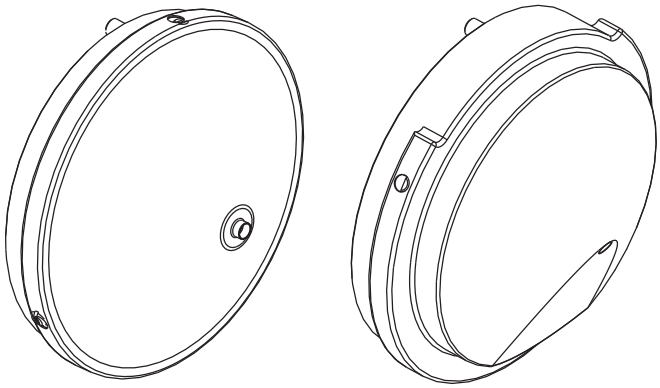
Figure 36. Ion source mount



2. Rotate the ion source housing locking levers 90 degrees to lock the ion source housing onto the ion source mount assembly.

   Figure 37 shows the two types of ion sweep cones available on Thermo Scientific mass spectrometers.

   Figure 37. Ion sweep cones



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.

3. Reinstall the source drain assembly as follows:

   a. Connect the source drain assembly to the ion source housing drain fitting (see "Ion Source Drain Assembly" on page 68).

   b. Attach the free end of the hose to a waste container. Vent the waste container to a fume exhaust system.

Ion Source Drain Assembly

When you install the Ion Max or Ion Max-S ion source, reconnect the drain at the bottom of the source housing to the solvent waste container (Figure 38 on page 69).

Figure 38. Source drain assembly and waste container

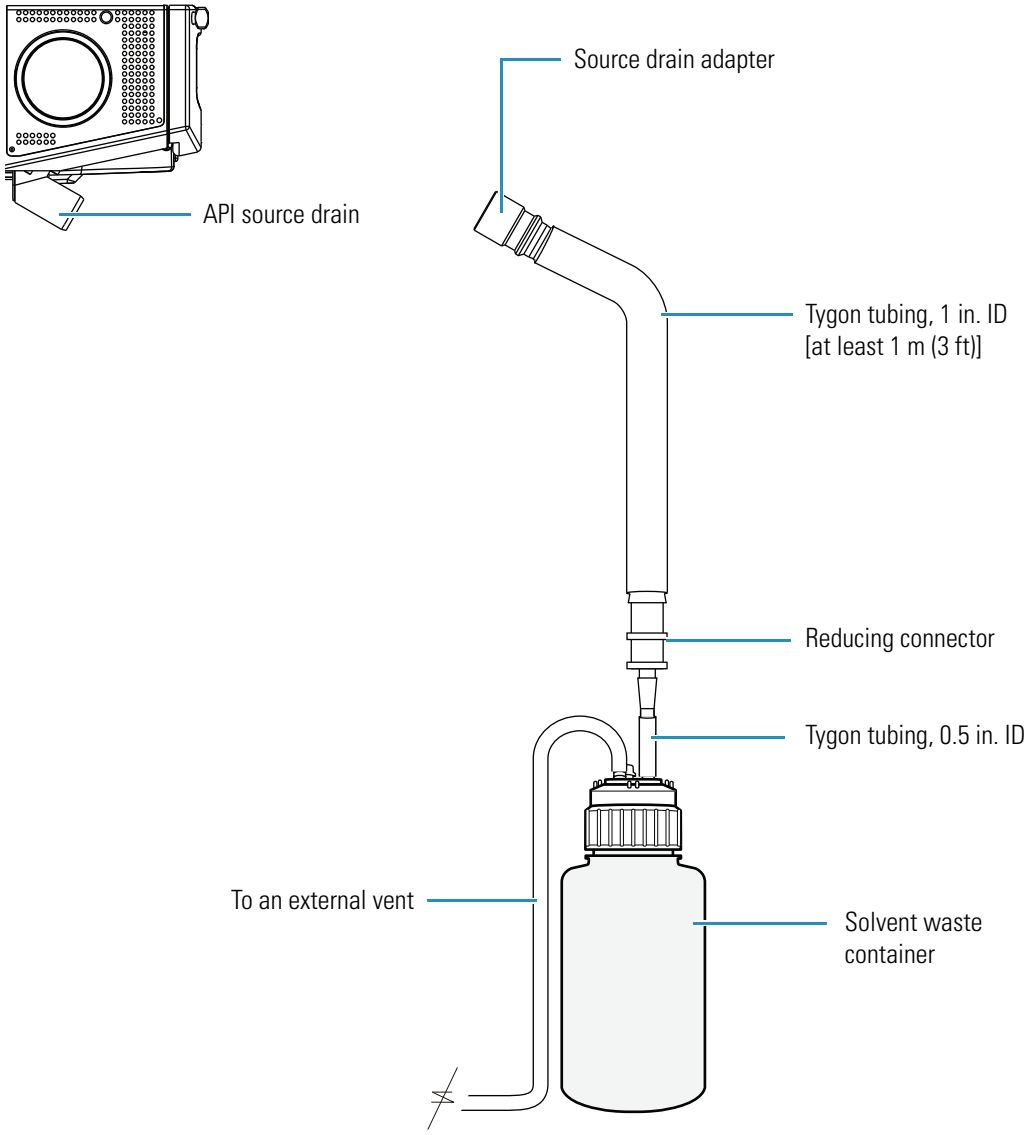


Table 6 on page 70 lists the components of the solvent waste system. During the initial installation of the mass spectrometer, a Thermo Fisher Scientific field service engineer installs the solvent waste system.

Table 6. Solvent waste system parts

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

When you reconnect the drain tubing to the drain at the bottom of the Ion Max or Ion Max-S API source, ensure that you connect the Teflon source drain adapter, which can withstand the high temperatures produced by the H-ESI or APCI source, to the source drain.

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

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

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

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

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

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

Daily Operation

To ensure the proper operation of your LTQ Series system, Thermo Fisher Scientific recommends that you perform daily preventive maintenance. This chapter provides details about the items you should check before you operate the system and the cleaning procedures you should perform after you complete your analyses.

Contents

Note You do not need to tune (optimize the tune parameters for the ESI calibration solution) and calibrate the LTQ Series system 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 must tune and calibrate the LTQ Series system (that is, optimize the tune for the ESI calibration solution and calibrate the mass accuracy using the ESI calibration solution) about once a quarter.

You must optimize the tune parameters (create a new tune method) whenever you change the type of experiment.

For information on tuning and calibration, refer to the *LTQ Series Getting Started Guide*.

Before Operating the LTQ Series System

Perform the following procedures every day before you begin your first analysis:

- "Checking the Helium and Nitrogen Supplies," next section
- "Checking the ESI Fused-Silica Sample Tube for Elongation" on page 72
- "Turning the System On" on page 72
- "Checking the System Vacuum Levels" on page 72
- "Checking the Disk Space" on page 74

Checking 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 275 ± 35 kPa (40 ±5 psi). 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. When nitrogen is on 24 hours per day, typical nitrogen gas consumption at 5560 L (200 ft^3) per day results in a maximum usage of up to 26700 L (960 ft^3). If necessary, replace the tank. Verify that the pressure of nitrogen reaching the MS detector is 690 ± 140 kPa (100 ± 20 psi). If necessary, adjust the pressure with the tank pressure regulator.

For more information about gas requirements, including those for a MALDI LTQ XL system and the reagent carrier gas needed for the LTQ XL/ETD system, refer to the *LTQ Series Preinstallation Requirements Guide*.

Checking the ESI Fused-Silica Sample Tube for Elongation

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

If you are running in the ESI mode with a fused-silica sample tube, verify that the sample tube is not elongated past the tip of the ESI spray needle. If the tube is elongated, cut and reposition it. See "Trimming the ESI Sample Tube" on page 87.

Turning the System On

Ensure that the system is turned on, and if it is not, turn it on as described in "Turning the Mass Spectrometer On" on page 56.

Checking the System Vacuum Levels

For proper performance, operate the LTQ Series system at the proper vacuum levels. Operating the system with poor vacuum levels can cause reduced sensitivity, tuning problems, and reduced electron multiplier life. Before you begin daily operation, check for major air leaks in the system, and check the vacuum levels of the system.

❖ To check the system for major air leaks

- Listen for a rush of air or a hissing sound inside the mass spectrometer.

  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.

❖ To check the vacuum pressure

1. On the Windows taskbar, choose **Start > All Programs > Thermo Instruments > LTQ > *model* Tune**.

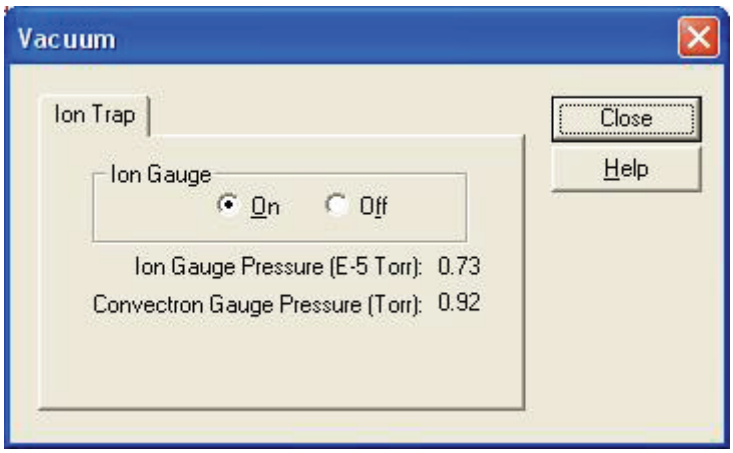
   Note For LTQ version 2.5.0 or earlier, the path is **Start > All Programs > Xcalibur > *model* Tune**.

   The Tune Plus window opens (Figure 33 on page 55).

2. Choose **Setup > Vacuum**.

   The Vacuum dialog box opens (Figure 39).

   Figure 39. Vacuum dialog box



3. Check the Ion Gauge Pressure readback.

   This readback displays the current pressure in the analyzer region.

4. Check the Convectron Gauge Pressure readback.

   This readback displays the current pressure in the capillary-skimmer and foreline region.

5. Compare the current values of the pressures in the vacuum manifold with the values listed in Table 7.

   If the observed pressures are higher than those in the table, your system might have an air leak. If the pressure is high (above 5 x 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 decreases with time, check the pressure periodically until it falls within the typical pressure range of the MS detector. If the pressure remains high, your system might have an air leak.

Table 7. Typical pressure readings

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

❖ **To remedy an air leak**

1. Shut down the system as described in "Shutting Down the Mass Spectrometer Completely" on page 57.
2. Make a visual inspection of the vacuum system and vacuum lines for leaks.
3. 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.
4. Make sure that the cover plates of the vacuum manifold are properly seated.

Checking the Disk Space

Periodically verify that your hard disk drive has enough free space for data acquisition.

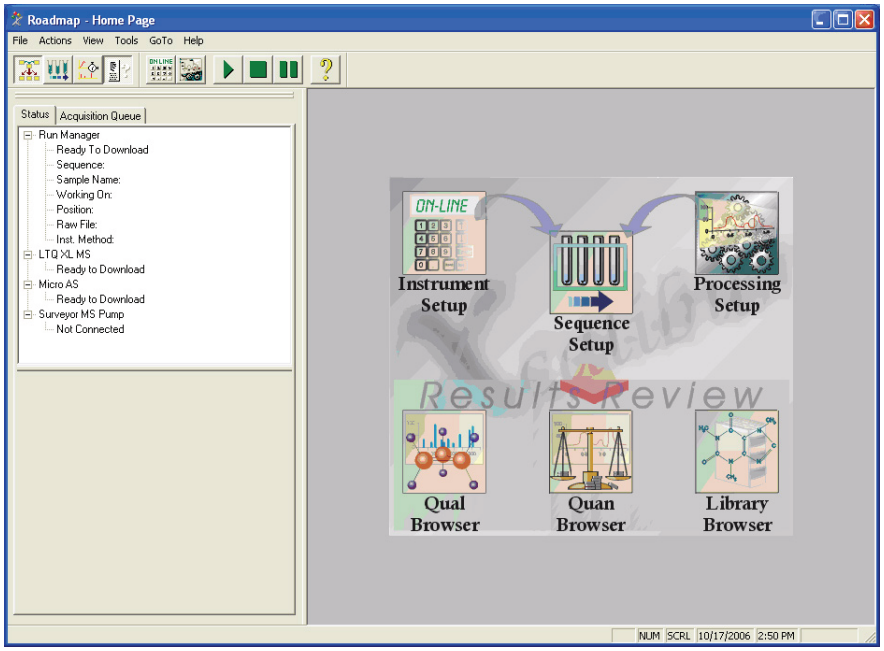
❖ **To determine the amount of available disk space**

1. On the Windows taskbar, choose **Start > All Programs > Thermo Xcalibur > Xcalibur**.

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

The Xcalibur Home Page opens (Figure 40).

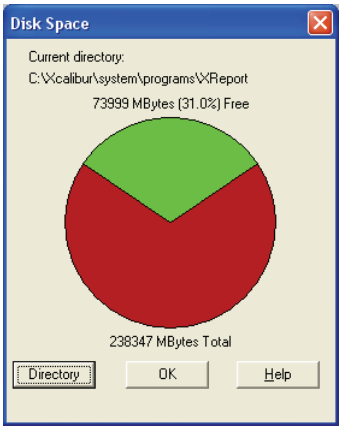
Figure 40. Xcalibur Home Page



2. Choose **Actions > Check Disk Space**.

The Disk Space dialog box opens (Figure 41 on page 75).

Figure 41. Disk Space dialog box



Review the following information:

- 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

3. To select another disk drive so that you can determine its disk space, click **Directory**.
4. When you have completed this procedure, click **OK**.

Tip 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 LTQ Series System

After operating the LTQ Series system, do the following procedures in sequence:

- "Flushing the Sample Transfer Line, Sample Tube, and API Probe," next section
- "Flushing the Ion Sweep Cone and Ion Transfer Capillary" on page 79
- "Purging the Oil in the Forepump" on page 81
- "Emptying the Solvent Waste Bottle" on page 82
- "Placing the System in Standby Mode" on page 82

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

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) with a mobile phase of 50:50 methanol/distilled water. Flushing the system with 50:50 methanol/distilled water at a flow rate of 200 to 400 µL/min for a period of approximately 15 minutes should be sufficient to remove contamination.

❖ **To flush the sample transfer line, sample tube, and API probe**

1. Wait until data acquisition, if any, is complete.
2. Make sure that the lid to the API chamber is closed and secured.
3. On the Windows taskbar, choose **Start > All Programs > Thermo Instruments > LTQ > *model* Tune**.

   Note For LTQ version 2.5.0 or earlier, the path is **Start > All Programs > Xcalibur > *model* Tune**.

   The Tune Plus window opens (Figure 33 on page 55).

On 
Standby 

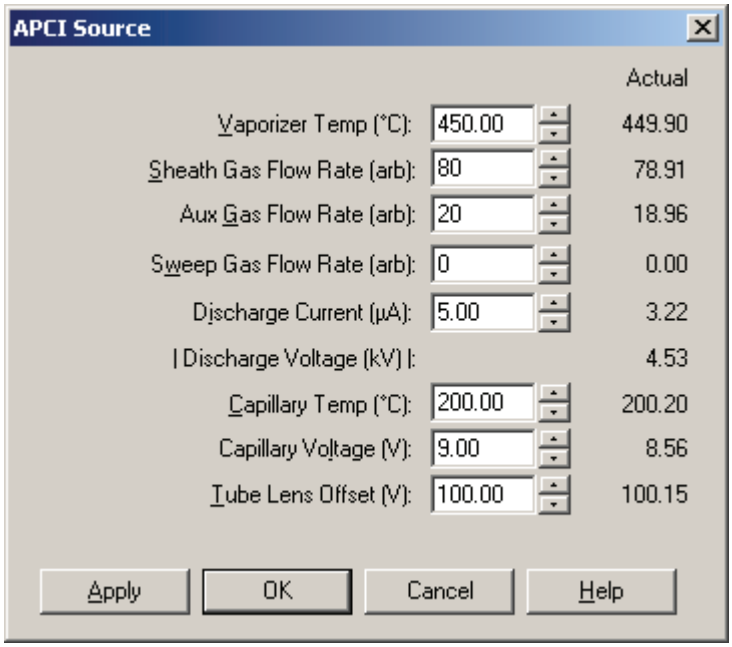
4. On the Control/Scan Mode toolbar, click **On/Standby** to turn on the voltages and gas flows to the API source.
   - If you are operating in APCI or APPI mode, go to step 5.
   - If you are operating in ESI mode, go to step 6.

5. To flush the APCI source:

   a. In the Tune Plus window, choose **Setup > APCI Source**.

      The APCI Source dialog box opens (Figure 42).

      Figure 42. APCI Source dialog box



   b. To set the APCI vaporizer temperature to 500 °C, type **500** in the Vaporizer Temperature box.

   c. To set the sheath gas flow rate to 30, type **30** in the Sheath Gas Flow Rate box.

   d. To set the auxiliary gas flow rate to 5, type **5** in the Aux Gas Flow Rate box.

   e. To set the sweep gas flow rate to 0, type **0** in the Sweep Gas Flow Rate box.

   f. To set the APCI spray current to 0, type **0** in the Spray Current box.

   g. Click **OK**.

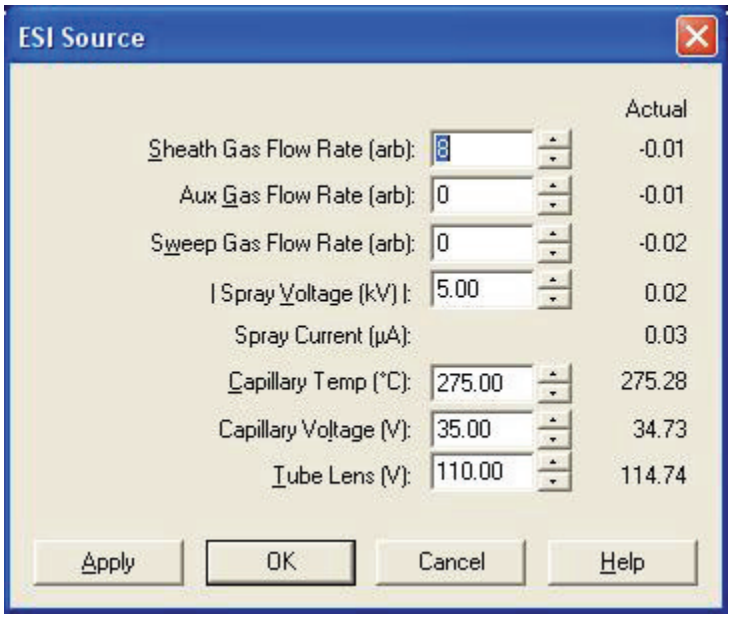
   h. Go to step 7.

6. To flush the ESI source:

   a. In the Tune Plus window, choose **Setup > ESI Source**.

      The ESI Source dialog box opens (Figure 43).

Figure 43. ESI Source dialog box



b. To set the sheath gas flow rate to 30, type **30** in the Sheath Gas Flow Rate box.

c. To set the auxiliary gas flow rate to 5, type **5** in the Aux Gas Flow Rate box.

d. To set the sweep gas flow rate to 0, type **0** in the Sweep Gas Flow Rate box.

e. To set the ESI spray voltage to 0, type **0** in the Spray Voltage box.

f. Click **OK**.

7. To set up and start a flow of 50:50 methanol/water solution from the LC system to the API source:

   a. Choose **Setup > Inlet Direct Control**.

      The Inlet Direct Control dialog box opens.

      The Xcalibur data system controls LC pumps from several manufacturers including Thermo Fisher Scientific Inc., Agilent Technologies, and Waters Corporation. Contact your Thermo Fisher Scientific sales representative for information on the liquid chromatography systems compatible with your LTQ Series mass spectrometer.

   b. Click the tab for the LC pump.

   c. Set the solvent proportions to 50% methanol and 50% water.

   d. Start the solvent flow.

8. Let the solution flow through the sample transfer line, sample tube, and API probe for 15 minutes.

9. After 15 minutes, turn off the flow of liquid from the LC to the API source as follows:
   a. Leave the API source (including the APCI vaporizer, sheath gas, and auxiliary gas) on for an additional 5 minutes.

   b. On the Control/Scan Mode toolbar, click the **Pump Off** or **Stop Pump** button to stop the LC pump.

On 

10. After 5 minutes, on the Control/Scan Mode toolbar, click the **On/Standby** button to put the mass spectrometer in Standby mode.

Standby 

Flushing the Ion Sweep Cone and Ion Transfer Capillary

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 pump a solution of 50:50 methanol/water solution through the sample transfer line, sample tube, and API probe (see "Flushing the Sample Transfer Line, Sample Tube, and API Probe" on page 76.) If you use a mobile phase that contains a nonvolatile buffer or inject 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. To turn off the solvent flow from the LC pump to the API source:
   a. On the Windows taskbar, choose **Start > All Programs > Thermo Instruments > LTQ > *model* Tune**.

   Note For LTQ version 2.5.0 or earlier, the path is **Start > All Programs > Xcalibur > *model* Tune**.

   The Tune Plus window opens (Figure 33 on page 55).
   b. Choose **Setup > Inlet Direct Control**.

   The Inlet Direct Control view opens.
   c. Click the **LC** tab.

   The LC page opens.

   d. Click the Pump **Off** or **Stop Pump** button to stop the LC pump.

On 

2. On the Control/Scan Mode toolbar, click the **On/Standby** button to turn the mass spectrometer off.

Standby 

CAUTION Avoid burns. At operating temperatures, the APCI vaporizer can severely burn you. The APCI vaporizer typically operates at 400 to 600 °C. Allow approximately 20 minutes for the vaporizer to cool to room temperature before you touch or remove either component.

3. Remove the Ion Max ion source from the front of the mass spectrometer, as described in "Removing the Ion Max or Ion Max-S API Source Housing" on page 65.
4. Use the spray bottle filled with the 50:50 solution of methanol/water and Kimwipes™ to clean contaminants from the accessible surfaces of the ion source chamber.
5. To remove the ion sweep cone (if it is installed):

CAUTION To prevent contaminating the ion optical elements, never clean the sweep cone or ion transfer capillary with solvent when they are attached to the system.

   a. Put on a new pair of lint- and powder-free gloves.
   b. Grasp the outer ridges of the ion sweep cone and pull the cone straight off of the API cone seal. You might need to loosen the set screws on the ion sweep cone in order to remove it.

Tip At this point, remove and clean the ion transfer capillary. See "Removing, Cleaning, and Reinstalling the Ion Transfer Capillary" on page 117.

6. To clean the ion transfer capillary and the ion sweep cone (if it is installed):
   a. Place the ion sweep cone and the ion transfer capillary in a beaker of 50:50 methanol/water.
   b. Place the beaker in an ultrasonic bath, and sonicate these components for 15 minutes.
   c. Dry the ion sweep cone.
7. To reinstall the ion sweep cone:
   a. Carefully align the gas inlet (Figure 45 on page 81) on the ion sweep cone with the sweep gas supply port (Figure 44 on page 81) in the API cone seal. Firmly press the ion sweep cone into position.
   b. If necessary, adjust the set screws around the perimeter of the ion sweep cone.

Figure 44. Sweep gas supply port in the API cone seal

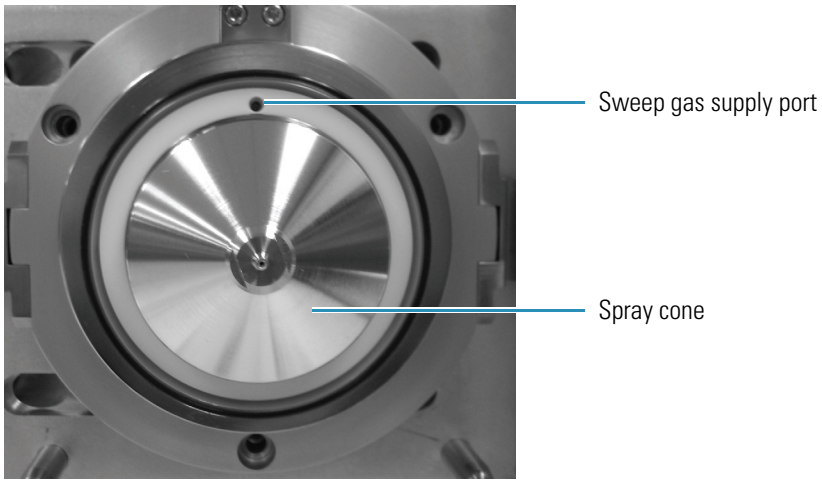
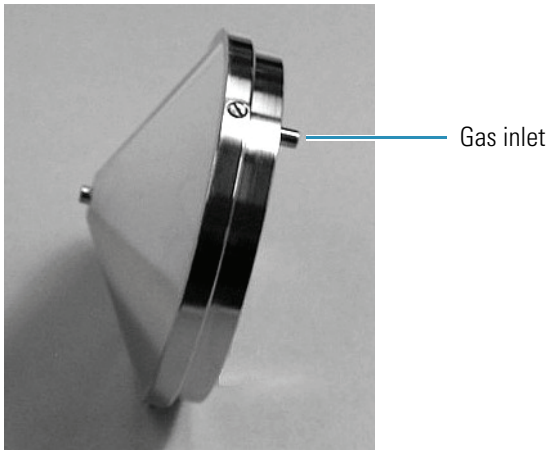


Figure 45. Gas inlet on the ion sweep cone



8. Reinstall the Ion Max ion source as described in "Installing the Ion Max or Ion Max-S API Source Housing" on page 66.

Purging the Oil in the Forepump

Plan to purge (decontaminate) the oil in the forepump (also known as a rotary vane pump, backing pump, roughing pump, or mechanical pump) on a daily basis to remove water and other dissolved chemicals from the pump oil. Water and other chemicals in the forepump can cause corrosion and decrease the lifetime of the forepump. The best 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.

Refer to the manufacturer's documentation for the necessary procedures.

Emptying the Solvent Waste Bottle

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

Placing the System in Standby Mode

After you complete the daily maintenance procedures, put the mass spectrometer in Standby mode as described in "Placing the Mass Spectrometer in Standby Mode" on page 55.

Maintenance

The performance of your LTQ Series mass spectrometer depends on the maintenance of all parts of the instrument. You are responsible for maintaining your system properly by performing the system maintenance procedures on a regular basis.

Contents

For optimal results when you perform the procedures in this chapter:

- Proceed methodically.
- Always wear a new pair of lint- and powder-free gloves when you handle 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.

Table 8 on page 84 lists the maintenance procedures and how frequently they should be performed.

