

TSQ Series

Hardware Manual

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DOCUMENTATION
SURVEY

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Software version: Xcalibur 2.1, TSQ 2.1

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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 below.

Changes that you make to your system might 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.

- [TSQ Quantum Access MAX](#)
- [TSQ Quantum Ultra](#)
- [TSQ Vantage](#)
- [TSQ Quantum Access](#)

TSQ Quantum Access MAX

EMC Directive 2004/108/EEC

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

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

FCC Class A: CFR 47 Part 15: 2007

Low Voltage Safety Compliance

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



TSQ Quantum Ultra

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

EMC compliance has been evaluated by Underwriters Laboratories Inc.

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

Low Voltage Safety Compliance

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

TSQ Vantage

EMC Directive 2004/108/EC

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

EN 55011: 1998, A1: 1999, A2: 2002	EN 61000-4-4: 2004
EN 61000-3-2: 2006	EN 61000-4-5: 2006
EN 61000-3-3: 1995, A1: 2001, A2: 2005	EN 61000-4-6: 2001
EN 61000-4-2: 2001	EN 61000-4-11: 2004
EN 61000-4-3: 2006	EN 61326-1: 2006

FCC Class A, CFR 47 Part 15: 2007	CISPR 11: 1999, A1: 1999, A2: 2002
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Low Voltage Safety Compliance

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

TSQ Quantum Access

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

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

EN 55011: 1998, A1: 1999, A2: 2002

EN 61000-4-4: 1995, A1: 2000, A2: 2001

EN 61000-3-2: 2000

EN 61000-4-5: 2001

EN 61000-3-3: 1995, A1: 2001

EN 61000-4-6: 2003

EN 61000-4-2: 2001

EN 61000-4-11: 2001

EN 61000-4-3: 2002

EN 61326: 1997, A1: 1998, A2: 2001, A3: 2003

FCC Class A, CFR 47 Part 15: 2005

CISPR 11: 1999, A1: 1999, A2: 2002

Low Voltage Safety Compliance

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

FCC Compliance Statement

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

Notice on Lifting and Handling of Thermo Scientific Instruments



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.

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.



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.

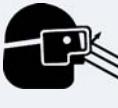
Conformité DEEE

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 Schutzbdeckung 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 éliminer 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 deberá apagarse y desconectarse de la línea de alimentación eléctrica. No opere el instrumento sin sus cubiertas exteriores quitadas. No remueva las cubiertas protectoras de las tarjetas de circuito impreso.	Shock da folgorazione. L'apparecchio è alimentato da corrente ad alta tensione che può provocare lesioni fisiche. Prima di effettuare qualsiasi intervento di manutenzione occorre spegnere ed isolare l'apparecchio dalla linea elettrica. Non attivare lo strumento senza lo schermo superiore. Non togliere i coperchi a protezione dalle schede di circuito stampato (PCB).
	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, cancérogènes, mutagènes, ou corrosifs/irritants. Utilisez des récipients et des procédures homologuées pour se débarrasser des déchets d'huile.	Química: El instrumento puede contener productos químicos peligrosos. Utilice guantes al manejar productos químicos tóxicos, carcinogénicos, mutagénicos 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 Température: Permettre aux composants chauffés de refroidir avant tout intervention.	Altas temperaturas: Permita que los componentes se enfrien, ante de efectuar servicio de mantenimiento.	Calore. Attendere che i componenti riscaldati si raffreddino prima di effettuare l'intervento di manutenzione.
	Fire: Use care when operating the system in the presence of flammable gases.	Feuer: Beachten Sie die einschlägigen Vorsichtsmaßnahmen, 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 salpicaduras de productos químicos o partículas que salten bruscamente pueden causar lesiones en los ojos. Utilice anteojos protectores al manipular productos químicos o al darle servicio 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 außerdem 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 categorías anteriores. Este símbolo también se utiliza en el instrumento para 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'un procédé 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 Técnica 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 Técnica 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.	電擊：この計測器は高電圧を使用し、人体に危害を与える可能性があります。保守・修理は、必ず操作を停止し、電源を切ってから実施して下さい。上部カバーを外したまま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考して下さい。	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ルサポートセンターご連絡ください。	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	xv
About This Guide	xv
Related Documentation	xv
Safety and Special Notices	xv
Safety Precautions	xvi
Solvent and Gas Purity Requirements	xvii
Service Philosophy	xvii
Level of Repair	xviii
Contacting Us	xviii
 Chapter 1 Introduction	 1
Ionization Modes	3
Ion Polarity Modes	3
Scan Modes	3
Q1MS and Q3MS Scan Modes	5
Product Scan Mode	5
Parent Scan Mode	6
Neutral Loss Scan Modes	7
Data Dependent Scan Mode	9
Scan Types	10
Full Scan	10
Selected Ion Monitoring	10
Selected Reaction Monitoring	11
AutoSIM	11
Data Types	11
Profile Data Type	11
Centroid Data Type	12
Mass/Charge Range	12
 Chapter 2 Functional Description.....	 13
Autosampler	14
Liquid Chromatograph	15
Syringe Pump	15
Divert/Inject Valve	16