Table 8. LTQ Series mass spectrometer maintenance procedures and frequency

MS detector component	Procedure	Frequency	Refer to
ESI probe	Trim sample tube	If polyimide coating on the end of the sample tube has become elongated	"Trimming the ESI Sample Tube" on page 87
API source	Flush (clean) sample transfer line, sample tube, and API probe	Daily	"Flushing the Sample Transfer Line and Sample Tube" on page 100
Ion source interface	Flush (clean) ion sweep cone and ion transfer capillary	Daily, or more often depending on analytical conditions	"Ion Source Interface Maintenance" on page 111
	Remove and clean ion transfer capillary	Weekly, or if ion transfer capillary bore is contaminated or obstructed	
	Replace ion transfer capillary	If ion transfer capillary bore is corroded	
	Clean tube lens and skimmer	As needed, depending on analytical conditions	
	Clean S-lens or exit lens	As needed, depending on analytical conditions	
Rotary vane pump	Purge (decontaminate) oil	Daily	Manufacturer's documentation
	Change oil	Every 3 months or if oil is cloudy or discolored	
	Add oil	As needed, depending on analytical conditions	
Cooling fans	Clean fan filters	Every 4 months	"Fan Filter Maintenance" on page 150
Q00 rf lens	Clean Q00 quadrupole and lens L0	As needed, depending on analytical conditions	"Cleaning the Q00 RF Lens Assembly Components" on page 125
APCI or ESI probe	Replace sample tube	If sample tube is broken or obstructed	"Installing a Fused-Silica Sample Tube and PEEK Safety Sleeve" on page 92

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

Tools and Supplies

The LTQ Series mass spectrometer requires very few tools to perform routine maintenance procedures. You can remove and disassemble many of the components by hand. Table 9 lists the tools, equipment, and chemicals needed for the maintenance of the API source, ion guides, mass analyzer, and ion detection system.

Table 9. Tools, equipment, and chemicals

Description	Part number
Screwdrivers, set, ball point, Allen (also referred to as ball drivers)	00025-03025
3/16 in. hex ball driver	00025-01700
7/64 in. hex ball driver	00025-01800
5/16 in., 9.5 in. long hex ball driver	00025-10015
5/32 in., 7.4 in. long hex ball driver	00025-10020
Ion transfer capillary removal tool	70111-20258
Screwdriver, slot head, large	
Screwdriver, slot head, small	
Screwdriver, Phillips, small	
5/16 in. open-end wrench	
3/8 in. open-end wrench	
1/2 in. open-end wrench	
Fused-silica cutting tool	
Beaker, 450 mL	
Gloves, lint- and powder-free	
Kimwipes or other lint-free industrial tissues	
Applicators (swabs), cotton-tipped	00301-02000
Detergent	
Clean, dry, compressed nitrogen gas	
Distilled water, LCMS grade	Fisher Chemical P/N W6-1
Methanol, LCMS grade	Fisher Chemical P/N A456-1
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 local and federal regulations.

Ion Source Probe Maintenance

This section contains information for maintaining the ion source probes:

- "ESI Probe Maintenance," next section
- "HESI-II Probe Maintenance" on page 99
- "APCI Probe Maintenance" on page 104

ESI Probe Maintenance

The ESI probe requires a minimum of maintenance. If the fused-silica sample tube is plugged or broken, replace it. You can trim or replace the sample tube without disassembling the ESI probe. However, to clean the nozzle bore or the interior surfaces of the manifold or to replace the electrospray needle or needle seal, you must disassemble the ESI probe.

To minimize cleaning of the probe components, flush the ESI probe at the end of each working day by pumping a 50:50 HPLC-grade methanol/distilled water solution through the ESI probe.

IMPORTANT Wear a new pair of lint- and powder-free gloves when you handle ESI probe components.

To maintain the ESI probe, follow these procedures:

- "Trimming the ESI Sample Tube," next section
- "Disassembling the ESI Probe" on page 88
- "Cleaning or Replacing the ESI Probe Components" on page 89
- "Assembling the ESI Probe" on page 91
- "Installing a Fused-Silica Sample Tube and PEEK Safety Sleeve" on page 92
- "Installing an Optional Metal Needle Sample Tube" on page 99

Trimming the ESI Sample Tube

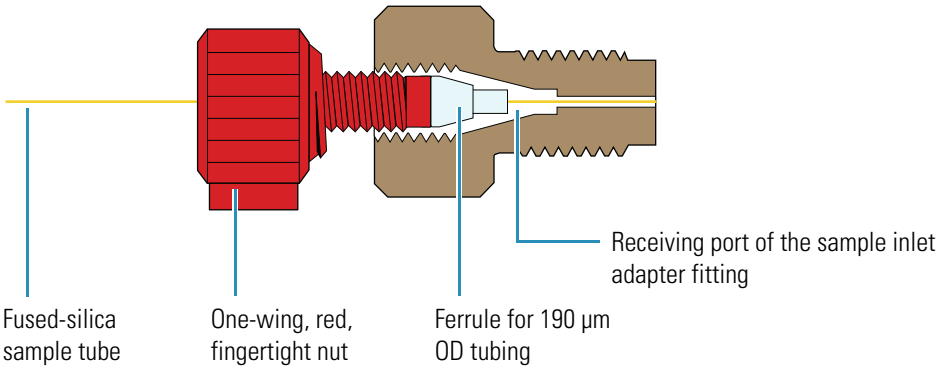
Operating the MS detector with acetonitrile in the mobile phase can cause elongation of the polyimide coating on the fused-silica sample tube. If the polyimide coating has elongated past the end of the electrospray needle, cut and reposition the end of the fused-silica sample tube.

❖ To cut and reposition the end of the fused-silica sample tube

1. Remove the ESI probe from the Ion Max or Ion Max-S source housing (see "ESI Probe Installation and Removal" in Chapter 2 of the *LTQ Series Getting Started Guide*).
2. Loosen the two-piece fingertight fitting that secures the position of the fused-silica sample tube and the PEEK safety sleeve at the ESI probe sample inlet (Figure 46).

> **Note** When the nut and ferrule assembly are properly seated in the receiving port, the receiving port compresses the ferrule so that it fits snugly to the tubing. When you loosen the fitting, the receiving port no longer compresses the ferrule and the tubing is free to move.

Figure 46. Two-piece fingertight fitting and loosened sample inlet adapter fitting



3. Gently pull back on the sample tube to free it from the ferrule.
4. Push the sample tube forward so that it extends beyond the end of the electrospray needle.
5. Using a fused-silica cutting tool, 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 flush with the ESI needle.

   The optimal sample tube protrusion depends on the solvent flow rate:

   - For flow rates below or equal to 100 µL/min, set the sample tube protrusion to 1 mm.
   - For flow rates above 100 µL/min, ensure that the sample tube is flush with the ESI needle or recessed inside the ESI needle by less than 1 mm.

7. Tighten the two-piece fingertight fitting securely to hold the sample tube in place.
8. Because the sample tube can move forward as you tighten the two-piece fingertight fitting, ensure that the sample tube is still set to the appropriate protrusion. If necessary, loosen the fitting and reposition the sample tube.
9. Reinstall the ESI probe in the API source housing (refer to "ESI Probe Installation and Removal" in the *LTQ Series Getting Started Guide*).

Disassembling the ESI Probe

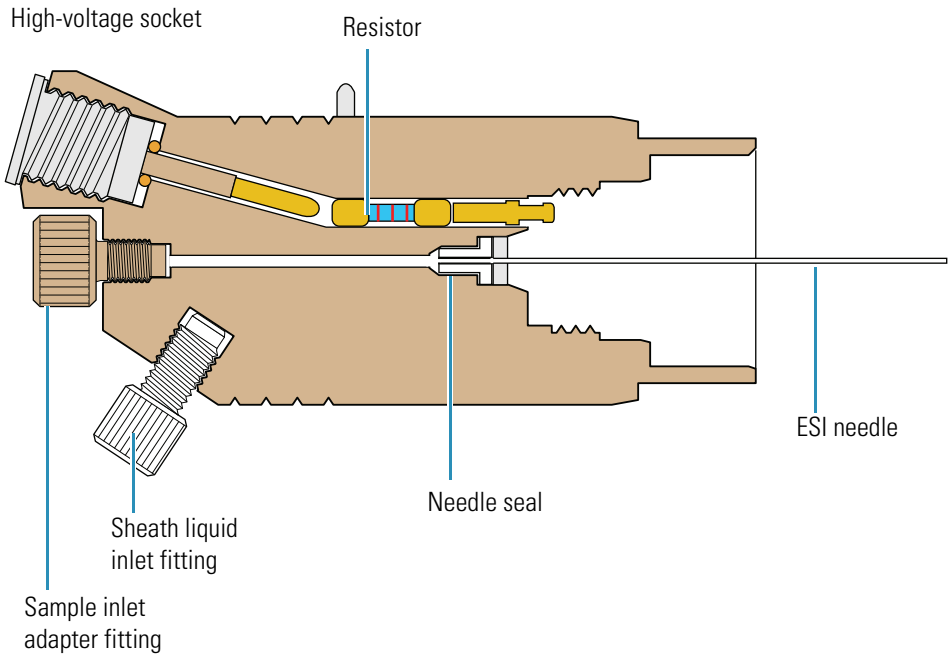
To replace or clean the ESI probe components, disassemble the ESI probe. Disassembling the ESI probe requires these tools:

- 5/16 in. open-end wrench
- 1/2 in. open-end wrench

❖ To disassemble the ESI probe

1. If you have not already done so, remove the ESI probe from the API source housing (refer to "ESI Probe Installation and Removal" in the *LTQ Series Getting Started Guide*).
2. Unscrew the two-piece fingertight fitting from the sample inlet adapter fitting and remove the sample tube from the ESI probe.
3. Because the ESI manifold contains loose components (resistor and battery), hold the ESI probe with the nozzle facing upward. With a 5/16 in. open-end wrench, loosen and remove the ESI nozzle from the ESI manifold.
4. If the nozzle requires cleaning, see "Cleaning the ESI Nozzle" on page 90.
5. Pull the ESI needle out of the ESI manifold (Figure 47 on page 89).

Figure 47. ESI probe with the nozzle removed (cross section)



6. To dislodge the needle seal, gently tap the ESI manifold against a hard surface. If necessary, use the needle or another appropriate tool to push the needle seal out of the ESI manifold.

   Tapping the manifold against a hard surface also dislodges the resistor and battery contact.

7. Using a 1/2 in. open-end wrench, disconnect the high-voltage socket from the back of the ESI probe.

8. Unscrew the fitting from the sheath liquid inlet.

9. If the ESI manifold needs cleaning, see "Cleaning the ESI Manifold" on page 91.

10. To reassemble the ESI probe, see "Assembling the ESI Probe" on page 91.

Cleaning or Replacing the ESI Probe Components

Maintaining the ESI probe requires occasional replacement of the 26-gauge needle, the needle seal, the ESI nozzle, and the high-voltage socket O-rings. In addition, the ESI nozzle and manifold occasionally require cleaning.

To clean or replace the ESI probe components, follow these procedures:

- "Cleaning the ESI Nozzle," next section
- "Replacing the Needle, Needle Seal, or Both" on page 90
- "Cleaning the ESI Manifold" on page 91

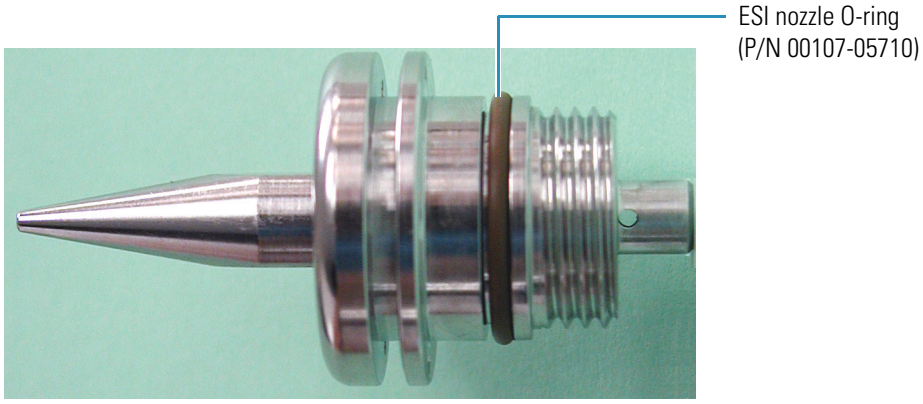
Cleaning the ESI Nozzle

❖ To clean the ESI nozzle

1. Remove the ESI probe from the API source housing (refer to "ESI Probe Installation and Removal" in the *LTQ Series Getting Started Guide*).
2. Disconnect the ESI nozzle from the ESI manifold (see "Disassembling the ESI Probe" on page 88, steps 2 and 3).
3. Clean the bore of the ESI nozzle with an appropriate solvent.

   The choice of solvent depends on the solubility of the chemical deposits.
4. Rinse the nozzle with methanol and dry with nitrogen gas.
5. Inspect the ESI nozzle O-ring and replace it if necessary (Figure 48).

   Figure 48. ESI nozzle and O-ring



6. Reconnect the ESI nozzle to the ESI manifold (see "Assembling the ESI Probe" on page 91, steps 4 through 6).

Replacing the Needle, Needle Seal, or Both

If the needle is damaged, replace it. If the sheath gas is leaking at the interface between the needle seal and the needle, replace the needle seal.

❖ To replace the needle, needle seal, or both

1. Remove the ESI probe from the API source housing (refer to "ESI Probe Installation and Removal" in the *LTQ Series Getting Started Guide*).
2. Disconnect the ESI nozzle from the ESI manifold (go to "Disassembling the ESI Probe" on page 88, steps 2 and 3).
3. Pull the ESI needle out of the ESI manifold.

4. To dislodge the needle seal, gently tap the ESI manifold against a hard surface. If necessary, use the needle or another appropriate tool to push the needle seal out of the ESI manifold.

   Tapping the manifold against a hard surface also dislodges the resistor and contact battery.

5. If necessary, replace the needle seal (P/N 00950-00952), the 26-gauge spray needle (P/N 00950-00990), or both.

6. Reassemble the ESI probe (see "Assembling the ESI Probe" on page 91, steps 1through 6).

Cleaning the ESI Manifold

❖ To clean and dry the ESI manifold

1. If you have not already done so, remove the ESI probe from the API source housing (refer to "ESI Probe Installation and Removal" in Chapter 2 of the *LTQ Series Getting Started Guide*).

2. Disassemble the ESI probe (see "Disassembling the ESI Probe" on page 88).

3. Rinse the ESI manifold with distilled water and then with LCMS-grade methanol. Remove excess methanol from the ESI manifold with a lint-free tissue.

4. Dry the ESI manifold with nitrogen gas.

5. Inspect the following parts.

Description	Part number
ESI nozzle O-ring	00107-05710
High-voltage socket O-ring	00107-02550
Needle seal	00950-00952
ESI 26-gauge spray needle	00950-00990

6. Replace damaged parts.

7. Reassemble the ESI probe.

Assembling the ESI Probe

❖ To assemble the ESI probe

1. Insert the resistor and contact battery into the ESI manifold.

2. Insert the entrance end of the ESI needle into the needle seal.

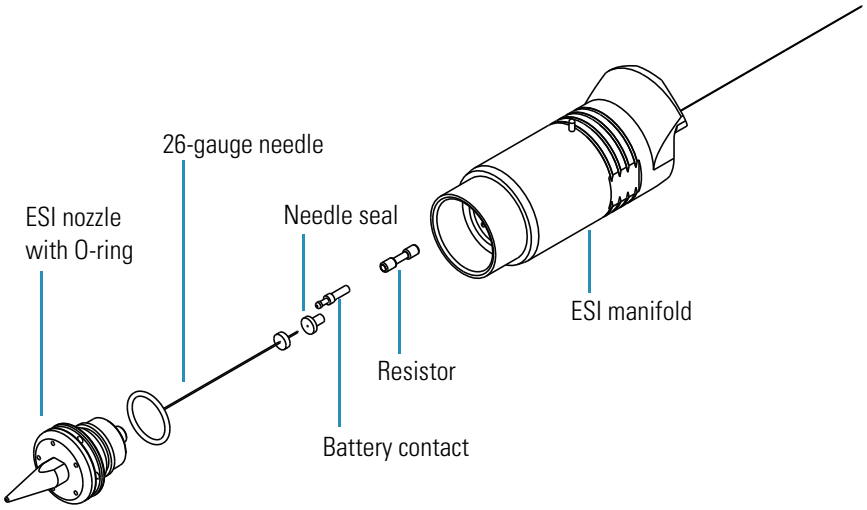
3. Seat the ESI needle and needle seal in the ESI manifold.

4. Ensure that the 0.676 in. ID O-ring is placed into the precut groove on the ESI nozzle (Figure 48 on page 90).

5. Thread the ESI nozzle over the needle and into the ESI manifold. Slightly wet the nozzle threads with LCMS-grade methanol for lubrication.
6. With a 5/16 in. open-end wrench, gently tighten the ESI nozzle until it is a little more than fingertight. Do not overtighten the nozzle.

   Figure 49 shows an exploded view of the front end of the ESI probe.

   Figure 49. Front end of the ESI probe (exploded view)



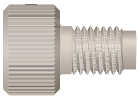
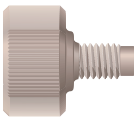
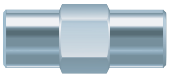
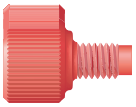
7. Insert the high-voltage socket into the back of the ESI manifold. Using a 1/2 in. wrench, tighten the socket.
8. Reconnect the sheath liquid fitting.
9. Install a new sample tube (see "Installing a Fused-Silica Sample Tube and PEEK Safety Sleeve," next).

Installing a Fused-Silica Sample Tube and PEEK Safety Sleeve

When you use a fused-silica sample tube with the ESI probe, cover the exposed portion of the sample tube with a PEEK safety sleeve.

CAUTION AVOID ELECTRICAL SHOCK. Cover the fused-silica capillary tube with the PEEK safety sleeve and associated PEEK ferrules provided in the Safety Sleeve Kit (P/N 70005-62015) before you operate the mass spectrometer. The PEEK tubing acts as a second level of protection against accidental electrical discharge.

Installing a fused-silica sample tube with the PEEK safety sleeve requires the following parts.

	Description	Part number
	Tubing, fused-silica, 0.1 mm ID × 0.190 mm OD	00106-10499
	Tubing, red PEEK, 0.005 in. ID × 1/16 in. OD	00301-22912
	PEEK safety sleeve, precut 25 cm (10 in.) length of natural PEEK tubing 0.23 mm ID × 0.61 mm OD (0.009 in. ID × 0.0240 in. OD)	00301-22806
	Fitting, adapter, 10-32 to 1/4-28, natural PEEK, 0.040 in. (1.0 mm) thru-hole (for the ESI probe sample inlet) (Upchurch P-669)	00101-18080
	Fitting, fingertight, natural PEEK, two wings, for 1/16 in. OD high-pressure tubing (Upchurch F-300)	00101-18081
	Ferrule, 0.027 in. ID, natural PEEK (for use with the 0.024 in. OD PEEK safety sleeve)	00101-18119
	Fitting, grounding union, stainless steel, 0.010 in. thru-hole (Upchurch U-435)	00101-18182
	Fitting, fingertight, for 1/16 in. OD high pressure tubing (Upchurch F-200)	00101-18195

To install a fused-silica sample tube, thread the 0.19 mm OD fused-silica sample tube through the ESI needle that protrudes from the ESI probe nozzle and the 0.23 mm ID safety sleeve. Because you must thread the fused-silica tubing through these small orifices, you might find a microscope useful.

❖ To install the new sample tube and PEEK safety sleeve

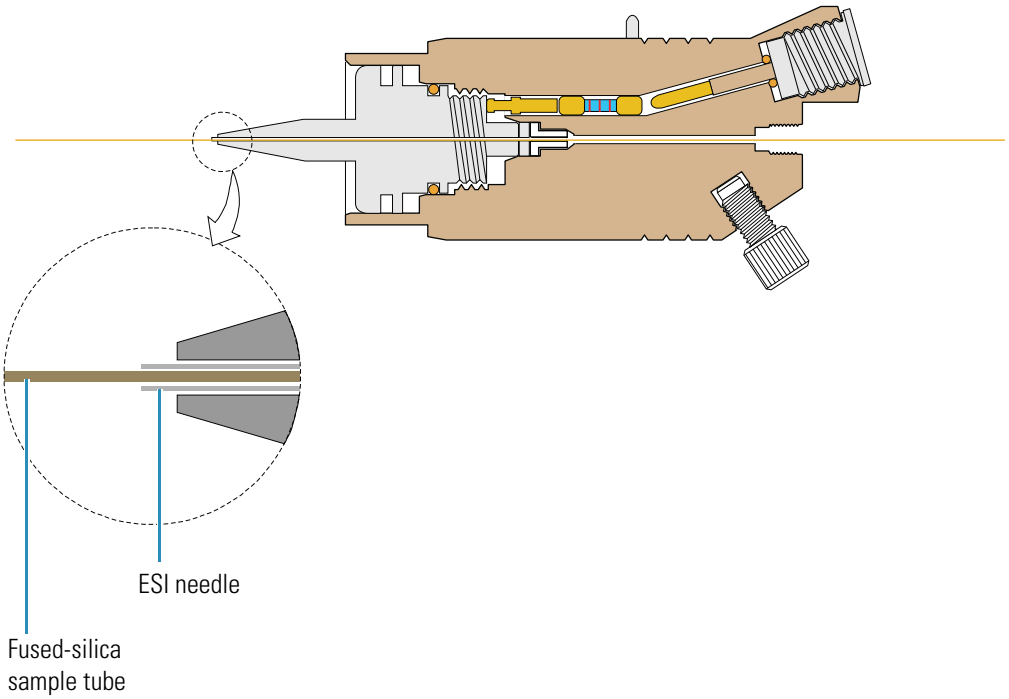
1. Using a fused-silica cutting tool to ensure square cuts, cut a length of fused-silica tubing approximately 38 cm (15 in.) long.

   The piece of fused-silica tubing must be long enough to extend through the ESI probe and the natural PEEK safety sleeve.

2. Remove the sample inlet adapter from the ESI probe sample inlet.

3. Insert the fused-silica sample tube through the ESI needle that protrudes from the ESI nozzle, and then push the sample tube through the ESI probe until approximately 3.5 cm (1.5 in.) of the sample tube protrudes from the front of the probe. The remaining length of sample tube protrudes from the ESI probe sample inlet at the back of the probe (Figure 50 on page 94).

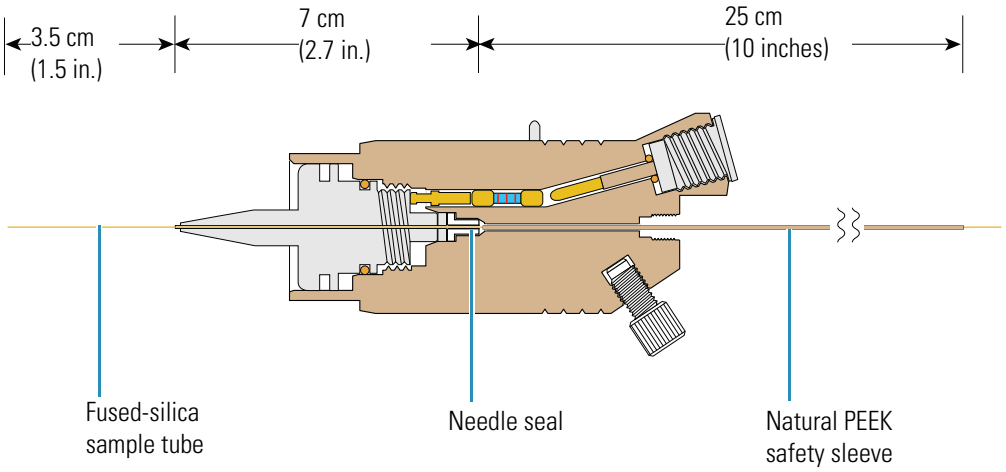
Figure 50. Fused-silica sample tube inserted through the front of the ESI probe



4. Slide the safety sleeve over the end of the fused-silica sample tube that protrudes from the probe sample inlet, and then push the safety sleeve into the probe until it meets resistance (Figure 51).

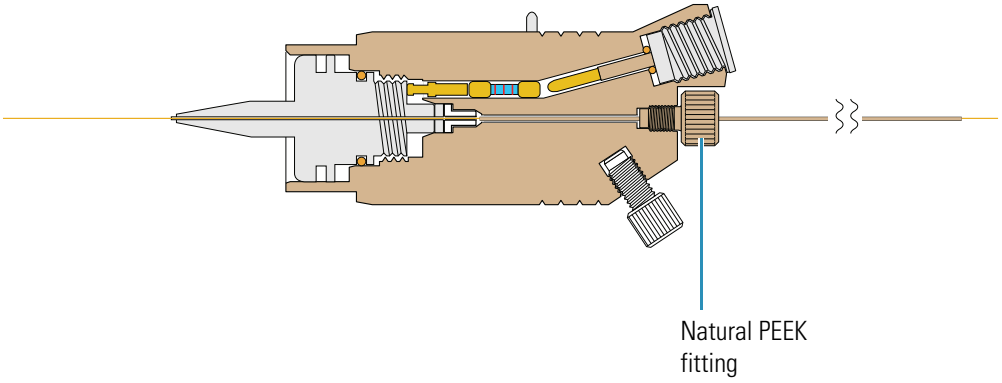
   The safety sleeve is a a precut length of natural PEEK tubing that acts as a second level of protection against accidental electrical discharge.

   Figure 51. Natural PEEK adapter installed in the sample inlet



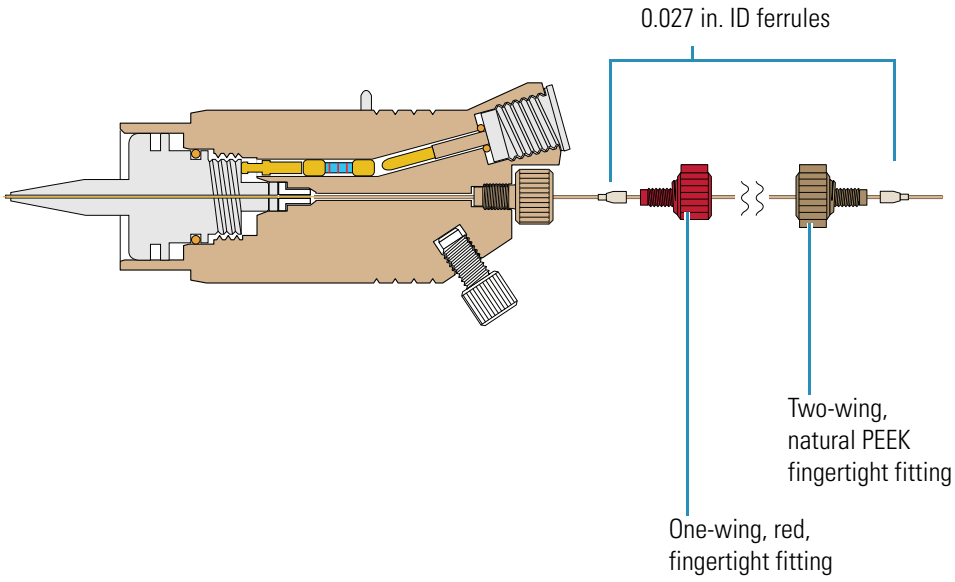
5. With the external threads facing the ESI probe sample inlet, slide the 10-32 ×1/4-28 natural PEEK fitting adapter over the safety sleeve, and then finger tighten the fitting into the ESI probe sample inlet (Figure 52 on page 95).

Figure 52. Natural PEEK fitting installed to secure the safety sleeve



6. Slide the other fingertight fittings onto the PEEK sleeve (Figure 53) as follows:
   a. Slide the 0.027 in. ID PEEK ferrule with the tapered end facing the sample inlet onto the PEEK safety sleeve.
   b. Slide the red, one-wing fingertight fitting with the threaded end facing the sample inlet onto the PEEK safety sleeve.
   c. Slide the natural PEEK, two-wing fingertight fitting with the threaded end facing away from the sample inlet onto the PEEK safety sleeve.
   d. Slide the 0.027 in. ID PEEK ferrule with the tapered end facing away from the sample inlet onto the PEEK safety sleeve.

Figure 53. Fingertight fittings installed over the safety sleeve



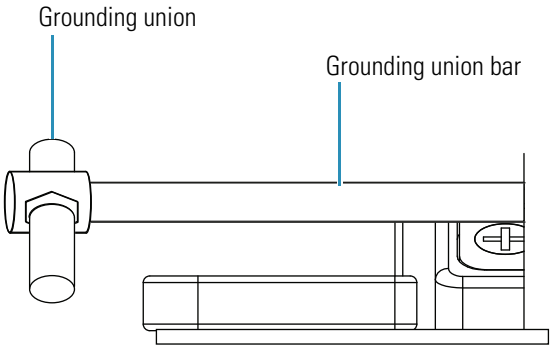
7. Connect the safety sleeve and fused-silica assembly to the grounding union as follows:

a. Adjust the position of the fused-silica sample tube so that it is flush with the end of the safety sleeve that protrudes from the back of the probe.

b. To provide leverage when you tighten the fitting to the union, seat the grounding union in the grounding union bar of the ion source housing (Figure 54).

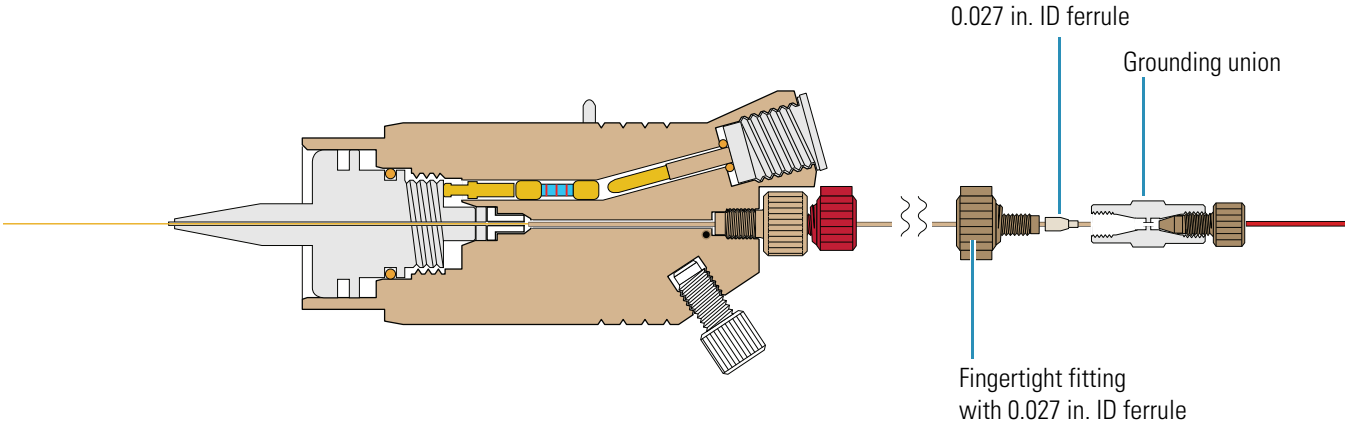
c. To prevent the 0.190 mm OD fused-silica sample tube from slipping through the 0.010 inch (0.25 mm) grounding union thru-hole and out the other end of the grounding union, connect a fingertight fitting and red PEEK tubing to the other end of the grounding union (Figure 54).

Figure 54. Grounding union seated in grounding bar



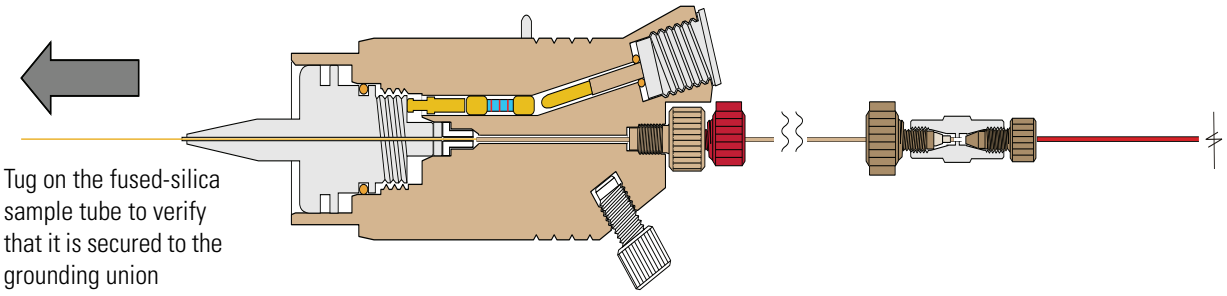
d. While holding the safety sleeve and fused-silica sample tube firmly against the grounding union receiving port, use your fingers to tighten the fitting as tight as you can (Figure 55, and Figure 56 on page 97).

Figure 55. Safety sleeve connection to the grounding union



e. Ensure that the fused-silica sample tube is held tightly in the grounded union by gently pulling the sample tube from the exit end of the ESI needle (Figure 56 on page 97).

Figure 56. Fused-silica sample tube securely tightened to the grounding union



8. Adjust the position of the fused-silica sample tube as follows:

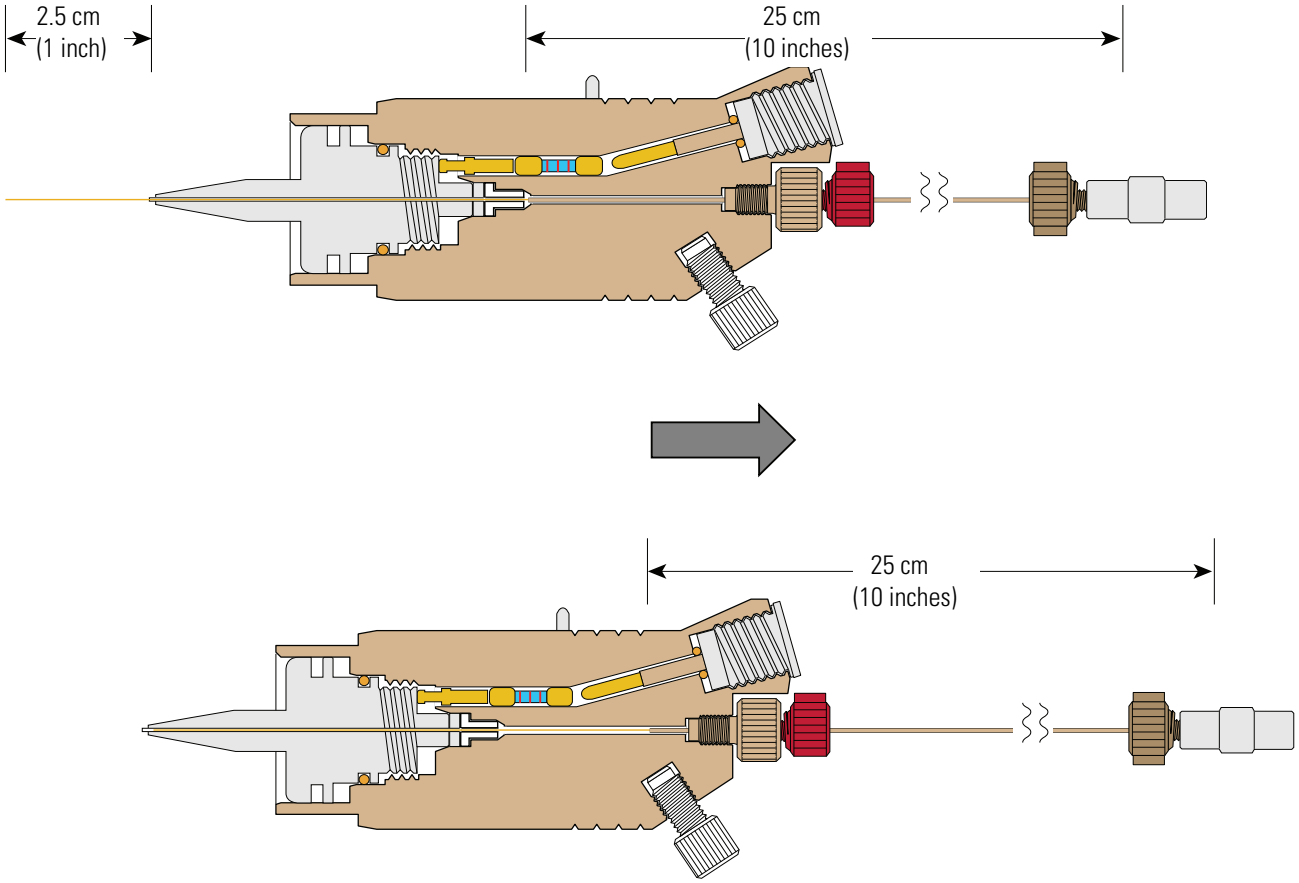
   a. Using a fused-silica cutting tool, cut the fused-silica sample tube so that 2.5 cm (1 in.) of the sample tube protrudes from the ESI needle.

   b. From the ESI sample inlet, loosen the red PEEK fitting, and then pull the PEEK safety sleeve backward so that the fused-silica sample tube is positioned appropriately within the ESI needle (Figure 57 on page 98).

      The optimal position of the sample tube depends on the solvent flow rate:

      - For flow rates below or equal to 100 µL/min, set the sample tube protrusion to 1 mm from the ESI needle tip.
      - For flow rates above 100 µL/min, ensure that the sample tube is flush with the ESI needle tip or recessed inside the ESI needle by no more than 1 mm (Figure 58 on page 99).

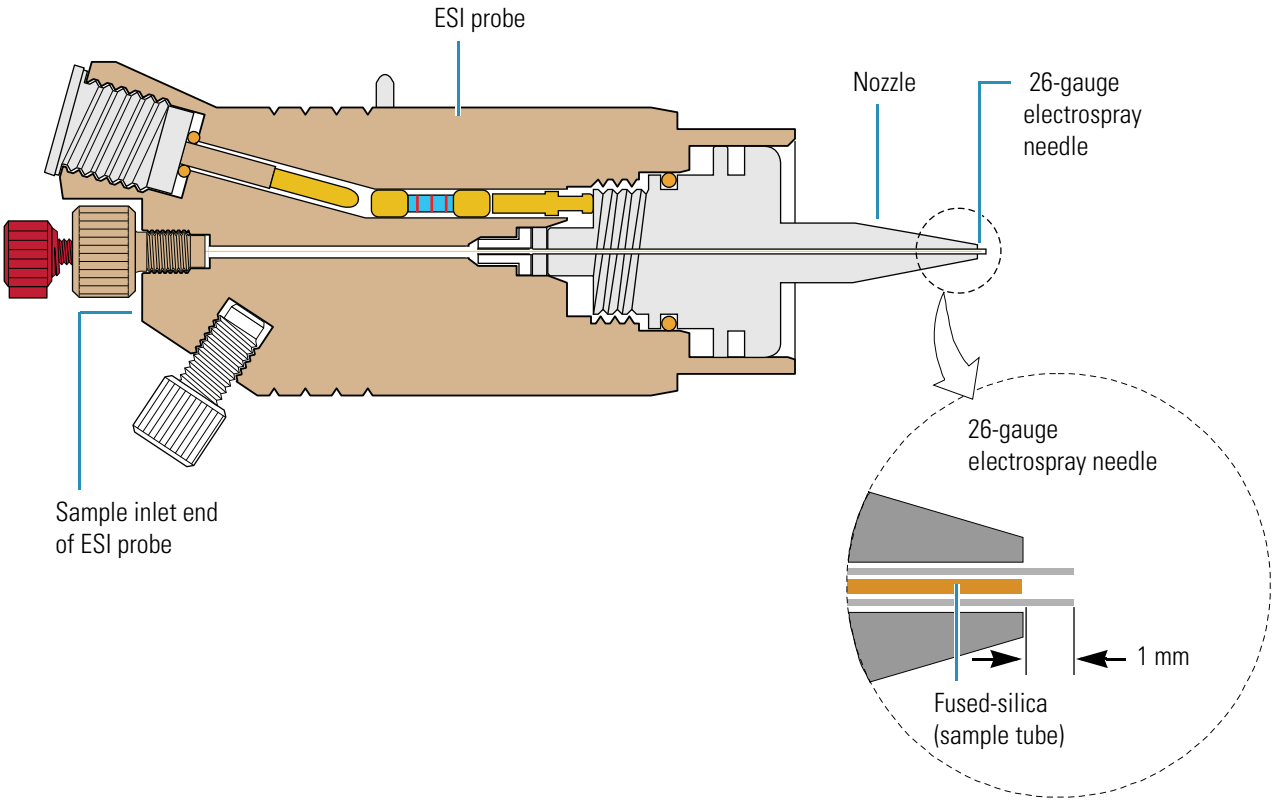
Figure 57. Position adjustment for the fused-silica sample tube



c. Tighten the fingertight fitting securely to hold the PEEK safety sleeve and sample tube in place.

d. Because the sample tube can move forward when you tighten the sample inlet fitting, ensure that the sample tube is recessed within the ESI needle. If necessary, loosen the red PEEK fitting and reposition the sample tube.

Figure 58. Position of the ESI fused-silica sample tube for flow rates above 100 µL/min



Installing an Optional Metal Needle Sample Tube

You can configure the ESI probe to use a stainless steel metal needle rather than a fused-silica sample tube. Two kits are available, one that includes a 32-gauge metal needle (OPTON-53003) for typical flow rates used in ESI and another with a 34-gauge metal needle (OPTON-30004) used for low-flow applications. Both kits include instructions for installing the stainless steel needle sample tube.

HESI-II Probe Maintenance

The HESI-II probe requires minimum maintenance. If the metal needle sample tube is plugged, replace it. Replacing the metal needle requires a partial disassembly of the probe.

This section contains the following maintenance procedures:

- "Flushing the Sample Transfer Line and Sample Tube," next section
- "Replacing the Needle Insert" on page 100

IMPORTANT For best results, avoid operating the HESI-II probe at elevated temperatures without solvent flow. Allowing the HESI-II probe to run dry at elevated temperatures can cause blockage of the replaceable metal needle.

IMPORTANT Wear a new pair of lint- and powder-free gloves when you handle HESI-II probe components.

CAUTION Avoid Burns. At operating temperatures, the vaporizer can severely burn you. The vaporizer typically operates between 350 and 450 °C. Allow approximately 20 minutes for the HESI-II probe to cool to room temperature before you touch or remove it.

Flushing the Sample Transfer Line and Sample Tube

For best results, flush the sample transfer line, sample tube, and HESI-II probe for 15 minutes at the end of each working day (or more often if you suspect they are contaminated). Use a 50:50 methanol/distilled water solution from the LC system through the API source. After 15 minutes, turn off the flow of liquid from the LC to the API source, but keep the API source on (including the sheath gas and auxiliary gas) for an additional 5 minutes. Refer to the daily operations chapter in the hardware manual for your mass spectrometer.

Replacing the Needle Insert

If the metal needle is plugged, you can replace the needle insert. The needle insert is assembled at the factory and consists of an adjustable union, a needle guide fitting, a ferrule, an O-ring, an ESI needle, and a metal needle (Figure 59). The ferrule is swaged onto the ESI needle. Factory adjusted, the metal needle protrudes 0.5 mm from the end of the ESI needle (Figure 60 on page 101).

Figure 59. Needle insert components

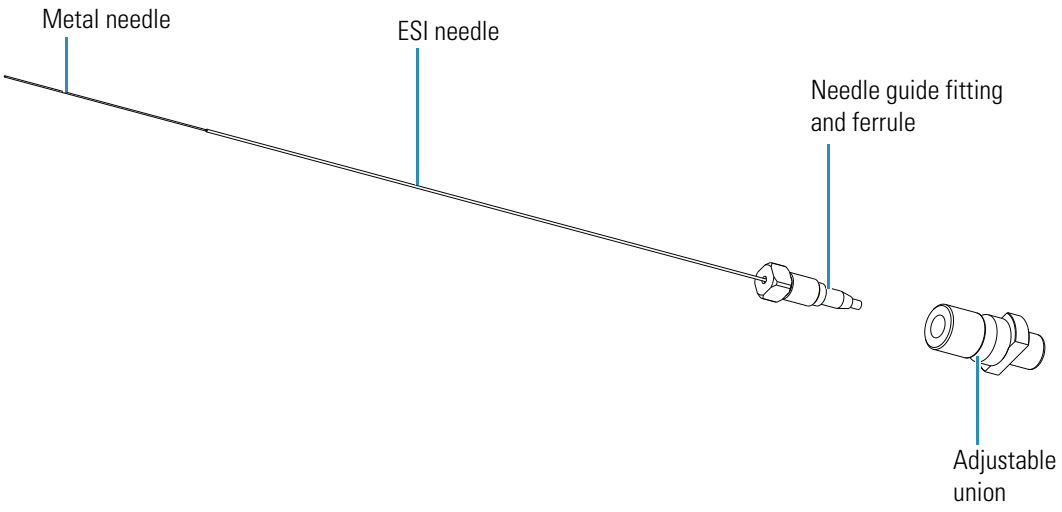
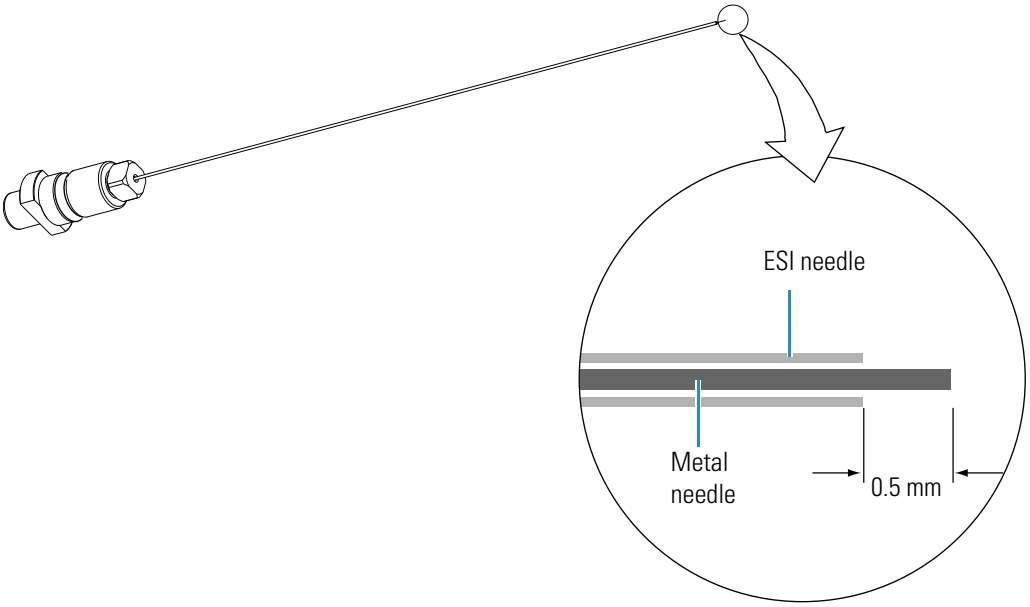


Figure 60. Metal needle insert assembly with an enlarged view of the stainless steel needle tip



To support flow rates from 5 to 2000 µL/minute, Thermo Fisher Scientific provides two metal needle inserts for the HESI-II probe. The difference between the two inserts is the size of the metal needle and supporting ferrule (Table 10).

Table 10. Metal needle inserts

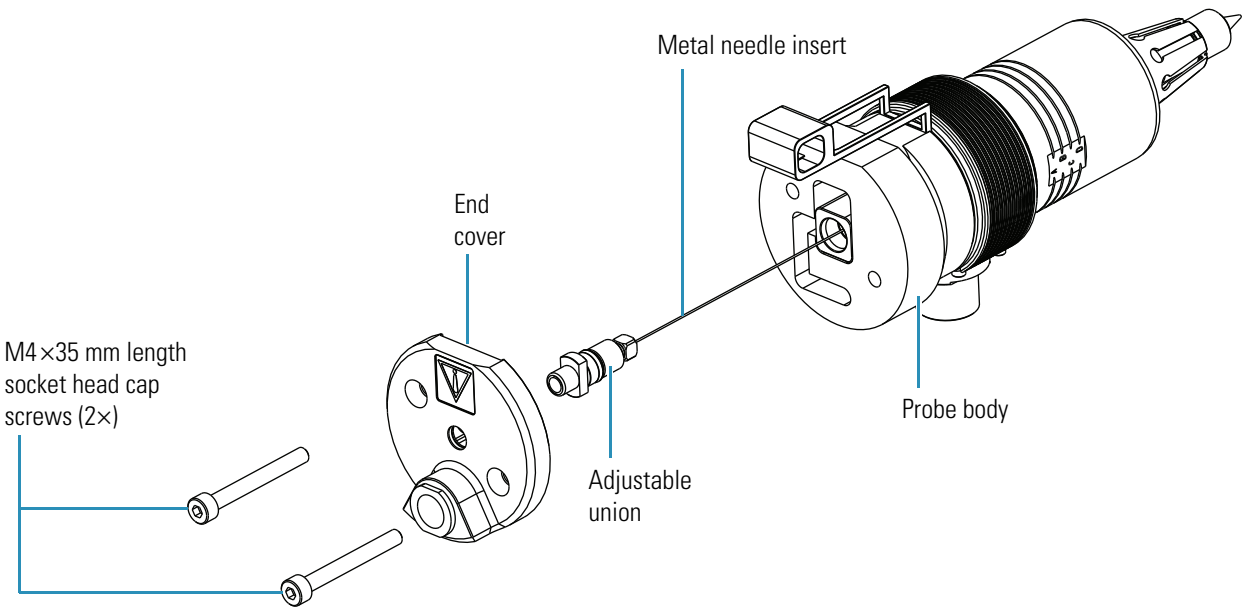
Description	Metal needle	Ferrule	Flow rate range	Part number
32-gauge needle insert, HESI-II probe	0.004 in. ID 0.009 in. OD	0.4 mm thru-hole	5 to 2000 µL/min	70005-60155
34-gauge needle insert, HESI-II probe	0.003 in. ID 0.007 in. OD	0.2 mm thru-hole	1 to 10 µL/min	70005-60180

To replace the metal needle insert, you must have a 3 mm (7/64 in.) hex wrench or ball driver.

❖ To replace the metal needle insert

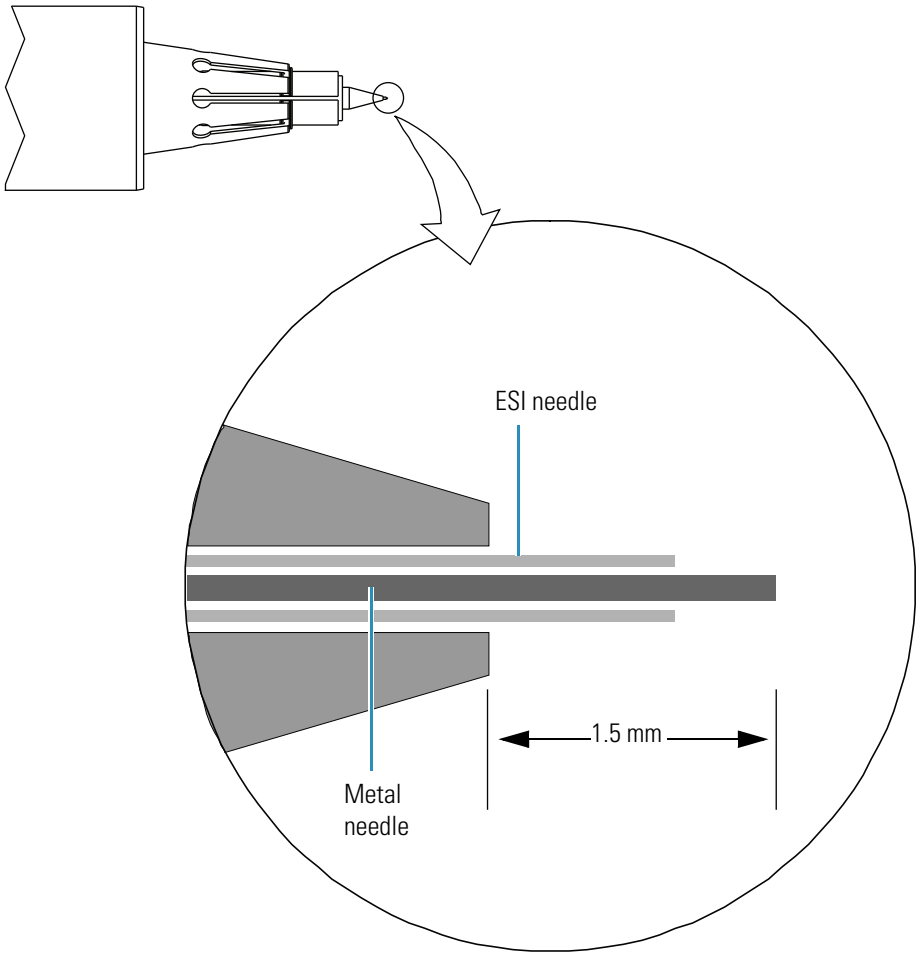
1. Remove the HESI-II probe from the Ion Max API source (refer to the *LTQ Series Getting Started Guide*).
2. Unscrew the fingertight fitting from the sample inlet port (refer to the *LTQ Series Getting Started Guide*).
3. Remove the metal needle insert from the probe as follows (Figure 61 on page 102):
   a. Using a 3 mm (7/64 in.) hex wrench or ball driver, remove the two M4×35 mm length, socket head cap screws.
   b. Pull the end cover off of the probe.
   c. Unscrew the metal needle insert, and then pull it out of the probe body.

Figure 61. HESI-II probe (exploded view)



4. Insert a new metal needle insert into the probe body.
5. Hand tighten the adjustable union fitting until the tip of the needle insert protrudes from the probe nozzle by 1.5 mm (Figure 62 on page 103).

Figure 62. HESI-II probe nozzle (exploded view)



6. Position the end cover on the probe body.
7. Insert the two M4×35 mm length, socket head cap screws into the end cover, and then tighten them with a 3 mm (7/64 in.) hex wrench or ball driver.
8. Reinstall the HESI-II probe (refer to the *LTQ Series Getting Started Guide*).

APCI Probe Maintenance

The APCI probe requires a minimum of maintenance. Occasionally, you must replace the APCI sample tube (150-µm ID×390-µm OD) fused-silica tubing) and clean the APCI nozzle.

Figure 63 and Figure 64 show the major components of the APCI probe.

Figure 63. APCI probe (cross section)

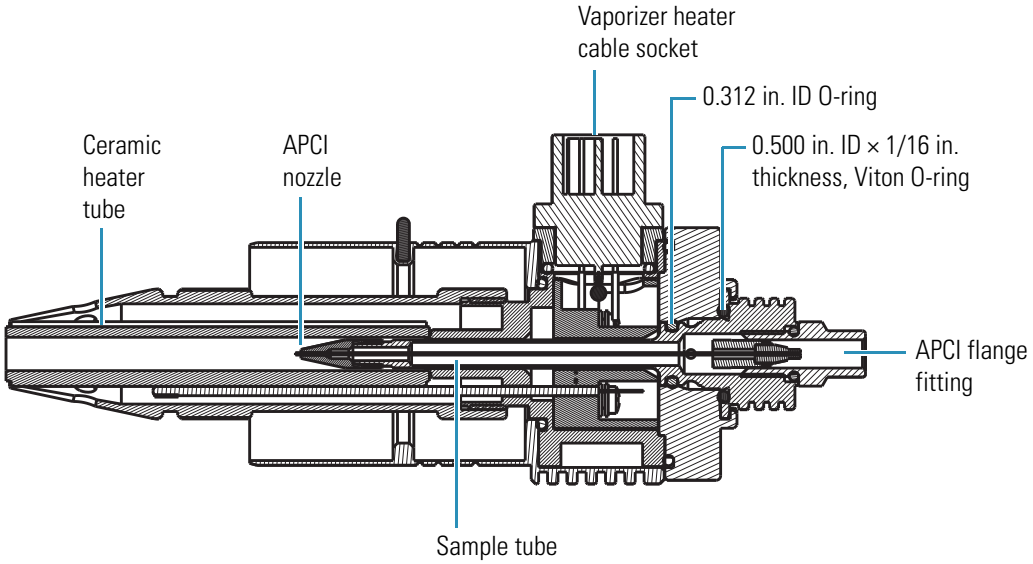
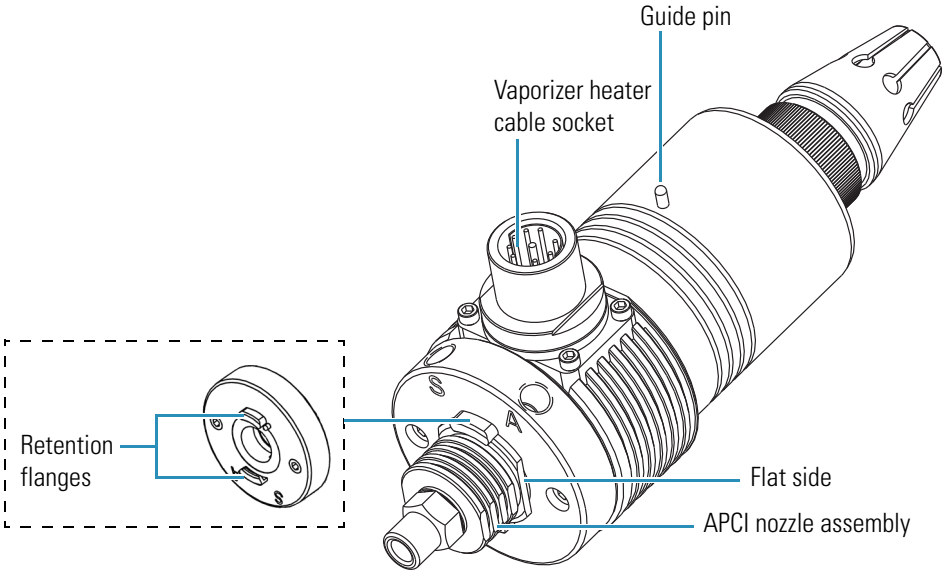


Figure 64. APCI probe (exterior view)



Note For best results, flush the APCI probe at the end of each work day by pumping a 50:50 methanol/water solution through the APCI source.

IMPORTANT Wear a new pair of lint- and powder-free gloves when you handle APCI probe components.

To maintain the APCI probe, follow these procedures:

- "Removing the APCI Nozzle," next section
- "Cleaning the APCI Nozzle" on page 106
- "Removing the APCI Sample Tube from the APCI Nozzle" on page 107
- "Installing the APCI Sample Tube" on page 109
- "Reassembling the APCI Probe" on page 110

Removing the APCI Nozzle

❖ **To remove the APCI nozzle from the APCI probe**

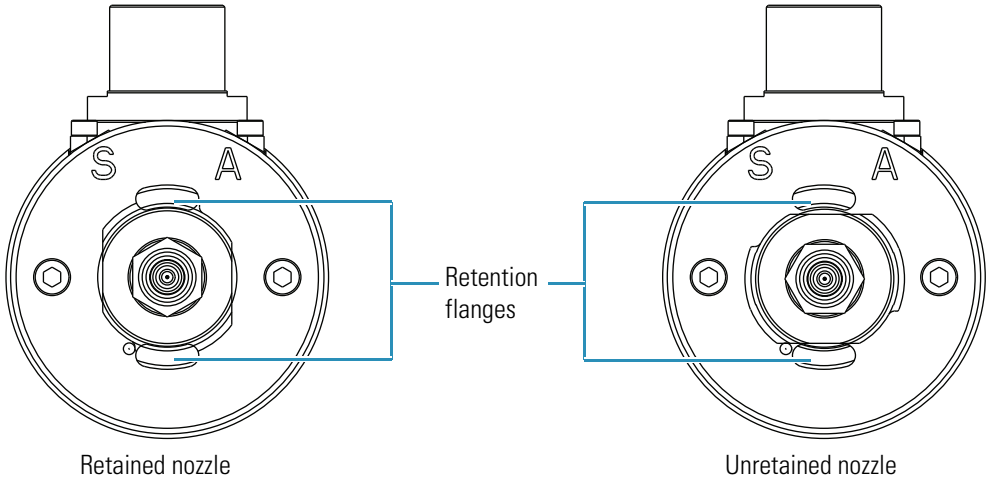
1. Place the mass spectrometer in Standby mode as described in "Placing the Mass Spectrometer in Standby Mode" on page 55.

CAUTION Until the APCI probe has cooled to room temperature, do not place, wrap, or store it in combustible materials (for example, plastic).

CAUTION **Avoid burns**. At operating temperatures, the APCI vaporizer an severely burn you. The APCI vaporizer typically operates at 400 to 600 °C. Allow approximately 20 minutes for the vaporizer to cool to room temperature before you touch or remove it.

2. Allow the heated components to cool to room temperature.
3. While holding the APCI probe body with one hand, grasp the head of the APCI nozzle assembly and rotate the head of the nozzle assembly counterclockwise until the flat sides of the head are facing toward the retention flanges (Figure 64 on page 104 and Figure 65 on page 106).

Figure 65. Sample inlet end of the APCI probe



4. Carefully pull the nozzle assembly straight out the back of the APCI probe.

CAUTION If the sample tube hits the sides of the vaporizer, it can break. To prevent breakage, carefully pull the APCI nozzle straight back from the APCI probe.

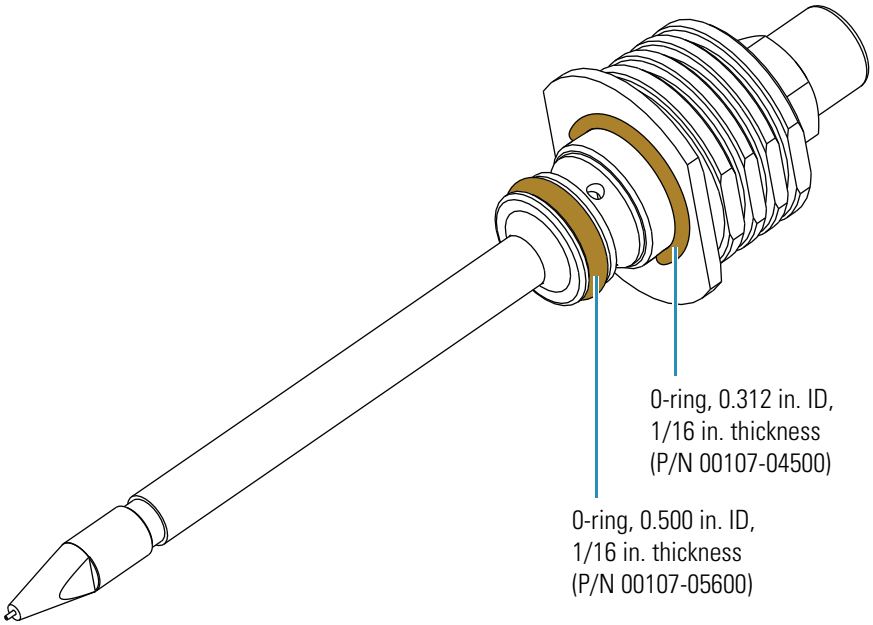
5. Place the nozzle assembly on a clean, lint-free tissue.

Cleaning the APCI Nozzle

❖ To clean the APCI nozzle

1. Remove the APCI nozzle from the probe body (see "Removing the APCI Nozzle" on page 105).
2. Check the condition of the O-rings on the APCI nozzle (Figure 66 on page 107).

Figure 66. APCI nozzle



3. Clean the interior APCI components (excluding the ceramic heater) with a 50:50 solution of LCMS-grade methanol/LCMS-grade water and a lint-free swab. Dry the components with nitrogen gas and place them on a lint-free tissue.
4. Reinstall any O-rings removed while cleaning.
5. Do one of the following:
   - If you do not want to replace the APCI sample tube, reinstall the APCI nozzle (see "Reassembling the APCI Probe" on page 110).
   - If you want to replace the sample tube, go to the next procedure "Removing the APCI Sample Tube from the APCI Nozzle."

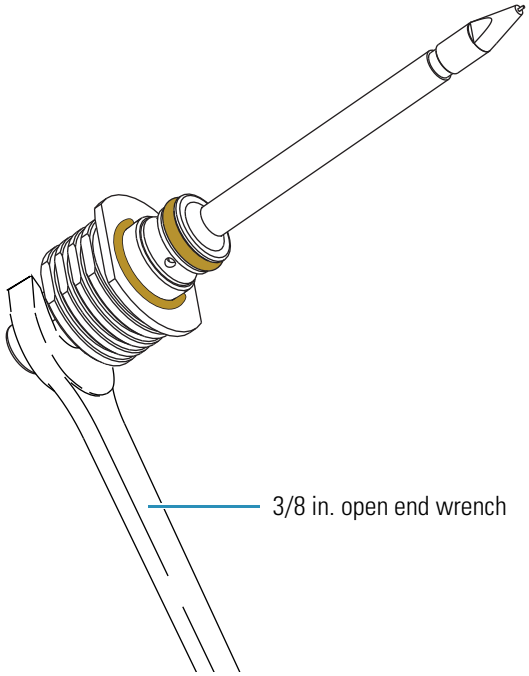
Removing the APCI Sample Tube from the APCI Nozzle

The sample tube for the APCI probe is an 8.6 cm length of 390 µm OD fused-silica tubing.

❖ To remove the APCI sample tube from the APCI Nozzle

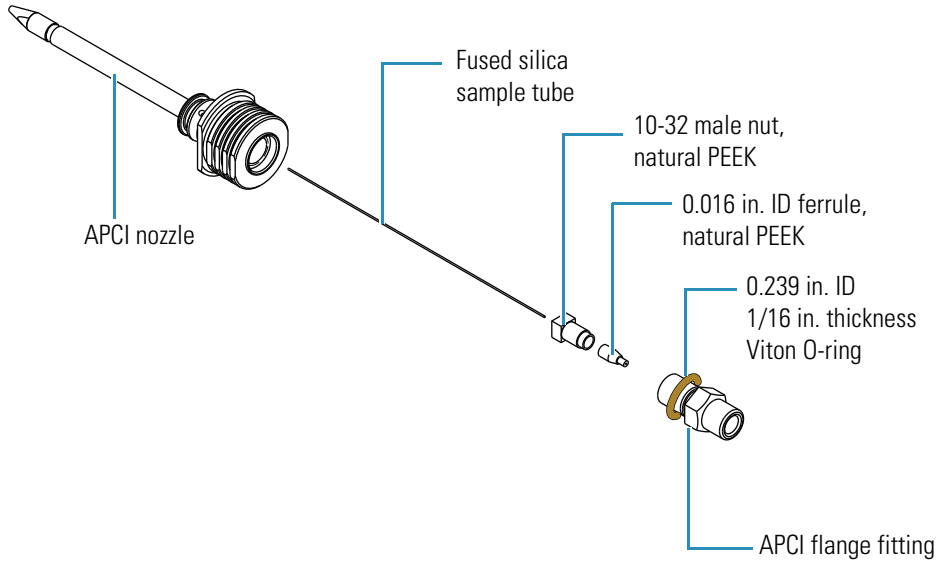
1. If you have not already done so, remove the APCI nozzle from the APCI probe (see "Removing the APCI Nozzle" on page 105).
2. Using a 3/8 in. open-end wrench, loosen the APCI flange fitting, and then pull the sample inlet fitting, exit nut, PEEK ferrule, and sample tube assembly from the APCI nozzle (Figure 67 on page 108).

Figure 67. 3/8 in. open-end wrench on the APCI flange fitting



3. Remove the fused-silica sample tube, nut, and ferrule assembly from the APCI flange fitting (Figure 68).

Figure 68. APCI sample tube connection



4. Discard the used fused-silica sample tube.

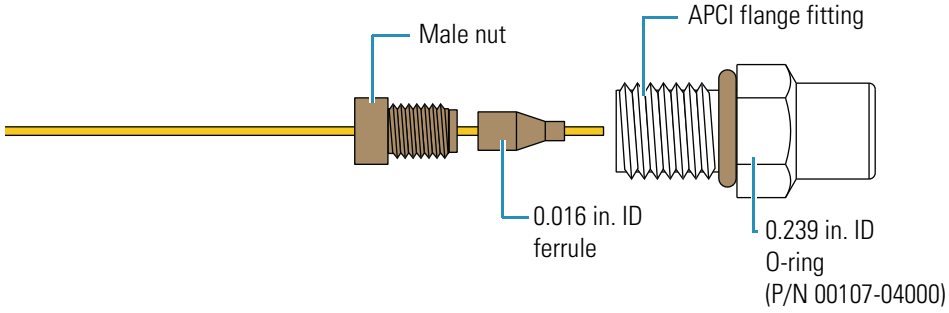
Installing the APCI Sample Tube

The APCI sample tube is an 8.6 cm length of 150 µm ID × 390 µm OD fused-silica tubing.

❖ To install a new APCI sample tube

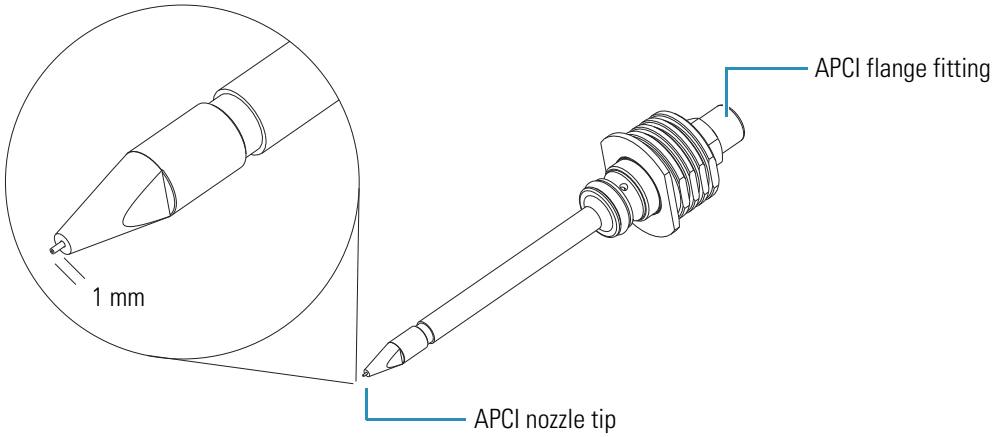
1. Check the condition of the 0.239 in. ID O-ring (P/N 00107-04000) on the APCI flange fitting (Figure 69). Replace it if necessary.
2. Using a fused-silica cutting tool, cut a piece of fused-silica tubing to a length of approximately 13 cm (5 in.). Ensure that you make square cuts to the ends of the fused-silica tubing.
3. Connect the fused-silica tubing to the APCI flange fitting:
   a. Slide the nut and the 0.016 in. ID ferrule onto the fused-silica tubing (Figure 69).
   b. While pressing the fused-silica tubing into the externally threaded end of the APCI flange fitting, finger tighten the two-piece fitting (Figure 69).

Figure 69. Fused-silica tubing connection to the APCI flange fitting



4. Carefully insert the free end of the fused-silica tubing into the back of the APCI nozzle and out the nozzle tip. Then finger tighten the APCI flange fitting.
5. Using a 3/8 in. open-end wrench, tighten the APCI flange fitting an additional quarter turn (Figure 67 on page 108).
6. Using a fused-silica cutting tool, cut the fused-silica sample tube so that approximately 1 mm protrudes past the tip of the APCI nozzle (Figure 70 on page 110).

Figure 70. Proper position of the exit end of the APCI sample tube

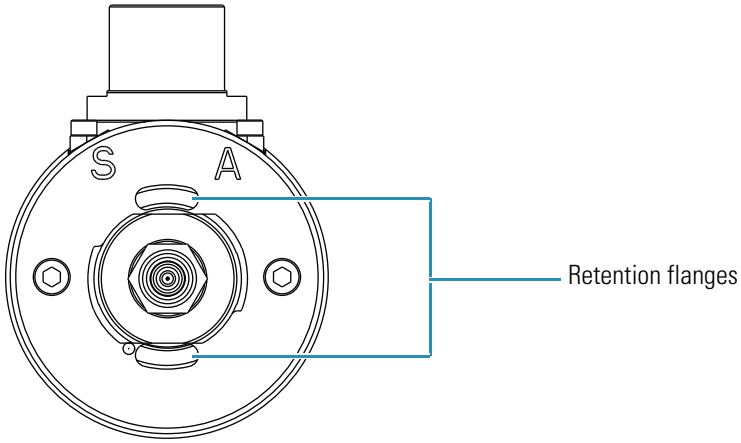


Reassembling the APCI Probe

❖ To reassemble the APCI probe

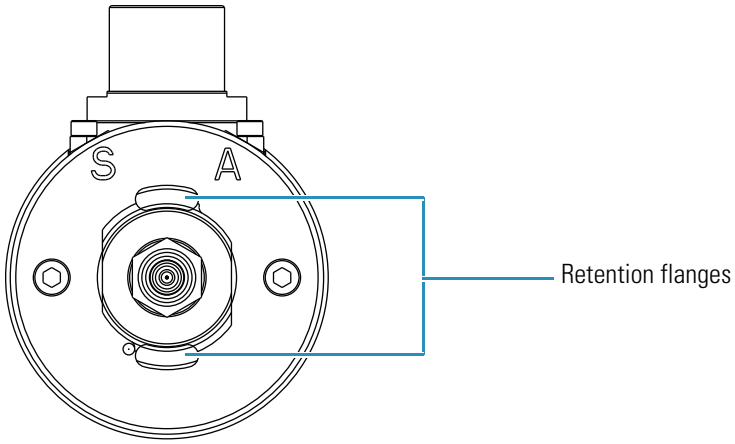
1. With one hand holding the APCI probe body to keep the probe from turning, carefully insert the APCI nozzle into the APCI probe.
2. With the flat sides of the APCI nozzle head facing the retention flanges on the probe body, seat the nozzle head into the APCI probe (Figure 71).

   Figure 71. Unsecured APCI nozzle seated in the APCI probe



3. To secure the APCI nozzle in the probe, rotate the head of the nozzle 90 degrees clockwise to secure the rounded sides of the nozzle head in the retention flanges (Figure 72 on page 111).

Figure 72. APCI nozzle secured by the retention flanges



To reinstall the probe in the Ion Max API source housing, refer to "APCI Probe Installation and Removal" in the *LTQ Series Getting Started Guide*.

Ion Source Interface Maintenance

To maintain the ion source interface, follow these procedures:

- "Removing the Ion Source Interface," next section
- "Removing, Cleaning, and Reinstalling the Tube Lens and Skimmer on the LXQ and LTQ XL Mass Spectrometers" on page 113
- "Removing, Cleaning, and Reinstalling the Exit Lens and S-Lens on the LTQ Velos" on page 116
- "Reinstalling the Ion Source Interface" on page 121

Removing the Ion Source Interface

❖ **To remove the ion source interface**

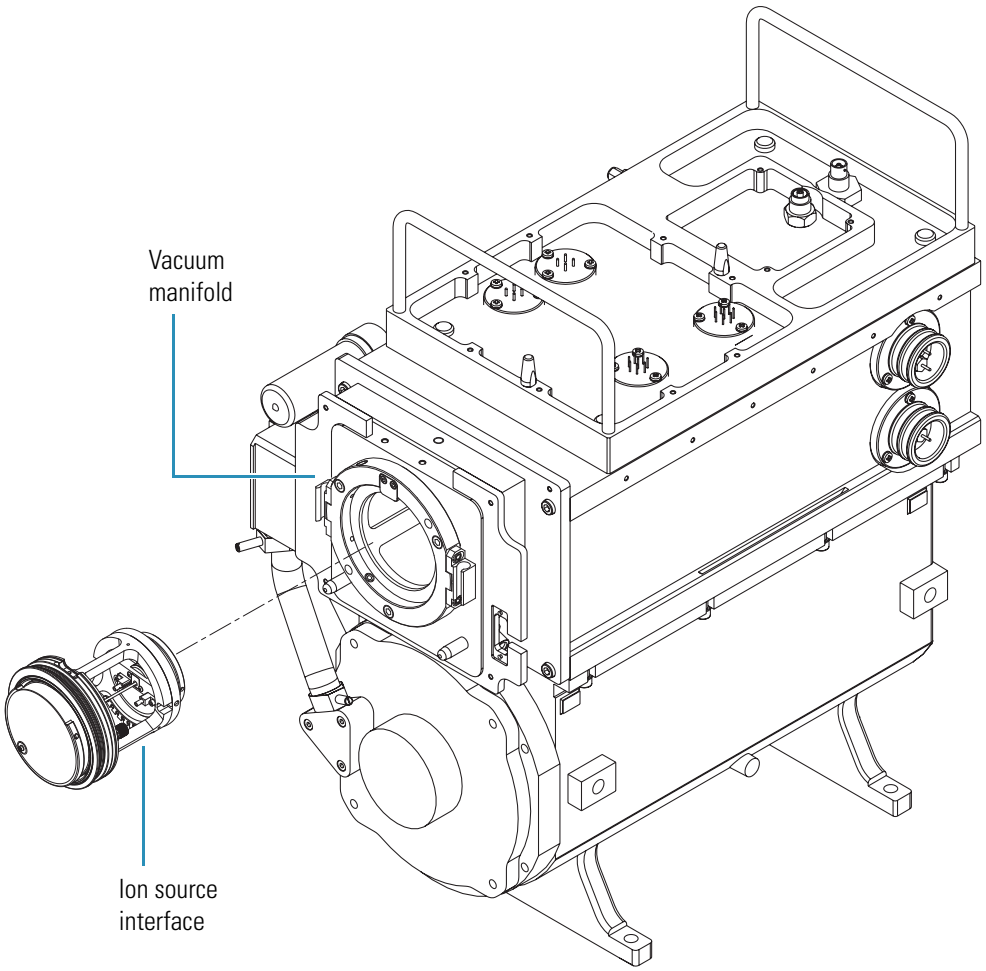
1. Shut down and vent the system as described in "Shutting Down the Mass Spectrometer Completely" on page 57. Wait several minutes for the LTQ Series mass spectrometer to vent.

CAUTION Unplug the mass spectrometer's power cord before you proceed.

CAUTION Allow approximately 20 minutes for the ion source interface to cool to ambient temperature before you remove it.

2. Put on a new pair of lint- and powder-free gloves.
3. Follow the instructions in "Removing the Ion Max or Ion Max-S API Source Housing" on page 65 to remove the housing.
4. Grasp the ridges on either side of the ion source interface (Figure 73).

Figure 73. Ion source removed from vacuum manifold



5. Carefully pull the ion source interface free from the vacuum manifold.
6. Place the ion source interface on a clean, lint-free surface.

Removing, Cleaning, and Reinstalling the Tube Lens and Skimmer on the LXQ and LTQ XL Mass Spectrometers

An accumulation of chemicals on the surfaces of the tube lens and skimmer forms an insulating layer, which 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 remove and clean the tube lens and skimmer**

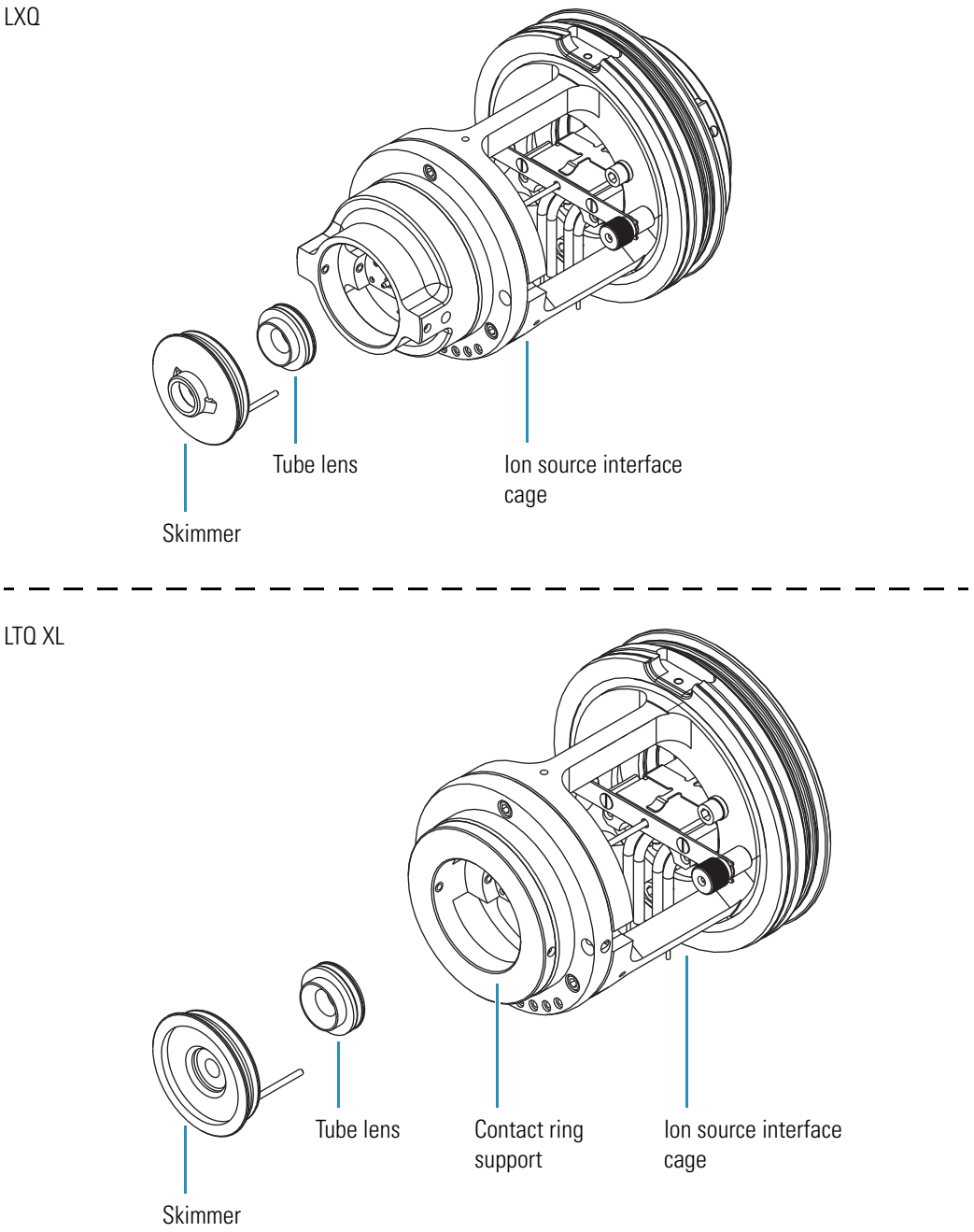
CAUTION Allow approximately 20 minutes for the ion source interface to cool to ambient temperature before disassembling it.

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

1. Prepare a clean work surface by covering the area with lint-free paper.
2. Put on a new pair of lint- and powder-free gloves.
3. Reach behind the skimmer with your fingers and gently press the skimmer out of the contact ring support. If necessary, loosen the set screws (Figure 74 on page 114).

Note Note the orientation of the skimmer.

Figure 74. Skimmer and tube lens separated from the LXQ or LTQ XL ion source interface cage



4. Place the skimmer on a clean, lint-free surface.
5. Push the tube lens, from the back, out of the contact ring support.
6. Place the tube lens on a clean, lint-free surface.

7. Sonicate the tube lens and skimmer alone in an organic or aqueous solution. Thermo Fisher Scientific recommends using LCMS-grade methanol.

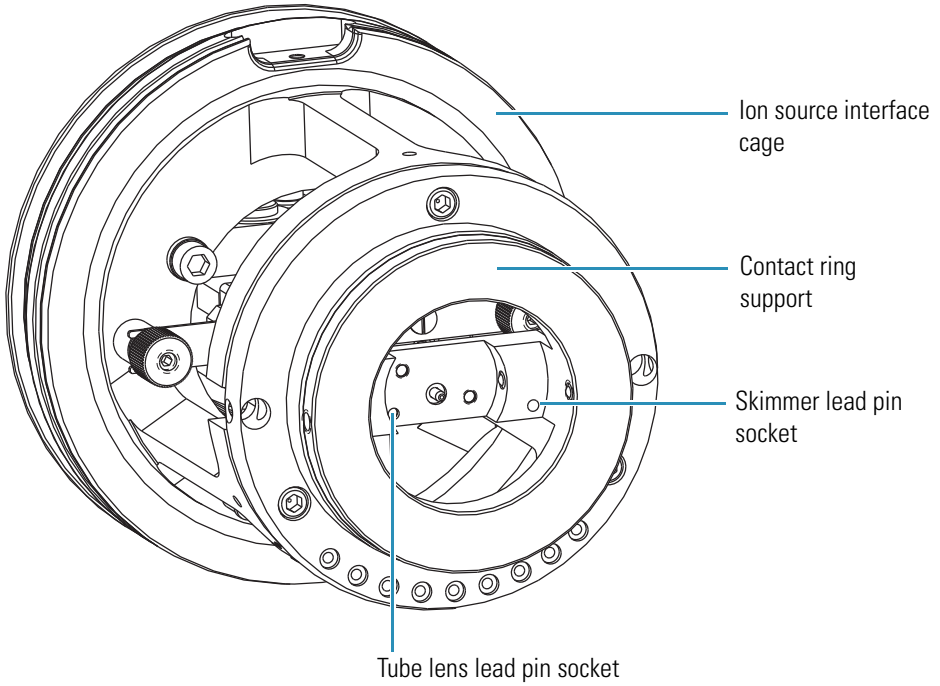
Note If you are using buffers or salt solutions in your MS detector, you might need to use an aqueous solution for cleaning. If you use an aqueous solution, flush the items with distilled water and then with methanol.

8. Air dry the skimmer and tube lens or blow them dry with nitrogen gas.
9. Ensure that all the solvent has evaporated from components before you reinstall them.

❖ To reinstall the tube lens and skimmer

1. Reinstall the tube lens into the ion source interface cage:
   a. Orient the tube lens so that the lead pin points toward the socket on the tube lens connection wire in the contact ring support (Figure 75).
   b. Insert the lead pin into the socket and firmly press the tube lens into the contact ring support until it snaps into place.

Figure 75. LXQ and LTQ XL ion source interface cage



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

2. Reinstall the skimmer into the ion source interface assembly:

a. Orient the skimmer so that the lead pin points toward the socket on the tube lens connection wire in the contact ring support.

b. Insert the lead pin into the socket and firmly press the skimmer into the contact ring support.

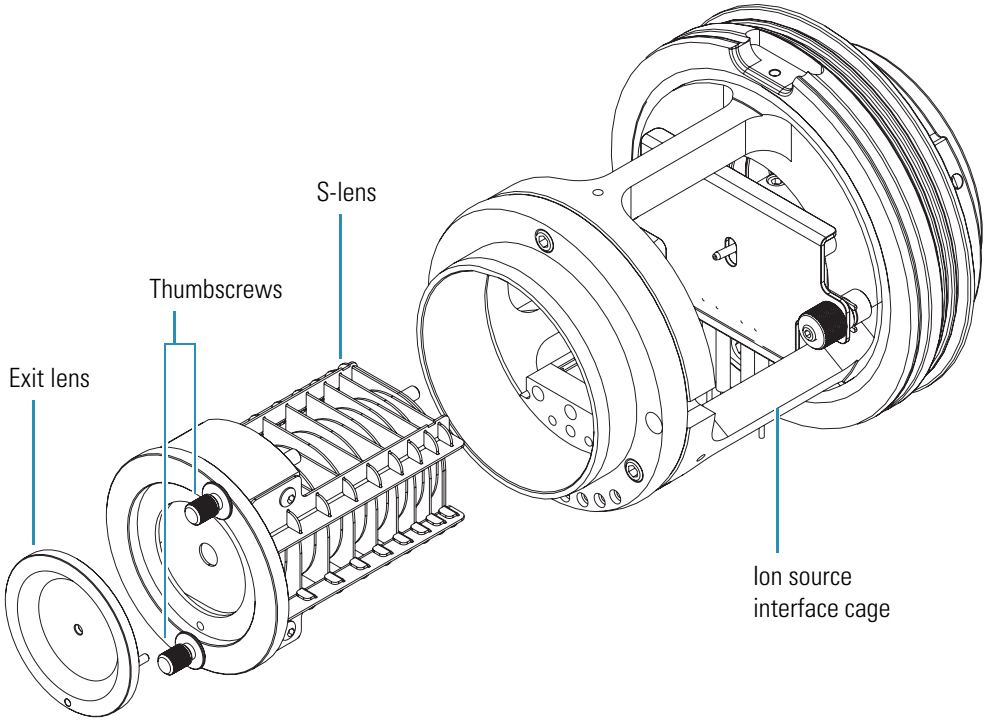
Removing, Cleaning, and Reinstalling the Exit Lens and S-Lens on the LTQ Velos

Remove the S-lens and exit lens from the ion source interface cage before cleaning them.

❖ **To remove the exit lens and S-lens from the ion source interface cage**

1. Prepare a clean work surface by covering the area with lint-free paper.
2. Put on a new pair of lint- and powder-free gloves.
3. Loosen and extend the two thumbscrews that secure the S-lens to the ion source interface cage and the exit lens to the S-lens (Figure 76).

Figure 76. Exit lens and S-lens separated from the LTQ Velos ion source interface cage



4. Remove the exit lens from the S-lens and place it on a clean, lint-free surface.
5. Grasp the two thumbscrews and carefully pull the S-lens straight out of the ion source interface cage and place it on a clean, lint-free surface.

❖ To clean the S-lens and exit lens

CAUTION Do not clean the S-lens or exit lens with detergents, acidic or caustic substances, or abrasives.

1. Put on a new pair of lint- and powder-free gloves.
2. Sonicate the exit lens and S-lens separately for 15 min. in a 50:50 solution of LCMS-grade methanol and water.
3. Rinse the exit lens and S-lens with fresh methanol.
4. Air dry the exit lens and S-lens or blow dry them with nitrogen gas.

   Ensure that all solvent has evaporated from the components before reassembly.

❖ To reinstall the S-lens and exit lens

1. Wearing a new pair of lint- and powder-free gloves, slide the S-lens into the ion source interface cage and align the thumbscrews with the screw holes (Figure 76 on page 116).
2. Insert the exit lens into the S-lens, aligning the lead pin with the lead pin socket, and press until you hear a click.
3. Hand tighten the thumbscrews to secure the exit lens and S-lens to the ion source interface cage.

Removing, Cleaning, and Reinstalling the Ion Transfer Capillary

The bore of the ion transfer capillary can become blocked by buffer salts or high concentrations of sample and must be cleaned. 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.

❖ To check the Convectron gauge pressure

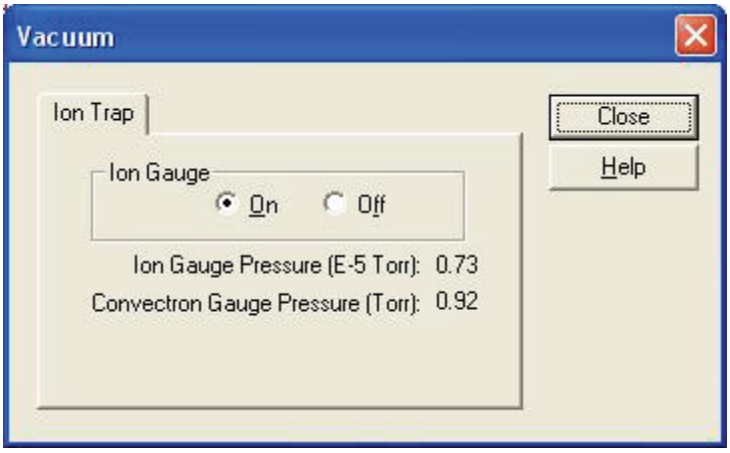
1. On the Windows taskbar, choose **Start > All Programs > Thermo Instruments > LTQ > *model* Tune**.

   Note For LTQ version 2.5.0 or earlier, the path is **Start > All Programs > Xcalibur > *model* Tune**.

   The LTQ Tune Plus window opens (Figure 33 on page 55).
2. Choose **Setup > Vacuum**.

   The Vacuum dialog box opens (Figure 77 on page 118).

Figure 77. Vacuum dialog box



3. Note the reading for the Convectron Gauge Pressure. If the reading is considerably below 1 Torr, clean the ion transfer capillary.

❖ To remove and clean the ion transfer capillary

1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source:

   a. On the Windows taskbar, choose **Start > All Programs > Thermo Instruments > LTQ > *model* Tune**.

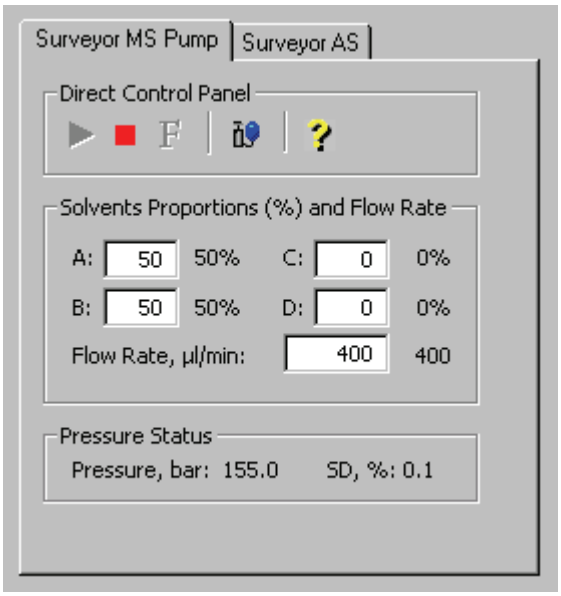
   > **Note** For LTQ version 2.5.0 or earlier, the path is **Start > All Programs > Xcalibur > *model* Tune**.

   The Tune Plus window opens (Figure 33 on page 55).

   b. Choose **Setup > Inlet Direct Control**.

   The Inlet Direct Control dialog box opens (Figure 78).

Figure 78. Inlet Direct Control dialog box for a Surveyor MS Pump



c. Click the **Pump Off** or **Stop Pump** button to stop the LC pump.

2. Place the electronics service switch (located on the right side of the mass spectrometer) in the Service position to turn off the nonvacuum system voltages.

CAUTION Make sure that the electronics service switch is in the Service position before proceeding.

3. Remove the ion source housing from the front of the mass spectrometer as described in "Removing the Ion Max or Ion Max-S API Source Housing" on page 65.

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.

5. Remove the ion transfer capillary 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. Wipe the inside and outside of the ion sweep cone with a Kimwipe tissue soaked in methanol.
9. Remove and inspect the O-ring that is seated in the spray cone under the entrance end of the ion transfer capillary (Figure 79 and Figure 80 on page 120). Clean it with methanol or replace it if necessary.

Figure 79. LXQ and LTQ XL ion source interface components

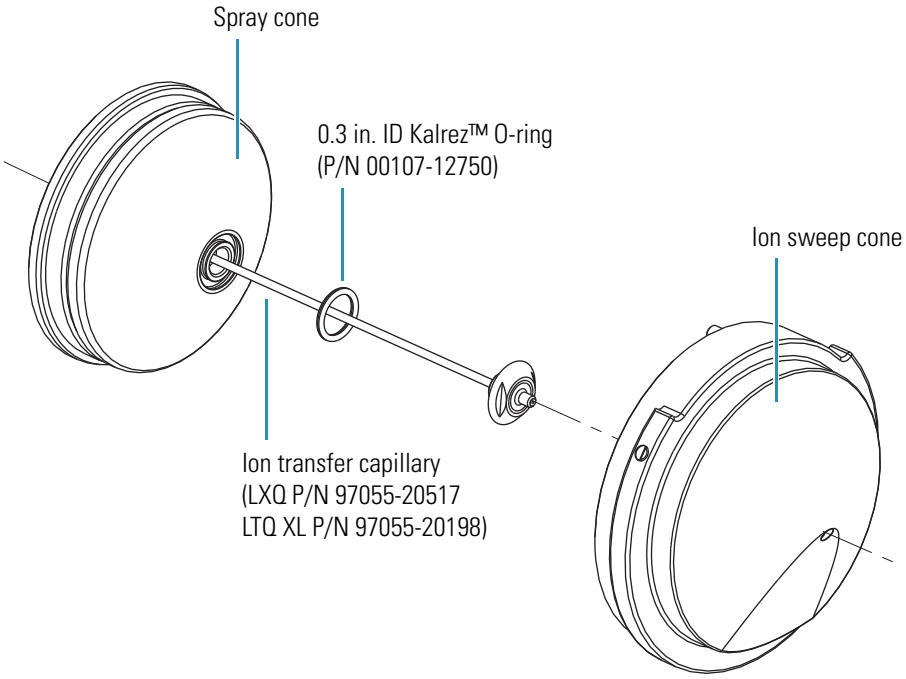
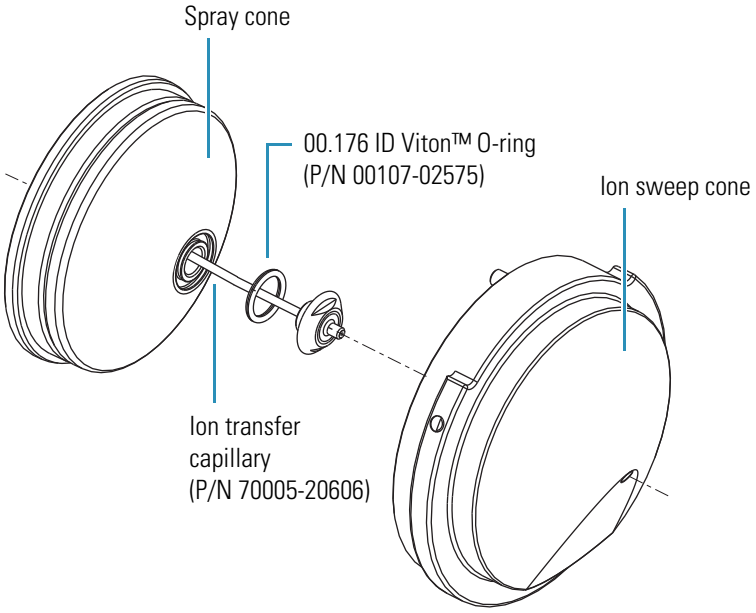


Figure 80. LTQ Velos ion source interface components



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. 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 on the mass spectrometer as described in "Installing the Ion Max or Ion Max-S API Source Housing" on page 66.

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 nonvacuum system voltages.

Reinstalling the Ion Source Interface

❖ **To reinstall the ion source interface**

1. Orient the ion source interface as shown in Figure 74 on page 114.
2. Carefully insert the ion source interface into the vacuum manifold until it is seated in the Q00 rf lens.
3. Reinstall the ion source housing as described in "Installing the Ion Max or Ion Max-S API Source Housing" on page 66.
4. Start up the system as described in "Starting the System after a Complete Shutdown" on page 58.

Q00 RF Lens Maintenance

An accumulation of chemicals on the surfaces of the Q00 quadrupole and lens L0 forms an insulating layer, which can modify the electrical fields that control ion transmission. Clean ion guide components are essential for the proper operation of the MS detector. The Q00 rf lens 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 follow these procedures:

- "Removing the Q00 RF Lens Assembly," next section
- "Disassembling the Q00 RF Lens Assembly" on page 123

- "Cleaning the Q00 RF Lens Assembly Components" on page 125
- "Reassembling the Q00 RF Lens Assembly" on page 126
- "Reinstalling the Q00 RF Lens Assembly" on page 126

Removing the Q00 RF Lens Assembly

❖ **To remove the Q00 rf lens assembly**

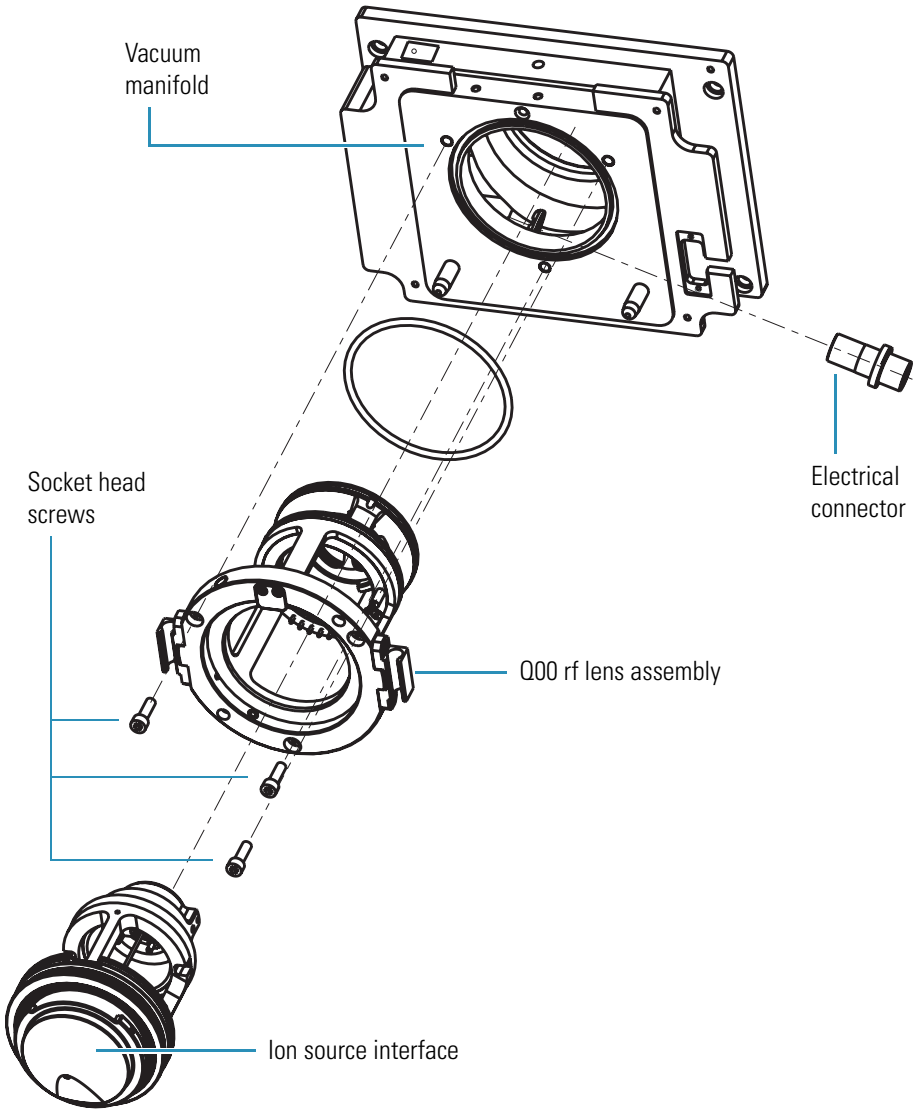
1. Shut down and vent the system as described in "Shutting Down the Mass Spectrometer Completely" on page 57. Wait several minutes for the LTQ Series mass spectrometer to vent.

CAUTION Unplug the mass spectrometer's power cord before you proceed.

CAUTION Allow approximately 20 minutes for the ion source interface to cool to ambient temperature before you remove it.

2. Remove the ion source interface as described in "Removing the Ion Source Interface" on page 111.
3. Reach into the opening in the vacuum manifold (where the ion source interface was) and disconnect the electrical connector to the Q00 rf lens assembly.
4. Loosen the three socket head screws that hold the Q00 rf lens assembly housing to the vacuum manifold (Figure 81 on page 123).

Figure 81. Q00 rf lens assembly removal



5. Carefully remove the Q00 rf lens assembly and place it on a clean surface.

Disassembling the Q00 RF Lens Assembly

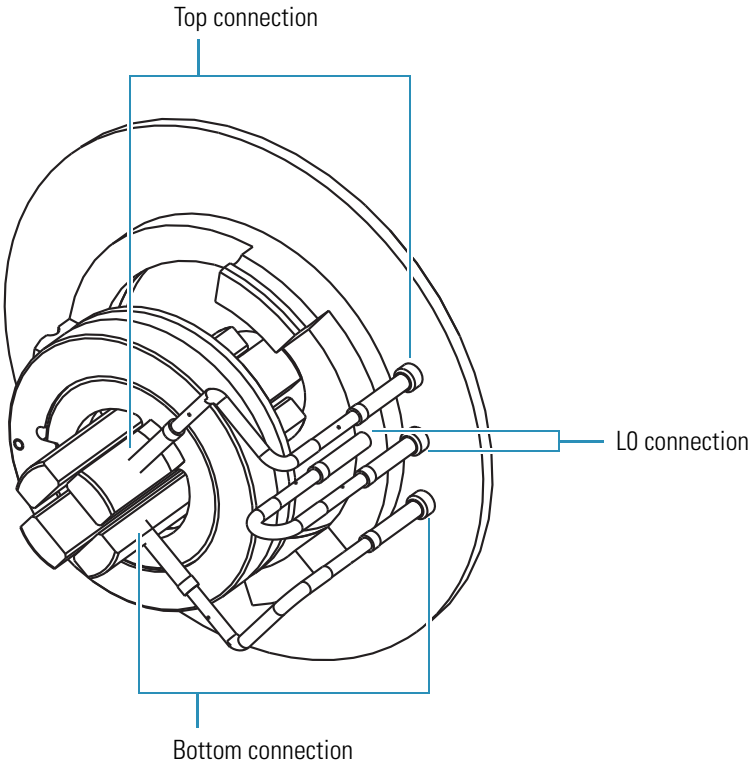
❖ **To disassemble the Q00 rf lens assembly**

CAUTION Be careful not to bend or break the lead pins on the Q00 rf lens.

1. Prepare a clean work surface by covering the area with lint-free paper.
2. Put on a new pair of lint- and powder-free gloves.

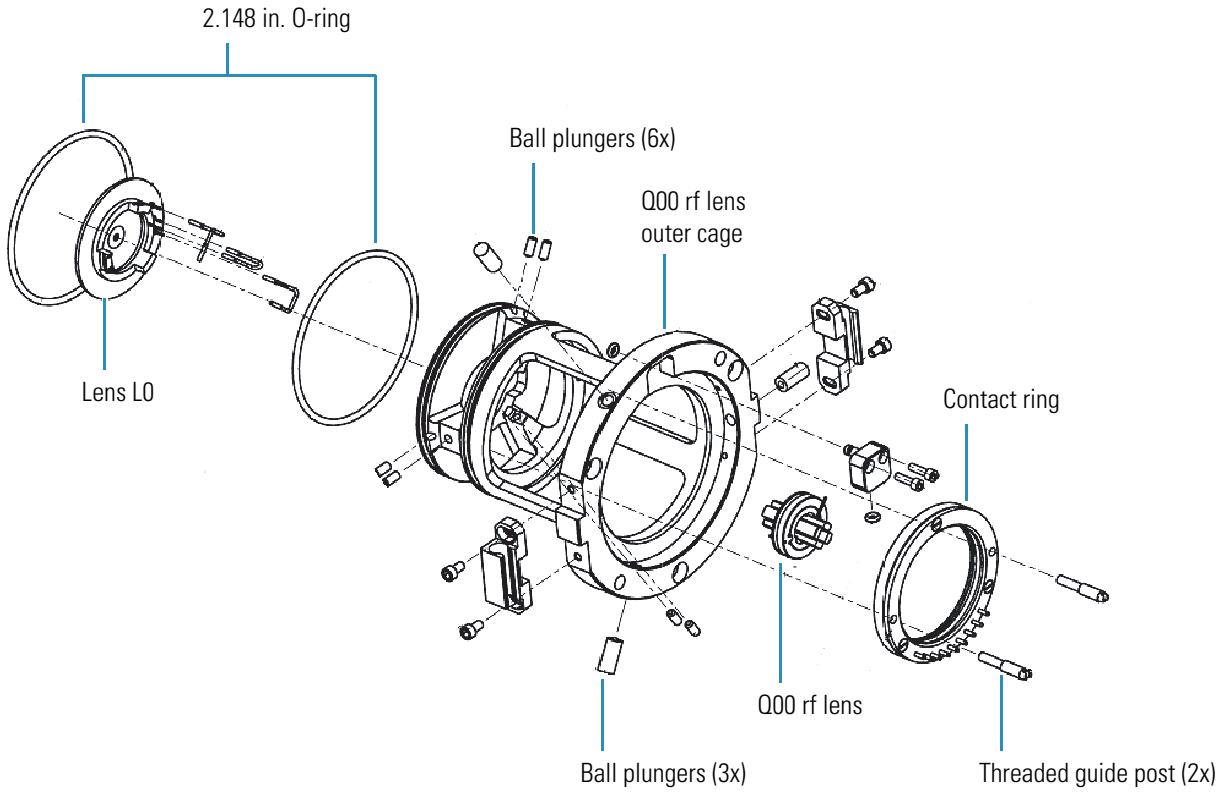
3. Carefully remove the leads from the lead pins on the Q00 rf lens and lens L0 (Figure 82).

Figure 82. Q00 quadrupole and lens L0 wiring connections



4. Remove lens L0 from the rear of the Q00 rf lens assembly (Figure 83 on page 125). (Lens L0 is secured to the Q00 rf lens assembly by ball plungers).

Figure 83. Q00 rf lens assembly



5. Remove the Q00 rf lens from the front of the Q00 rf lens outer cage. (The Q00 rf lens is secured to the Q00 rf lens outer cage by ball plungers.)

Cleaning the Q00 RF Lens Assembly Components

❖ **To clean the Q00 rf lens and lens L0**

1. Put on a new pair of lint- and powder-free gloves.
2. With a soft toothbrush or lint-free swab, scrub the part with a solution of detergent and water.
3. Rinse the part with tap water to remove the detergent.
4. Rinse the part with distilled water.
5. Place the part in a beaker and immerse it completely in LCMS-grade methanol. Move the part up and down in the methanol for 15 seconds.
6. Remove the part from the methanol bath; then rinse it thoroughly with fresh methanol.
7. Dry the part with a rapid stream of nitrogen gas.
8. Inspect each part for contamination and dust. If necessary, repeat the cleaning procedure.

Reassembling the Q00 RF Lens Assembly

❖ **To reassemble the Q00 rf lens assembly**

1. Insert the Q00 rf lens through the front of the Q00 rf lens outer cage until it is seated in the cage.
2. Insert lens L0 through the rear of the cage until it is seated in the cage.

CAUTION Be careful not to bend or break the lead pins on the Q00 rf lens.

3. Carefully reconnect the leads to the lead pins on the Q00 rf lens and lens L0 as shown in Figure 83 on page 125.

Reinstalling the Q00 RF Lens Assembly

❖ **To reinstall the Q00 rf lens assembly in the vacuum manifold**

1. Ensure that the two 2.148 in. O-rings (P/N 00107-15542) are properly installed on the rear of the outer cage.
2. Orient the Q00 rf lens outer cage assembly as shown in Figure 83 on page 125.
3. Carefully insert the Q00 rf lens outer cage assembly into the vacuum manifold.
4. Reconnect the electrical connections.
5. Reinstall the ion source interface as described in "Reinstalling the Ion Source Interface" on page 121.
6. Start up the system as described in "Starting the System after a Complete Shutdown" on page 58.

Q0 and Q1 Ion Guides Maintenance

An accumulation of chemicals on the surfaces of the Q0 and Q1 ion guides forms an insulating layer, which can modify the electrical fields that control ion transmission. 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 ion guide. 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:

- "Removing the Top Cover of the Mass Spectrometer," next section
- "Removing the Top Cover Plate of the Vacuum Manifold" on page 129

- "Removing the Q0 and Q1 Ion Guides" on page 131
- "Cleaning the Q0 and Q1 Ion Guides" on page 135
- "Reinstalling the Q0 and Q1 Ion Guides" on page 135
- "Cleaning the Ion Detection System" on page 140
- "Reinstalling the Top Cover of the Mass Spectrometer" on page 140

Removing the Top Cover of the Mass Spectrometer

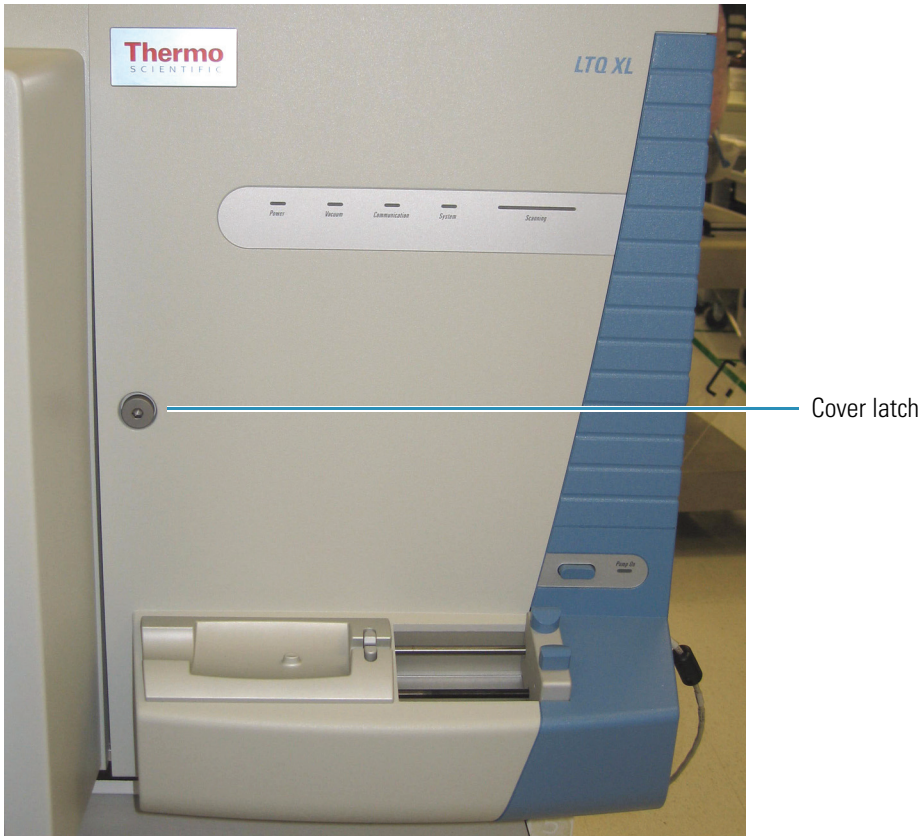
❖ **To remove the top cover of the mass spectrometer**

1. Shut down and vent the system as described in "Shutting Down the Mass Spectrometer Completely" on page 57. Wait several minutes for the LTQ Series mass spectrometer to vent.

CAUTION Unplug the mass spectrometer's power cord before you proceed.

2. Disconnect any tubing between the syringe pump and the API source.
3. Use a 1/4 in. hex wrench to loosen the cover latch (Figure 84).

Figure 84. Front cover latch



4. Open the front cover and loosen the two Phillips head captive screws that hold the top cover on (Figure 85).

Figure 85. Top cover screws

5. Slide the top back and off (Figure 86).

Figure 86. Top cover removal

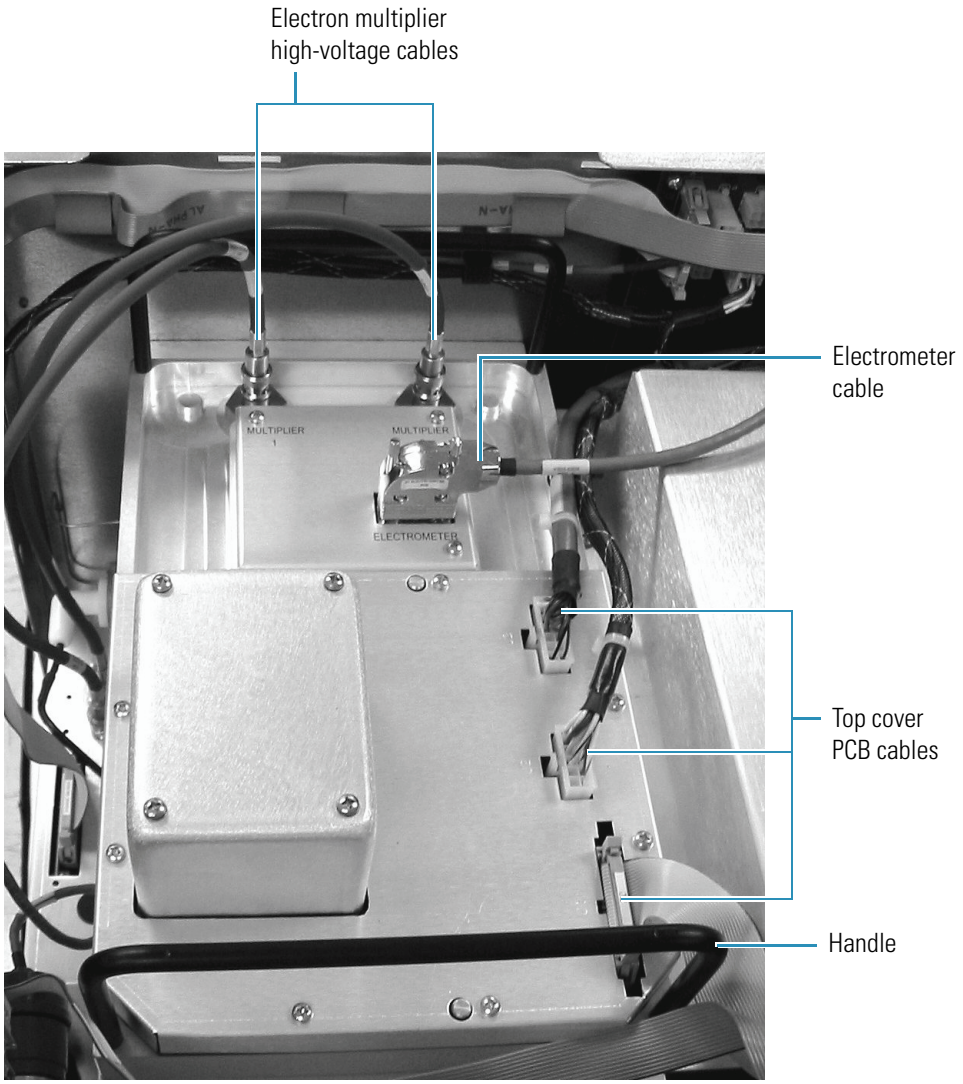
Removing the Top Cover Plate of the Vacuum Manifold

To access the Q0 and Q1 ion guides, mass analyzer, and ion detection system, remove the top cover of the vacuum manifold. The top cover is held in place by gravity and by the air pressure differential between the vacuum manifold and atmospheric pressure. Six cables are connected to the top cover plate.

❖ To remove the top cover plate of the vacuum manifold

1. Disconnect the electron multiplier high-voltage coaxial cables (Figure 87).

Figure 87. Electrical connections to the top cover plate of the vacuum manifold



2. Disconnect the electrometer cable. (If necessary, use a small screwdriver 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.

Removing the Q0 and Q1 Ion Guides

❖ **To remove the Q0 and Q1 ion guides from the top cover plate**

1. Prepare a clean work surface by covering the area with lint-free paper.
2. Put on a new pair of lint- and powder-free gloves.

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

3. Disconnect the electrical leads to the Q0 quadrupole, lens L1, gate lens (or split gate lens), and Q1 octapole (Figure 88 on page 132, Figure 89 on page 133, and Figure 90 on page 134).

Figure 88. LXQ Q0 and Q1 ion guides (exploded view)

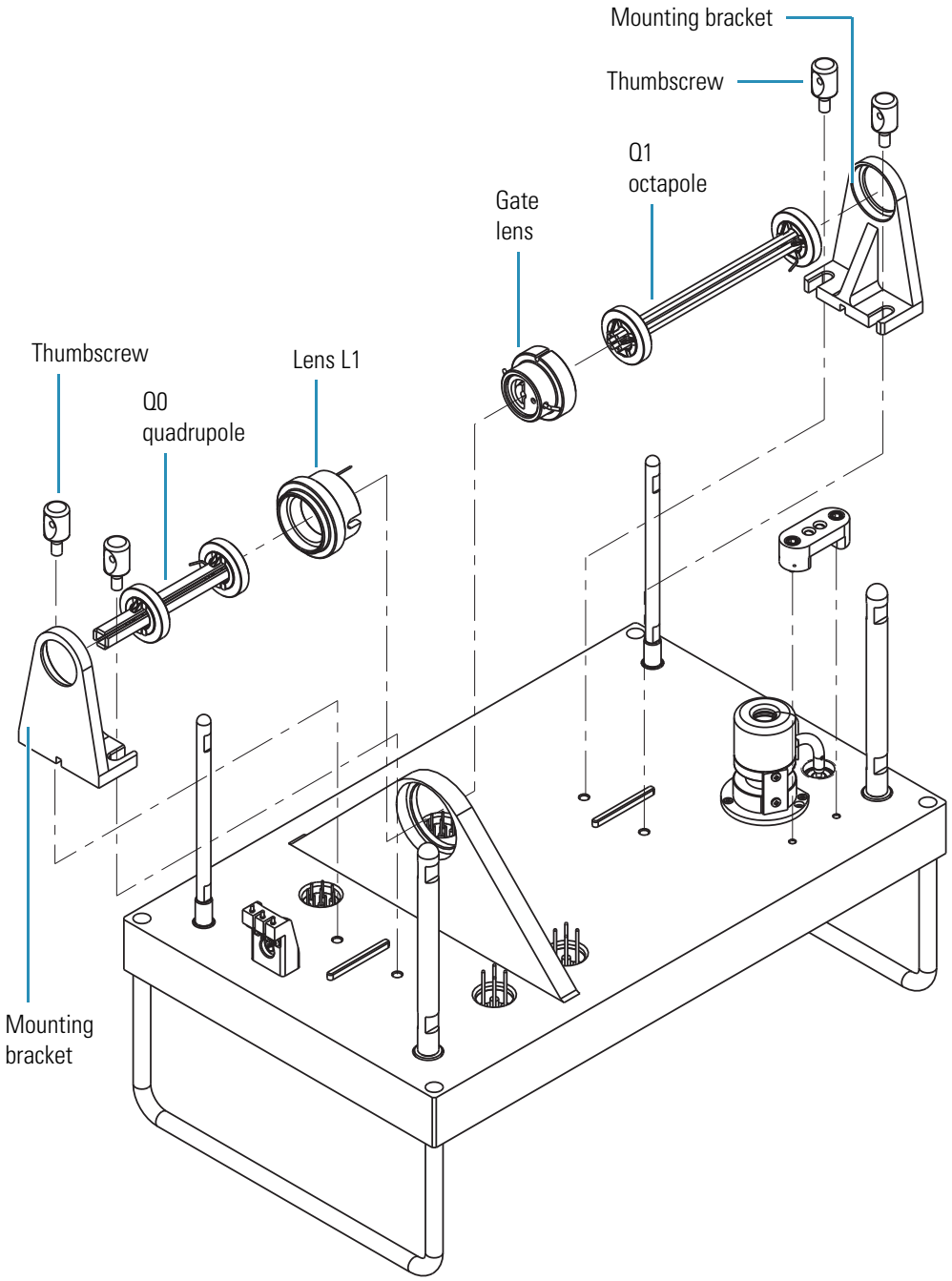


Figure 89. LTQ XL Q0 and Q1 ion guides (exploded view)

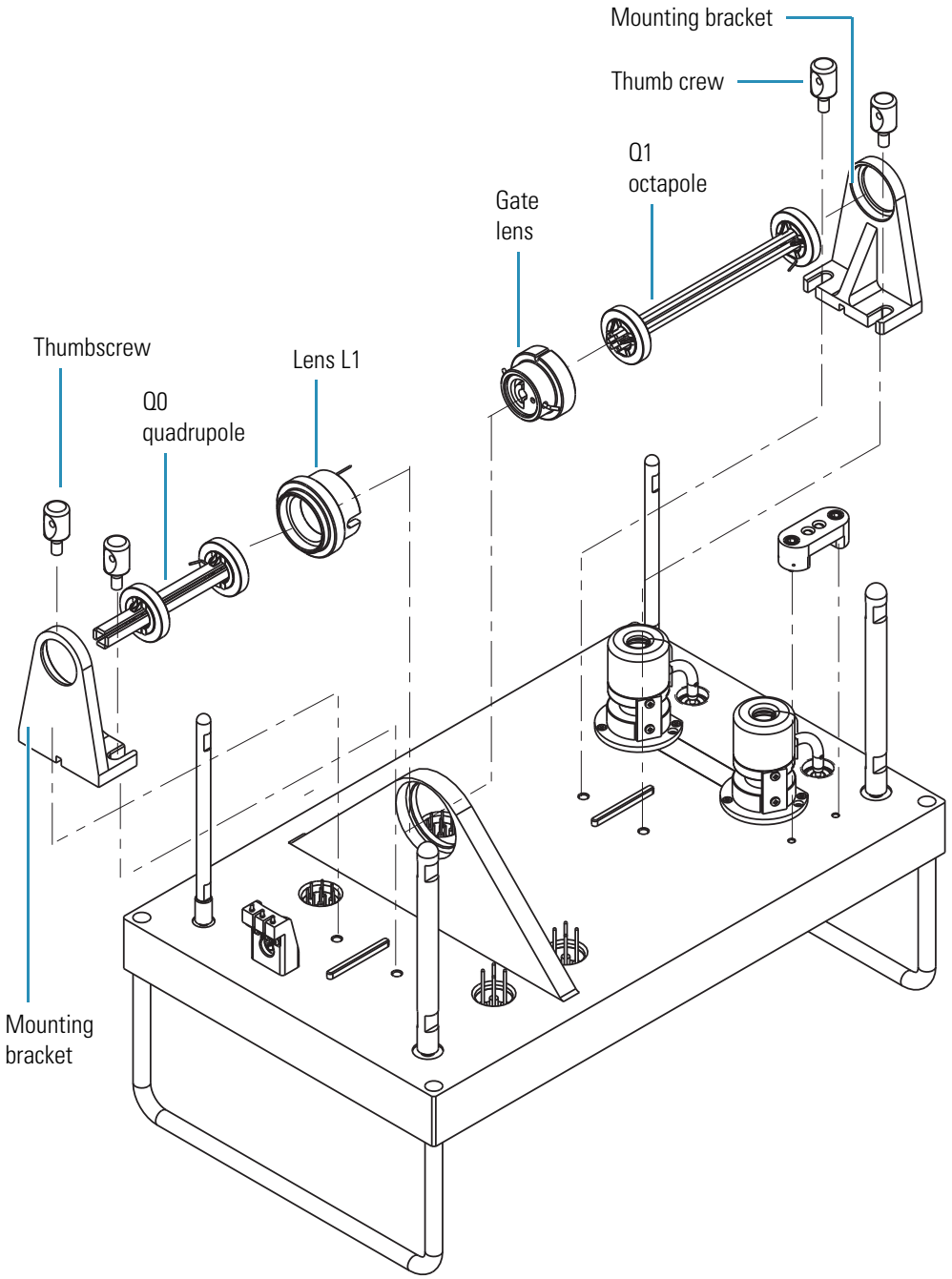
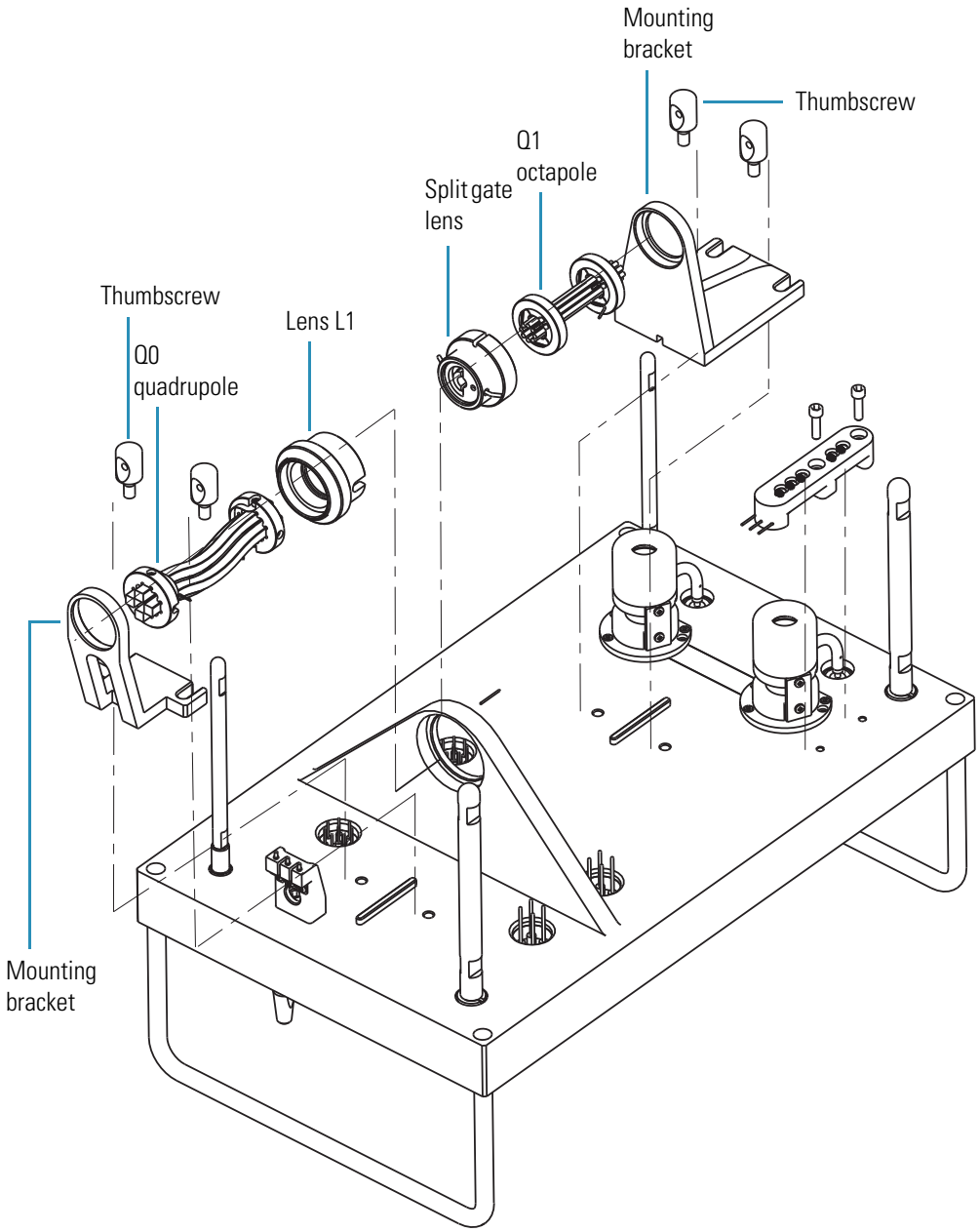


Figure 90. LTQ Velos Q0 and Q1 ion guides (exploded view)



4. Hold the Q1 octapole and gate lens (or split gate lens) with one hand; loosen and remove the two thumbscrews that hold the Q1 ion guide mounting bracket to the top cover plate of the vacuum manifold (Figure 88 on page 132 and Figure 90 on page 134).
5. Remove the Q1 octapole and gate lens (or split gate lens).
6. Hold the Q0 quadrupole and lens L1 with one hand; loosen and remove the two thumbscrews that hold the Q0 ion guide mounting bracket to the top cover plate of the vacuum manifold.
7. Remove the Q0 quadrupole and lens L1.

Cleaning the Q0 and Q1 Ion Guides

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

❖ **To clean the Q0 and Q1 ion guides**

1. Put on a new pair of lint- and powder-free gloves.
2. With a soft tooth brush or lint-free swab, scrub the ion guide parts with a solution of detergent and water.
3. Rinse the part with tap water to remove the detergent.
4. Rinse the part with distilled water.
5. Place the part in a tall beaker and immerse it completely in LCMS-grade methanol. Move the part up and down in the methanol for 15 seconds.
6. Remove the part from the methanol bath; then rinse it thoroughly with fresh methanol.
7. Dry the part with a rapid stream of nitrogen gas.
8. Inspect each part for contamination and dust. If necessary, repeat the cleaning procedure.

Reinstalling the Q0 and Q1 Ion Guides

❖ **To reinstall the Q0 and Q1 ion guides**

1. Put on a new pair of lint- and powder-free gloves.
2. To reinstall the Q0 ion guide:
   a. Insert lens L1 into the opening in the baffle (Figure 88 on page 132 and Figure 90 on page 134).
   b. With one hand, hold the Q0 quadrupole against the lens L1 and press L1 against the opening in the baffle with the contact pin up. away from the top cover plate.
   c. 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.

Note If the Q0 quadrupole is not positioned correctly, it will be too far forward and will make contact with the manifold.

d. Tighten the two thumbscrews 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. To reinstall the Q1 ion guide:
   a. Insert the gate lens (or split gate lens) into the opening in lens L1 (Figure 88 on page 132 and Figure 90 on page 134).
   b. With one hand, hold the Q1 octapole against the gate lens (or split 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 (or split gate lens).
   c. Tighten the two thumbscrews that hold the Q1 ion guide mounting bracket to the top cover plate.
4. Reconnect the electrical leads to the Q0 quadrupole, lens L1, gate lens, and Q1 octapole according to the wiring diagram shown in Figure 91, Figure 92 on page 138, and Figure 93 on page 139.
5. Check all leads to ensure that they are secure and that they are attached to the proper electrodes (Figure 91, Figure 92 on page 138, and Figure 93 on page 139).

Figure 91. LXQ Q0 and Q1 ion guides (wiring diagram)

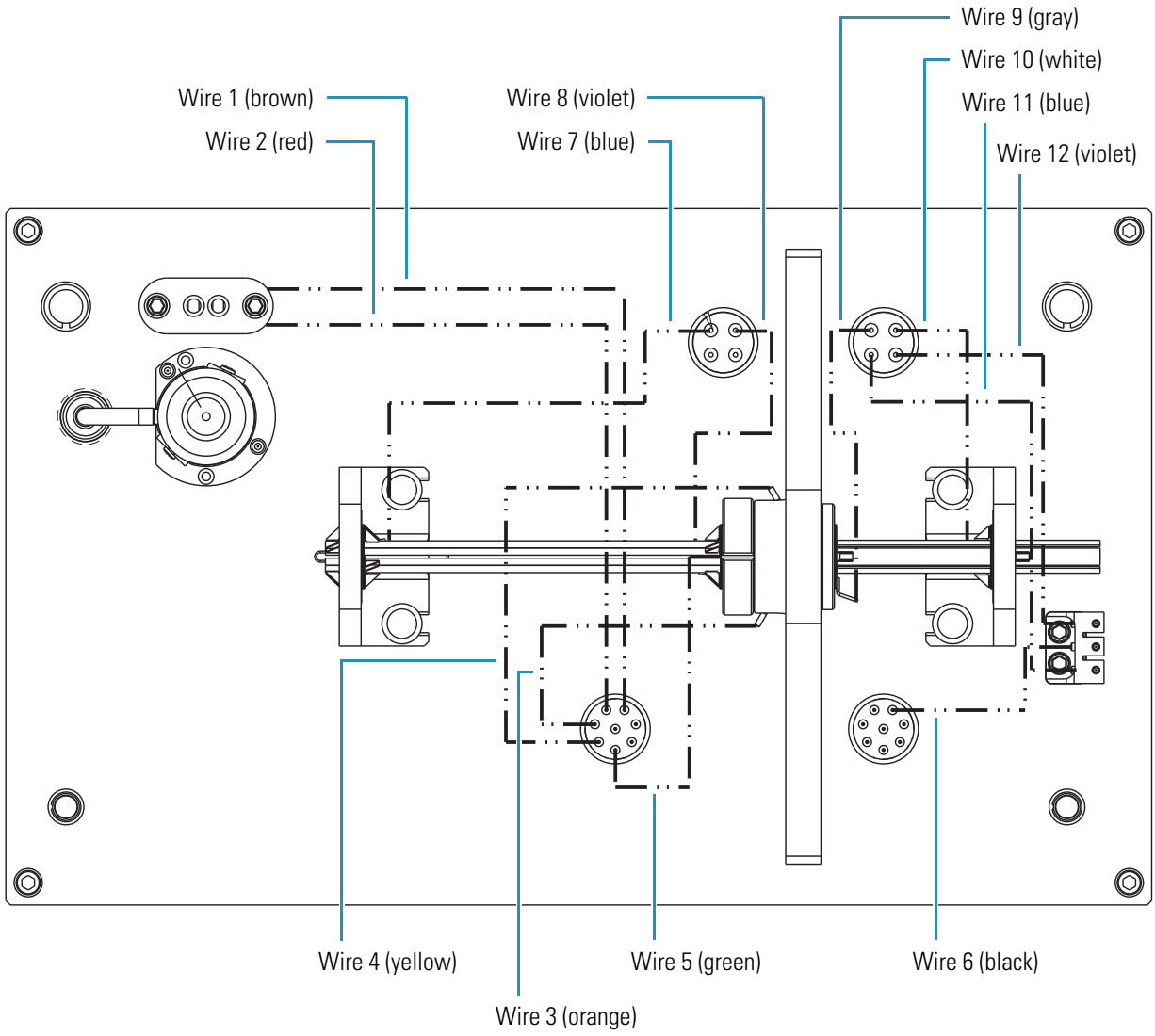


Figure 92. LTQ XL Q0 and Q1 ion guides (wiring diagram)

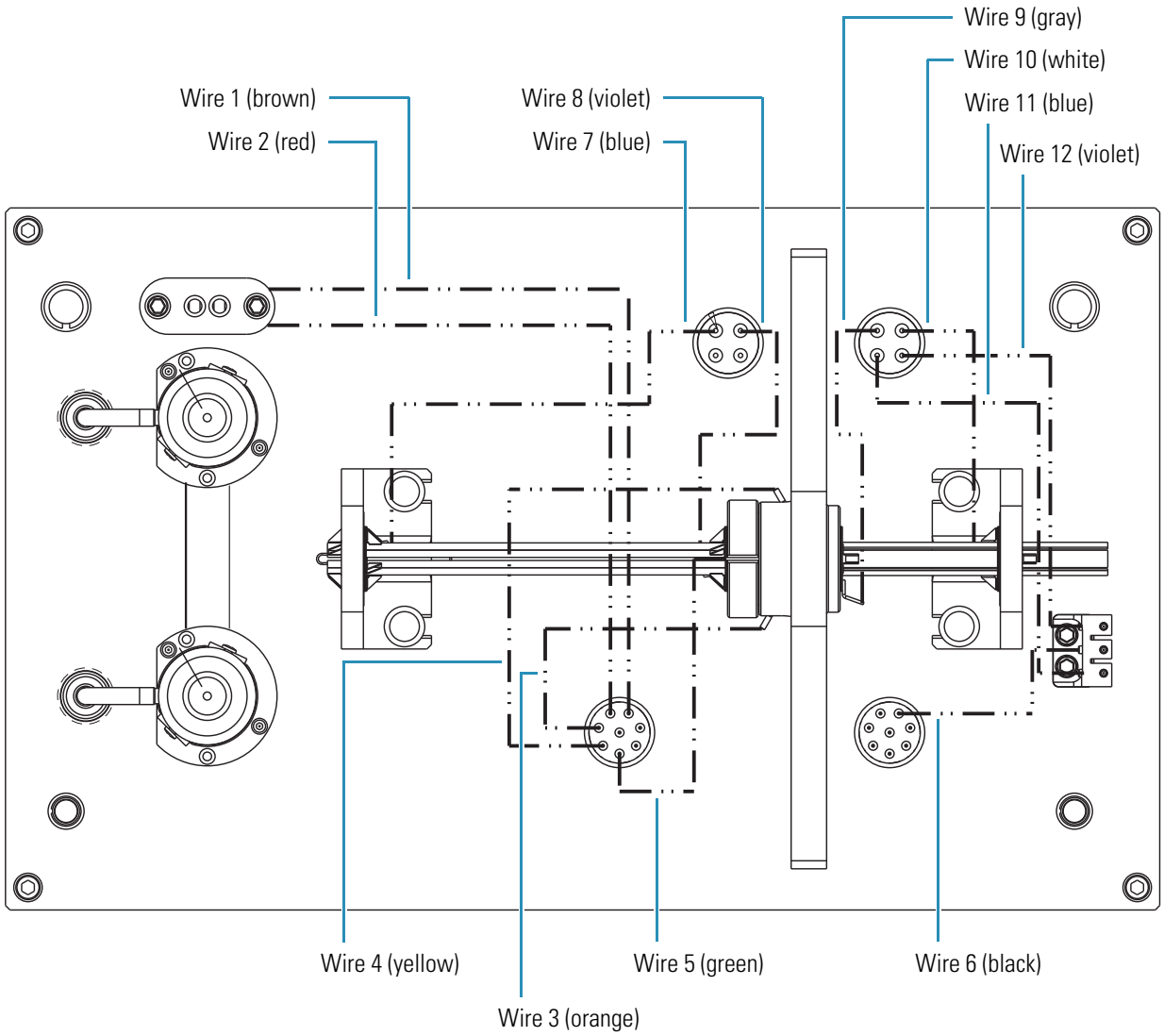
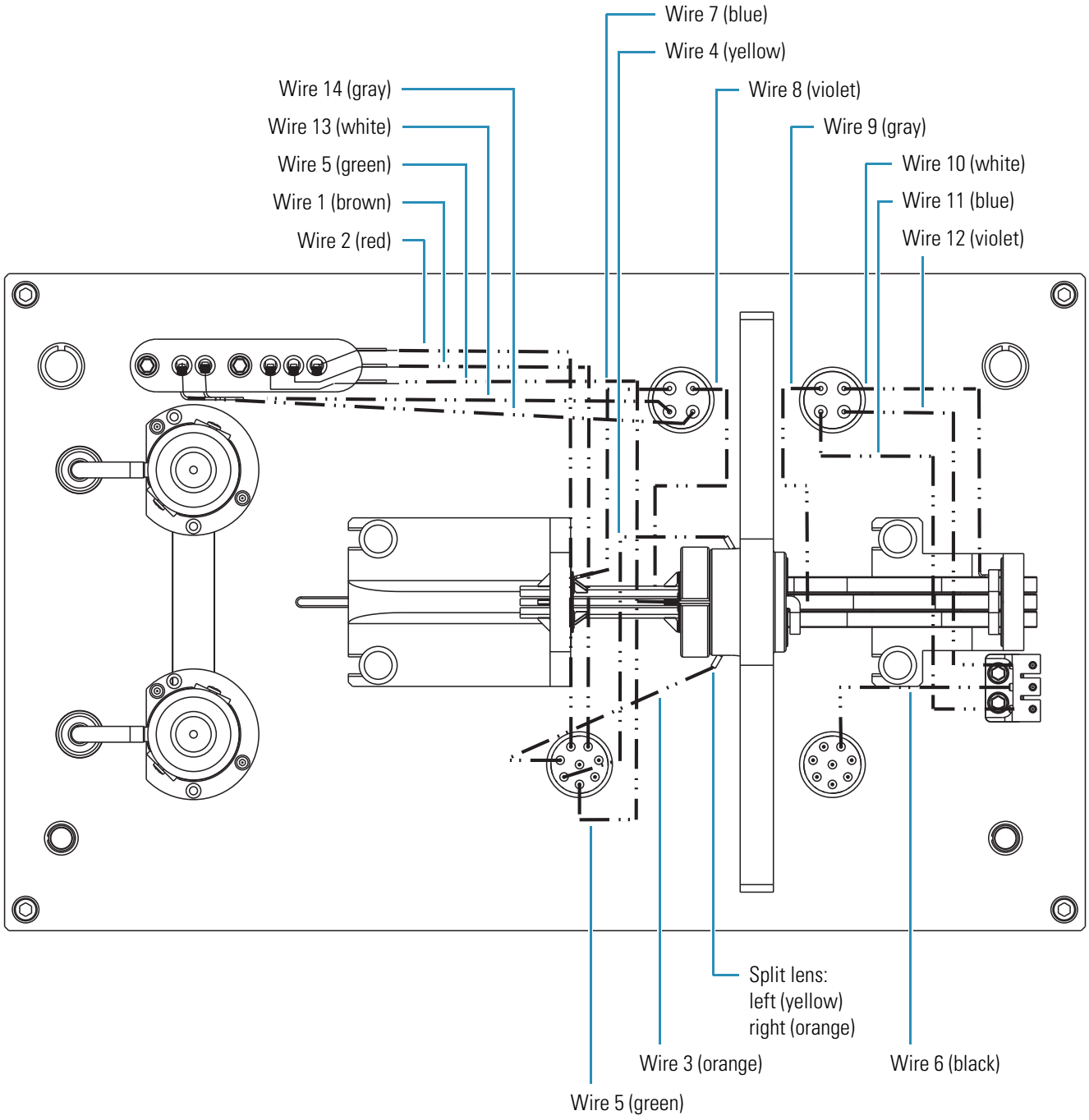


Figure 93. LTQ Velos Q0 and Q1 ion guides (wiring diagram)



Cleaning the Ion Detection System

Keep the conversion dynode and electron multiplier of the ion detection system dust free. Clean the conversion dynodes and electron multipliers by blowing them with clean, dry gas such as nitrogen. However, avoid using Freon gas. Do not use liquids to clean the ion detection system components.

Reinstalling the Top Cover of the Vacuum Manifold

❖ To reinstall the top cover 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 them with a lint-free cloth soaked in HPLC-grade methanol. Use a cotton-tipped applicator soaked in methanol to clean around the inlets and feedthroughs.

3. Carefully lift the top cover plate up by its two handles and turn it over.
4. Orient the top cover plate so that the electron multiplier is over the conversion dynode.
5. Carefully insert the guide posts on the underside of the top cover plate into the guide holes in the vacuum manifold.
6. 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.
7. Ensure that the cover plate is seated properly on the vacuum manifold.
8. Reconnect the three cables to the top cover PCB. See Figure 87 on page 130.
9. Reconnect the electron multiplier, high-voltage coaxial cables that come from the electron multiplier power supply.
10. Reconnect the electrometer cable to the electrometer PCB.

Reinstalling the Top Cover of the Mass Spectrometer

❖ To reinstall the top cover of the mass spectrometer

1. If the front door of the mass spectrometer is not open, use a 1/4 in. hex wrench to loosen the cover latch (Figure 85 on page 128).
2. Place the top cover over the mass spectrometer and slide it forward until it is flush with the front doors (when they are closed).
3. Tighten the two Phillips head captive screws to secure the top cover.

4. Close the front door of mass spectrometer and use a 1/4 in. hex wrench to tighten the cover latch.
5. Reconnect any tubing between the syringe pump and the API source to accommodate your instrument configuration.

Electron Multiplier Replacement

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

You might need to replace one or both of the electron multipliers if either of these symptoms persists:

- Excessive noise in the mass spectrum
- Inability of the multiplier gain calibration procedure to achieve a gain of 4×10^5 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. In the Tune Plus window, choose **Setup > Ion Detection System**.

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

❖ To replace the electron multiplier assembly

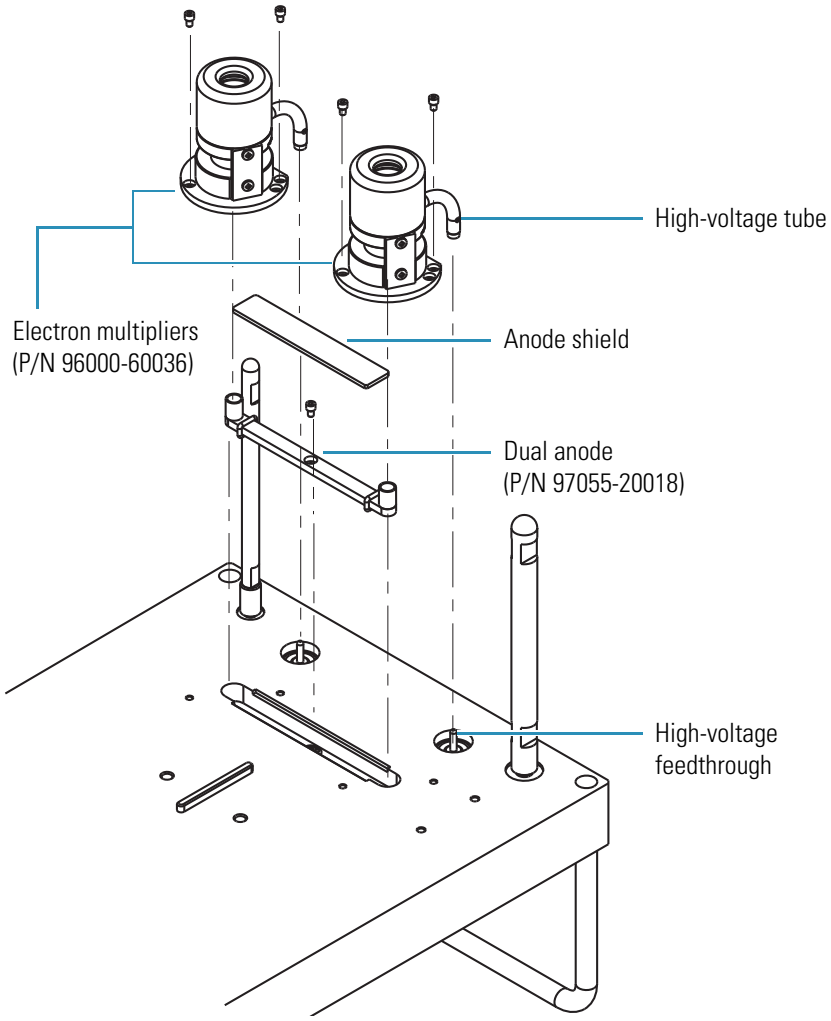
1. Shut down and vent the system according to the instructions in "Shutting Down the Mass Spectrometer Completely" on page 57.

CAUTION Unplug the mass spectrometer's power cord before you proceed.

2. Open the front door of the mass spectrometer by using an Allen wrench to loosen the Allen screw on the right side of the door.
3. Remove the top cover of the mass spectrometer as described in "Removing the Top Cover of the Mass Spectrometer" on page 127.
4. Remove the top cover plate of the vacuum manifold as described in"Removing the Top Cover Plate of the Vacuum Manifold" on page 129.
5. Put on a new pair of lint- and powder-free gloves.

6. With an Allen wrench, remove the two socket-head screws that hold one of the electron multiplier supports to the top cover plate of the vacuum manifold (Figure 94).
7. With one hand, hold the high-voltage tube and with the other hand hold the electron multiplier support.

Figure 94. Electron multipliers and dual anode



8. 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.)
9. Repeat steps 6 and 7 with the second electron multiplier.
10. Remove the anode shield (Figure 94).
11. Loosen the socket-head screw that secures the dual anode. Remove the dual anode from the anode feedthrough.
12. Install a new dual anode (P/N 97055-20018) in the anode feedthrough in the top cover plate. Secure the dual anode with the socket-head screw.

13. Reinstall the anode shield over the dual anode.

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

14. With one hand holding the high-voltage tube and the other 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.
15. Reinstall the two socket-head screws that secure the electron multiplier support to the top cover plate. Tighten the screws with an Allen wrench.
16. Repeat steps 14 and 15 with the second electron multiplier.
17. Reinstall the top cover plate of the vacuum manifold over the opening in the vacuum manifold as described in "Reinstalling the Top Cover of the Mass Spectrometer" on page 140.
18. Reinstall the top cover of the mass spectrometer as described in "Reinstalling the Top Cover of the Mass Spectrometer" on page 140.
19. Start up the LTQ XL system as described in "Starting the System after a Complete Shutdown" on page 58.

❖ To set the electron multiplier voltages

After you replace the electron multiplier you must first set the voltages, then save the settings (), and finally calibrate the electron multiplier voltage ().

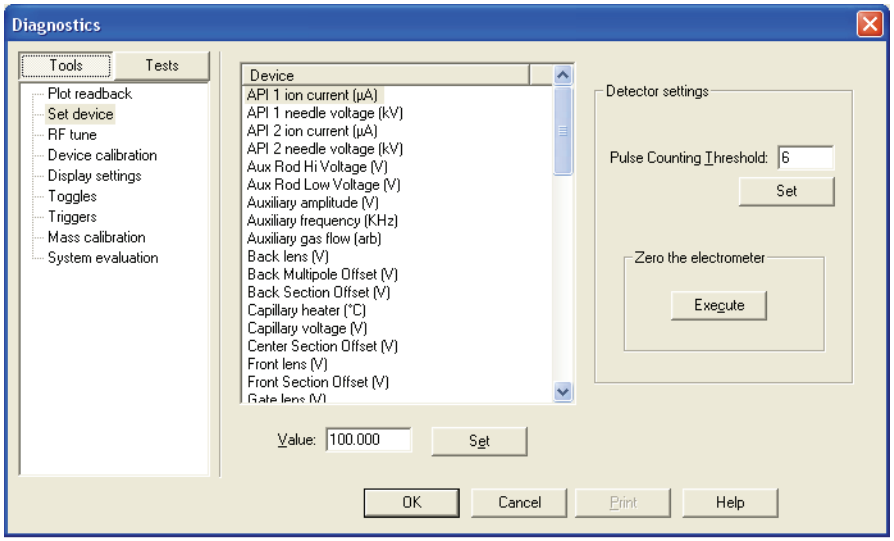
1. On the Windows taskbar, choose **Start > All Programs > Thermo Instruments > LTQ > *model* Tune**.

   Note For LTQ version 2.5.0 or earlier, the path is **Start > All Programs > Xcalibur > *model* Tune**.

2. Choose **Diagnostics > Diagnostics**.

   The Diagnostics dialog box opens (Figure 95 on page 144)

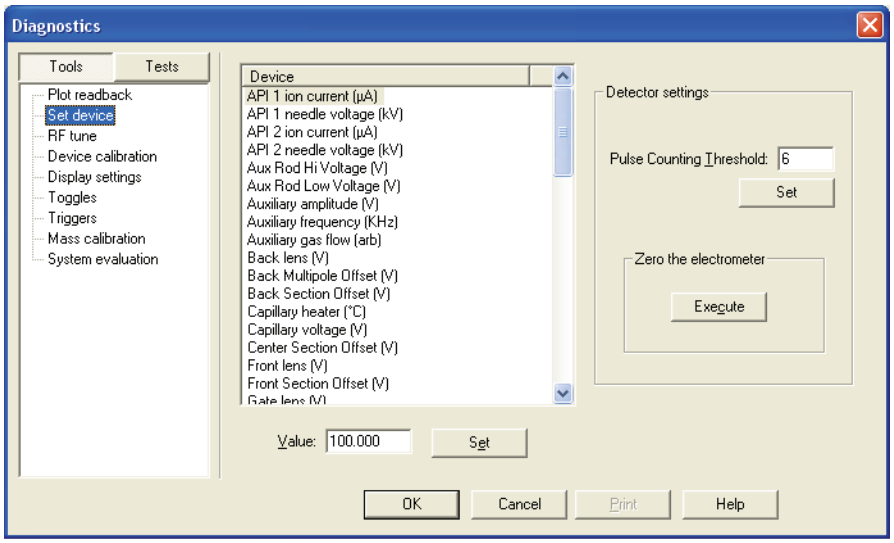
Figure 95. Diagnostics dialog box



3. In the Tools list, select **Set device**.

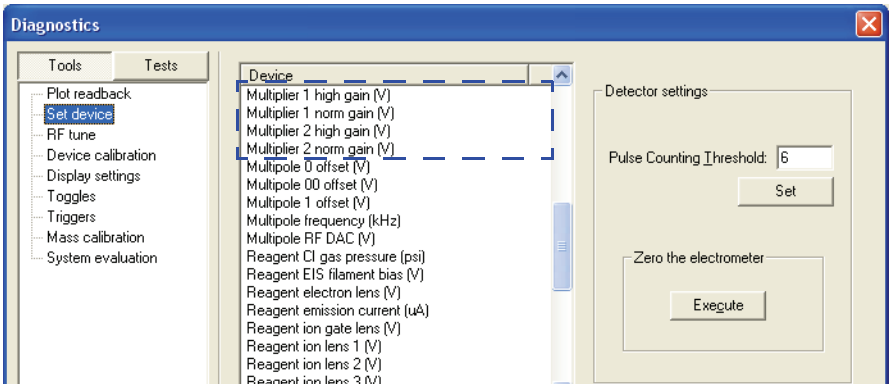
   The Set device list is displayed (Figure 96).

Figure 96. Set device list



4. Scroll the Device list to display the electron multiplier selections (Figure 97 on page 145).

Figure 97. Electron multiplier selections



5. Select **Multiplier 1 high gain (V)**.
6. In Value box below the list, type **-800**.
7. Click **Set**.
8. Select **Multiplier 1 normal gain (V)**.
9. In Value box below the list, type **-800**.
10. Click **Set**.
11. Select **Multiplier 2 high gain (V)**.
12. In Value box below the list, type **-800**.
13. Click **Set**.
14. Select **Multiplier 2 normal gain (V)**.
15. In Value box below the list, type **-800**.
16. Click **Set**.

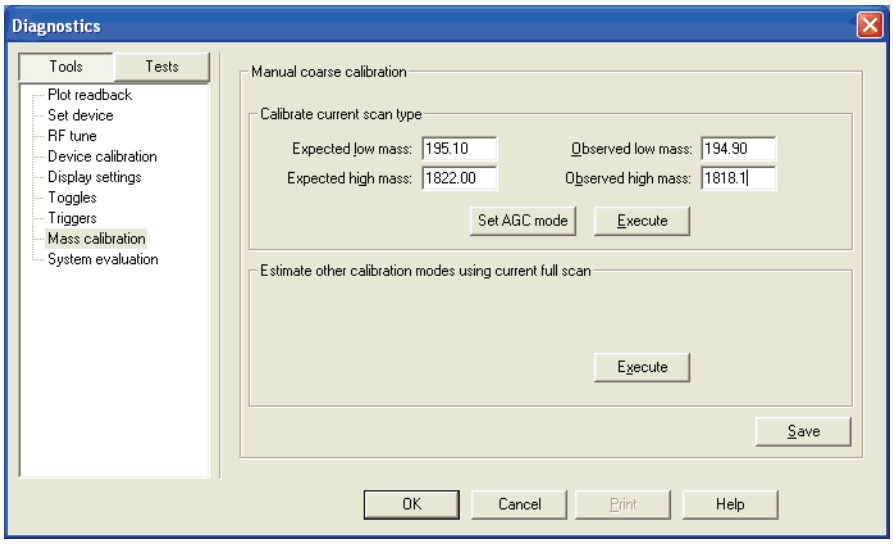
    Go to the next procedure to save the multiplier settings or they are lost when you close the Diagnostics dialog box.

❖ To save the electron multiplier voltage settings

1. In the Diagnostics dialog box, from the Tools list, choose **Mass Calibration**.

   The Mass Calibration dialog box opens (Figure 98 on page 146).

Figure 98. Mass calibration dialog box



2. Click **Save**.
3. Click **OK**.

   To complete the process of changing the electron multipliers, you must calibrate the electron multiplier voltage, as described in the next procedure.

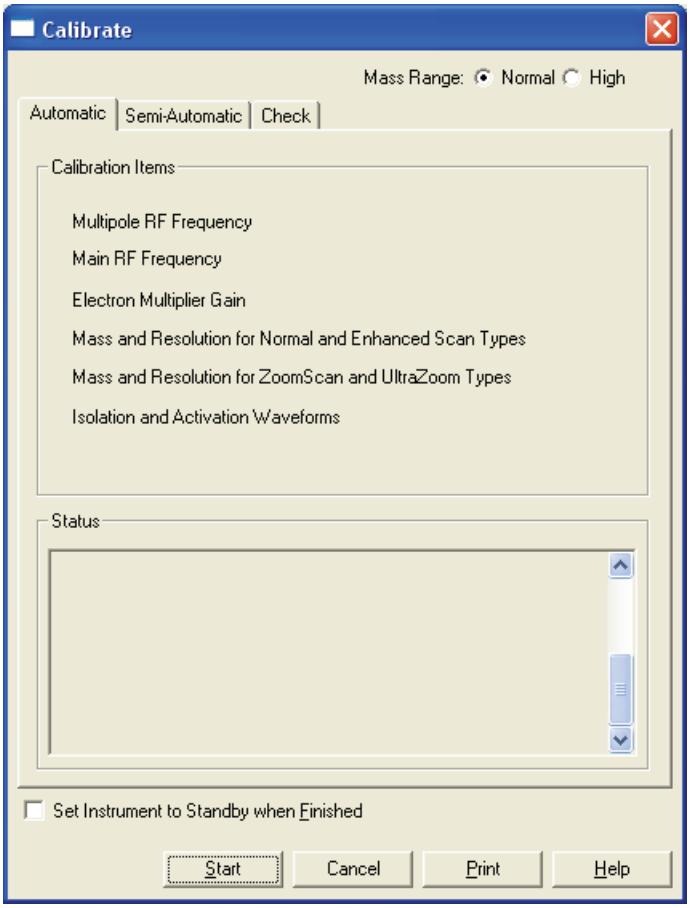
❖ To calibrate the electron multiplier voltage

1. Allow the system to pump down for at least one hour before you turn on the high voltages.
2. Set up for infusing the tuning solution into the mass spectrometer as described in the *LTQ Series Getting Started Guide*.

3. In the Tune Plus window, click the **Calibrate** button.

   The Calibrate dialog box opens with the Automatic page displayed by default (Figure 99 on page 147).

Figure 99. Calibrate dialog box



4. Click the **Semi-Automatic** tab.

   The Semi-Automatic page opens (Figure 100 on page 148 or Figure 101 on page 149) depending on your system.

Figure 100. Semi-Automatic page for LXQ and LTQ XL

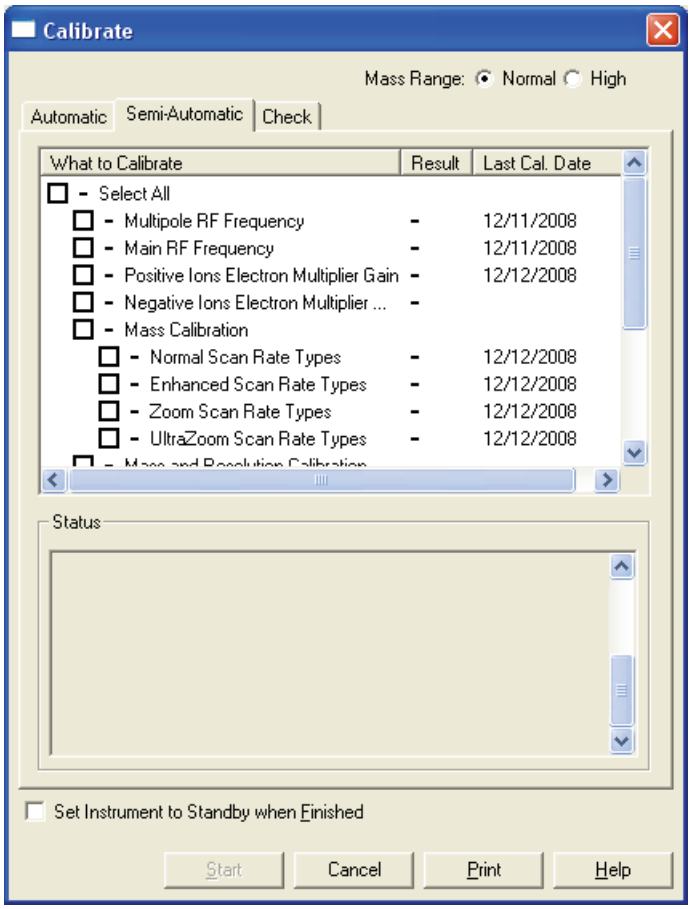
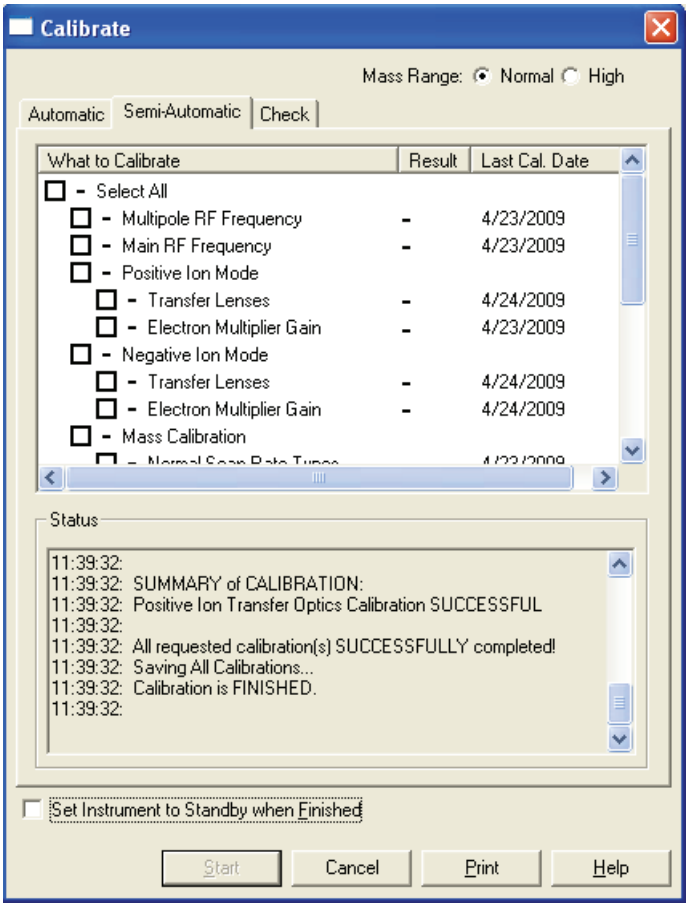


Figure 101. Semi-Automatic page for LTQ Velos



5. Do one of the following:
   a. For the LXQ or LTQ XL, select both the **Positive Ions Electron Multiplier Gain** and **Negative Ions Electron Multiplier Gain** options.
   b. For the LTQ Velos, under both Positive Ion Mode and Negative Ion Mode, select **Electron Multiplier Gain**.
6. Click **Start**.
7. After the electron multiplier gain calibrations are complete, set up for operation as described in the *LTQ Series Getting Started Guide*.

Forepump Maintenance

The forepump or forepumps require minimal maintenance. Inspecting, adding, purging, and changing the pump oil are all that is required to maintain the forepump.

Check the rotary vane pump oil (P/N A0301-15101) often. It is a translucent light amber color. During normal operation, oil must always be visible in the oil level sight glass between the MIN and MAX marks. If the oil level is below the MIN mark, add oil. If the oil is cloudy or discolored, purge the oil to decontaminate dissolved solvents. If the pump oil is still discolored, change it. You should change the pump oil every 3,000 hours (or about every four months) of operation.

Refer to the manufacturer's documentation for procedures for purging, adding, and changing the forepump oil.

Fan Filter Maintenance

Clean the fan filters every four months. The fan filters are located on the back of the mass spectrometer on the left side.

❖ To clean the fan filters

1. Remove the fan filter from the back of the mass spectrometer by pulling it up and out of the fan filter bracket.
2. Wash the fan filters in a solution of soap and water.
3. Rinse the fan filters with tap water.
4. Squeeze the water from the fan filters and allow them to air dry.
5. Reinstall the fan filter in the fan filter bracket.

Diagnostics

The diagnostics test the major electronic circuits within the MS detector and indicate whether the circuits pass or fail the tests. If there is a problem with the instrument electronics, the diagnostics can often locate it.

The 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 improper tuning. For such reasons, only someone who is familiar with system operation and basic hardware theory should run the diagnostics and use them to isolate 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 mass spectrometer, 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.

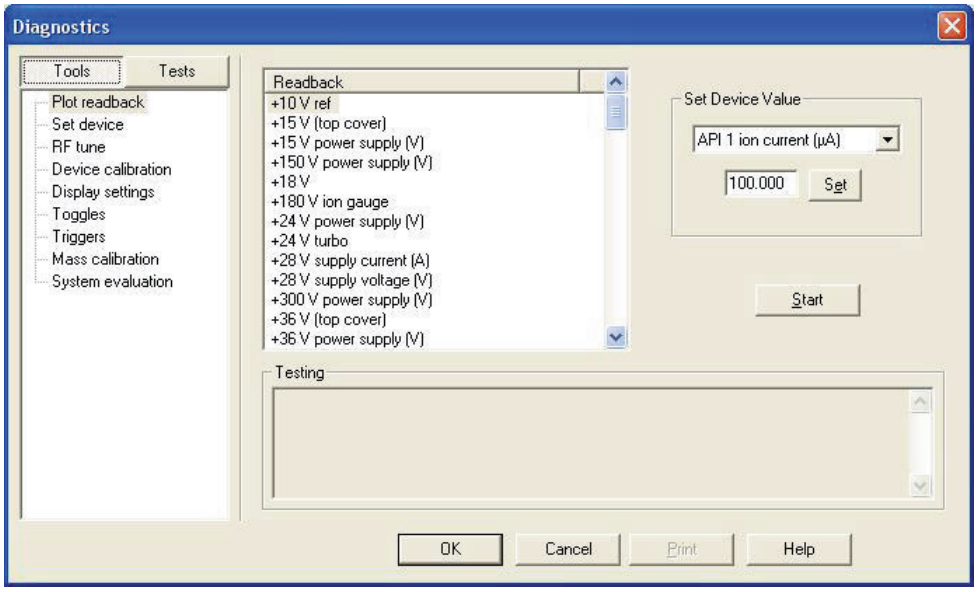
If the answer is yes to one of the last two items above, the problem is probably mechanical, not electrical. Check again that alignment, configurations, and cable connections are correct before you run the diagnostics.

❖ To run the diagnostics

1. In Tune Plus, choose **Diagnostics > Diagnostics**.

   The Diagnostics dialog box opens (Figure 102).

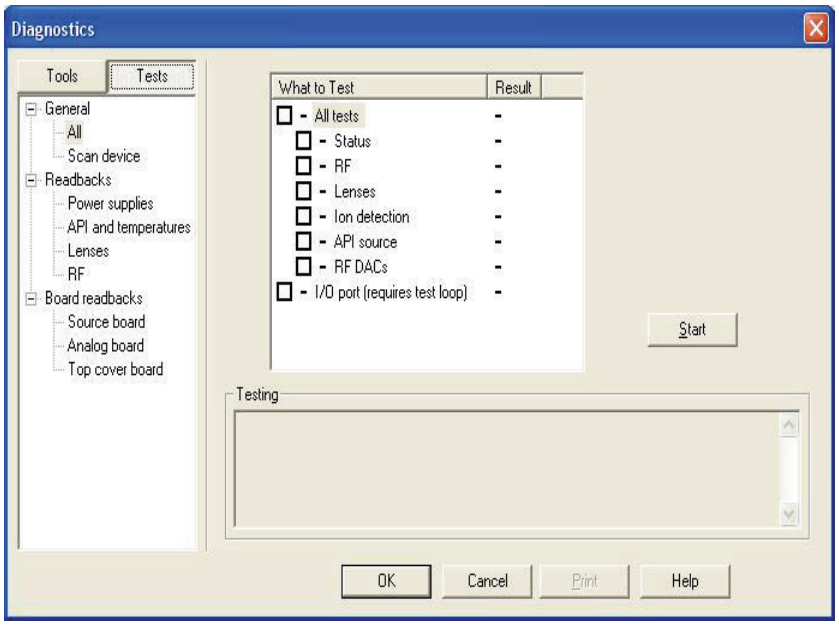
   Figure 102. Diagnostics dialog box



2. Click **Tests**.

   The list of tests is displayed (Figure 103).

   Figure 103. Diagnostic tests list



3. Select one of the following options:

   - To test all of the electronic subsystems (that is, the vacuum system, power supplies, lenses, ion detection system, and rf voltage electronics), under General, click **All** and under What to Test, select the **All Tests** check box.
   - To test an individual subsystem, click the item corresponding to that subsystem and select the appropriate options.

4. Select how many times you want to run the tests, and whether or not you want to print reports or to stop on a failure.

5. Click **Start**.

   Testing starts and a chronological log of all diagnostic tests is displayed in the Testing text box. After testing for a specific subsystem is completed, either Pass or Fail is displayed in the Result column. If the diagnostics indicates a problem, perform the maintenance procedure indicated. For more information on the diagnostics, see the online Help.

Replaceable Parts

Contents

Accessory Kits

Note Accessory kits for the ETD module and MALDI source are listed in their respective Getting Started guides.

Table 11 lists the mass spectrometer accessory kits.

Table 11. Accessory kits

Model	Vacuum hose accessory kit	Special accessory kit
LXQ	97055-60135	97055-62045
LTQ XL	97055-62007	97055-62044
LTQ Velos	97455-62007	97055-62044

Ion Source Probes and Parts

Table 12 lists the part numbers for the ion source probes and components of the ion source, and Table 13 lists the part numbers for the HESI-II probe metal needle kits.

Table 12. ESI, APCI, HESI-II, and probes and parts

Description	Part number
ESI Probe Kit	OPTON-20011
Safety Sleeve Kit	70005-62015
Stainless Steel Needle Kit, 32 gauge	OPTON-53003
Stainless Steel Needle Kit, 34 gauge	OPTON-30004
APCI Probe Kit	OPTON-20012
APCI Probe Nozzle Assembly	97055-60089
HESI-II Probe Kit (see Table 13 for needle kits)	OPTON-20037
High-flow Needle Insert Assembly	OPTON-53010
Low-flow Needle Insert Assembly	OPTON-53011

Table 13. HESI-II probe metal needle kits

Description	Metal needle	Ferrule	Flow rate range	Part number
32-gauge needle insert, HESI-II probe	0.004-in. ID 0.009-in. OD	0.4 mm thru-hole	5 to 2000 µL/min	70005-60155 OPTON-53010
34-gauge needle insert, HESI-II probe	0.003-in. ID 0.007-in. OD	0.2 mm thru-hole	1 to 10 µL/min	70005-60180 OPTON-53011

Ion Source Interface Parts

Table 14 lists the ion source interface parts for the LXQ, LTQ XL, and LTQ Velos mass spectrometers.

Table 14. Ion source interface parts (Sheet 1 of 2)

System	Description	Part number
LXQ	Ion source interface assembly	97055-60181
	Tube lens	97055-20463
	Skimmer	97055-20516
	Ion transfer capillary	97055-20517

Table 14. Ion source interface parts (Sheet 2 of 2)

System	Description	Part number
LTQ XL	Ion source interface assembly	97055-60040
	Tube lens	97055-20251
	Skimmer	97055-20253
	Ion transfer capillary	97055-20198
LTQ Velos	Ion source interface assembly	70005-60187
	Exit lens	70005-20419
	S-lens	70005-60182
	Ion transfer capillary	70005-20606
All	O-ring, 2-033 Viton V884 (2 × 1/16)	00107-01-00006
	O-ring, 2.625 ID x 3/32, AS-146, Viton	00107-11002
	O-ring, 2-74 × 0.063, 2-039, Viton	00107-12550
	O-ring, 0.030 ID x 0.054, graphite, Vespel™	97055-20442

Q00 rf Lens Parts

Table 15 lists the Q00 rf lens parts for the LXQ, LTQ XL, and LTQ Velos mass spectrometers. l

Table 15. Q00 rf lens parts

Description	Part number
Outer cage assembly (LXQ)	97055-60180
Outer cage assembly (LTQ XL and LTQ Velos)	97055-60036
O-ring, 0.101 ID × 0.070, Viton (all)	00107-02456
O-ring, 2-148, Viton 884 (all)	00107-15542

Q0 and Q1 Ion Guide Parts

LXQ and LTQ XL

The LXQ and LTQ XL Q0and Q1 ion guide parts are listed in Table 16. The LXQ assembly is shown in Figure 104 on page 159 and the LTQ XL assembly is shown in Figure 105 on page 160.

Table 16. LXQ and LTQ XL ion guide parts

Description	Part number
Thumbscrews, 10-32	97000-20235
Lens L1	97055-20022
Gate lens	97055-20482 (LXQ) 97055-20023 (LTQ XL)
Multipole bracket	97055-20054
Q1 octapole	97055-60034
Q0 quadrupole	97055-60035

Figure 104. LXQ Q0 and Q1 ion guide parts

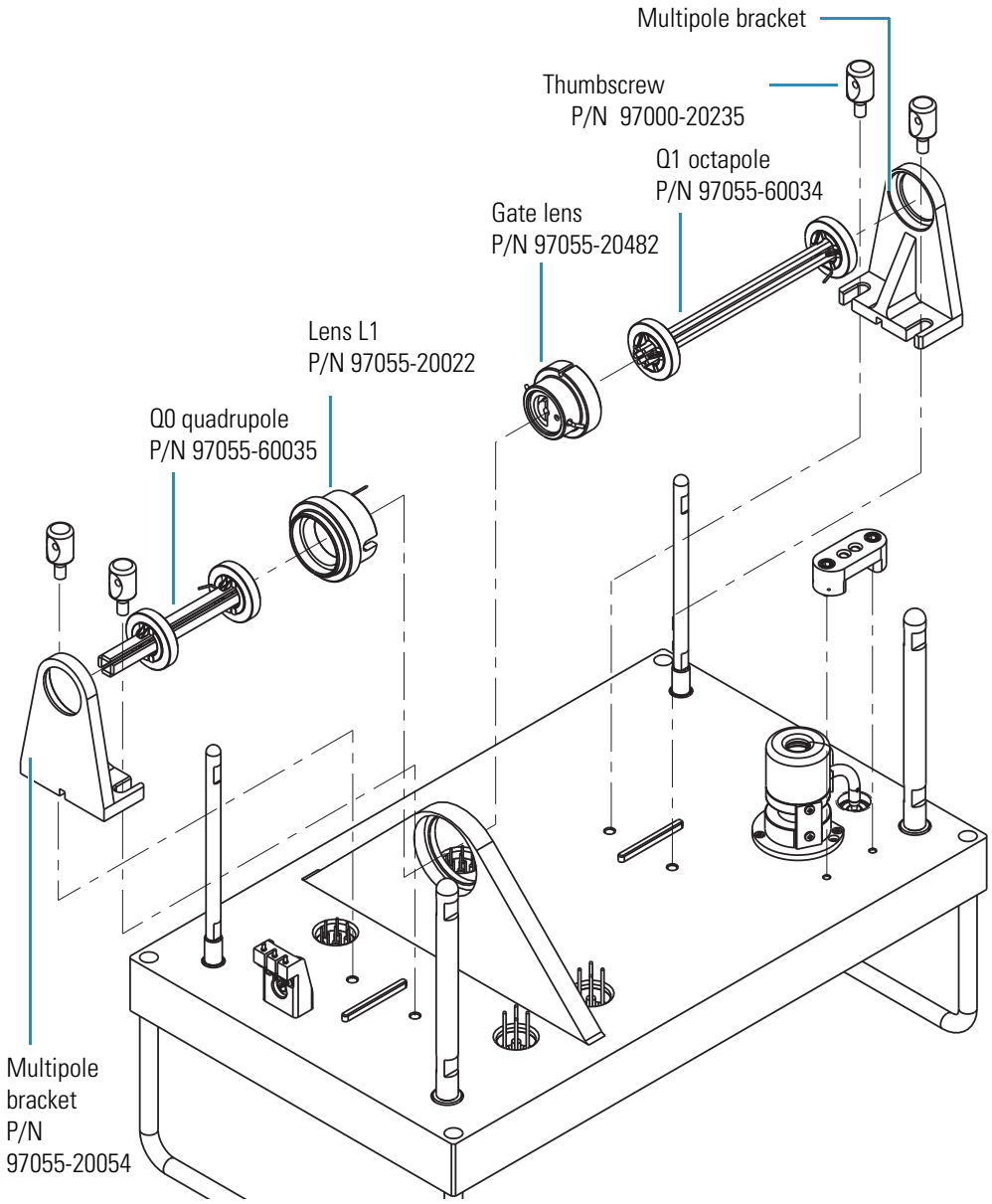
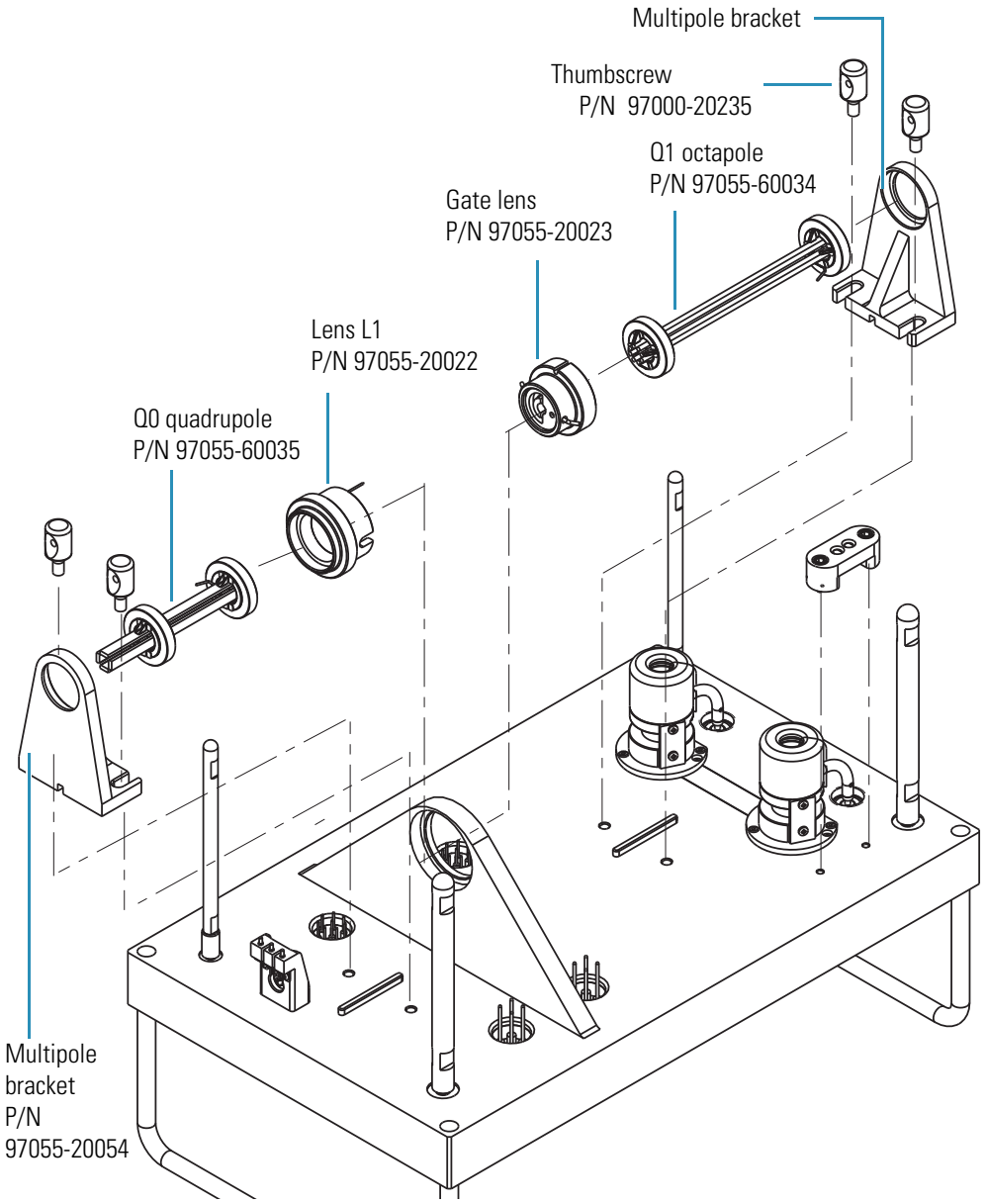


Figure 105. LTQ XL Q0 and Q1 ion guide parts



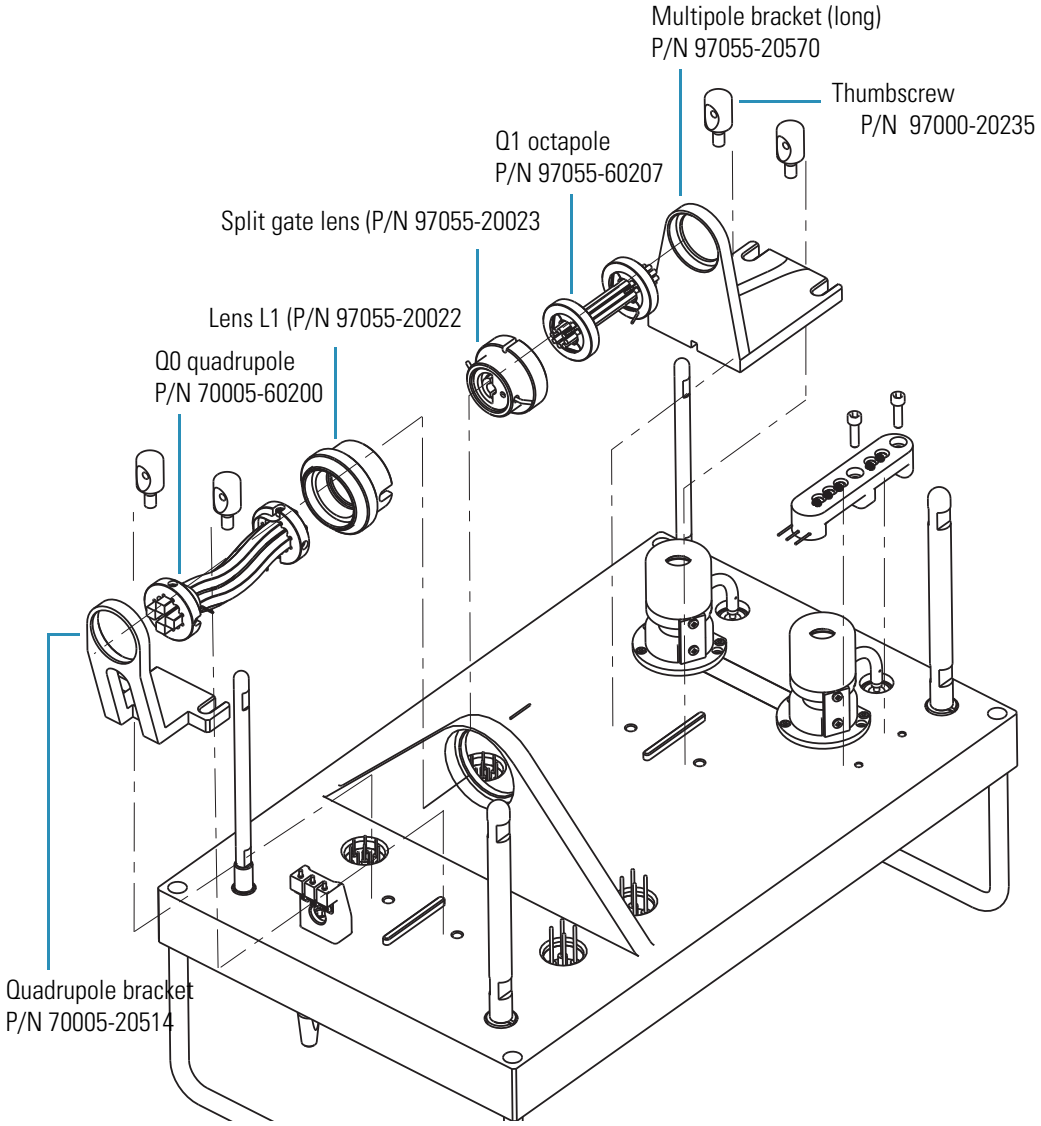
LTQ Velos

The LTQ Velos Q0 and Q1 ion guide parts are listed in Table 17 and shown in Figure 106 on page 162.

Table 17. LTQ Velos ion guide parts

Description	Part number
Thumbscrews, 10-32	97000-20235
Lens L1	97055-20022
Split gate lens	97055-20023
Multipole bracket (long)	97055-20570
Q1 octapole	97055-60207
Q0 quadrupole	70005-60200
Quadrupole bracket	70005-20514

Figure 106. LTQ Velos Q0 and Q1 ion guide parts



Electron Multipliers

All systems use the same electron multiplier assembly (P/N 96000-60036). LXQ uses a single anode (P/N 97055-20342); LTQ XL and LTQ Velos use a dual anode (P/N 97055-20018).

Stainless Steel Sample Loops

Table 18 lists the part numbers for the stainless steel sample loops.

Table 18. Stainless steel sample loops

Type	Part number
5 µL	001100-22010
10 µL	00110-22012
20 µL	00110-22014
50 µL	00110-22016
100 µL	00110-22018
500 µL	00110-22020
1 mL	00110-22022

Chemical Kit

All mass spectrometers use the chemical kit P/N 97455-62045

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