Mass Spectrometer	18
Controls and Indicators	19
API Source	22
Ion Source Interface	22
Ion Optics	24
Mass Analyzer	28
Ion Detection System	35
Vacuum System and Inlet Gases Hardware	36
Electronic Assemblies	42
Data System	44
Computer Hardware	44
Data System / Mass Spectrometer / LC Interface	45
Data System / Local Area Network Interface	45
Printer	45
Chapter 3 System Shutdown, Startup, and Reset	47
Shutting Down the System in an Emergency	47
Placing the System in Standby Condition	49
Shutting Down the System Completely	50
Starting Up the System after a Complete Shutdown	52
Starting Up the LC	52
Starting Up the Data System	52
Starting Up the Mass Spectrometer	52
Starting Up the Autosampler	53
Setting Up Conditions for Operation	54
Resetting the Mass Spectrometer	55
Resetting the Data System	55
Resetting the Data System by Using the Windows Shutdown and Restart Procedure	56
Resetting the Data System by Turning the Personal Computer Off Then On	56
Turning Off Selected Mass Spectrometer Components	57
Chapter 4 Daily Operation	61
Things to Do Before Operating the TSQ System	61
Checking the Argon and Nitrogen Supplies	62
Checking the ESI Fused-Silica Sample Tube for Elongation	62
Checking the System Vacuum Levels	62
Things to Do After Operating the TSQ System	64
Flushing the Sample Transfer Line, Sample Tube, and API Probe	64
Placing the System in Standby Condition	65
Cleaning the Ion Sweep Cone and Ion Transfer Tube	66
Emptying the Solvent Waste Bottle	66

Chapter 5	Removing and Reinstalling the Ion Source Housing	67
	Removing the Ion Max or Ion Max-S Ion Source Housing	67
	Installing the Ion Max or Ion Max-S Ion Source Housing	69
	Ion Max and Ion Max-S Housing Maintenance	71
Chapter 6	Maintenance	73
	Frequency of Cleaning	75
	Maintaining the Ion Sweep Cone and Ion Transfer Tube	76
	Removing and Cleaning the Ion Transfer Tube	76
	Maintaining the Ion Source Interface Assembly	82
	Shutting Down and Venting the System	82
	Removing the Ion Max or Ion Max-S Ion Source Housing	82
	Removing the Ion Source Interface	83
	Removing the S-Lens and Exit Lens (TSQ Vantage)	84
	Cleaning the S-Lens and Exit Lens (TSQ Vantage)	85
	Removing the Tube Lens and Skimmer (TSQ Quantum Access, TSQ Quantum Access MAX, or TSQ Quantum Ultra)	85
	Cleaning the Tube Lens and Skimmer (TSQ Quantum Access, TSQ Quantum Access MAX, or TSQ Quantum Ultra)	86
	Reinstalling the S-Lens and Exit Lens (TSQ Vantage)	87
	Reinstalling the Tube Lens and Skimmer (TSQ Quantum Access, TSQ Quantum Access MAX, or TSQ Quantum Ultra)	87
	Reinstalling the Ion Source Interface Assembly	88
	Reinstalling the Ion Max or Ion Max-S Ion Source Housing	88
	Starting Up the System	88
	Cleaning the Q00 Ion Optics	89
	Shutting Down and Venting the System	89
	Removing the Ion Max or Ion Max-S Ion Source Housing	89
	Removing the Ion Source Interface Assembly	89
	Removing the Ion Optics Cage Assembly	90
	Disassembling the Ion Optics Cage Assembly	94
	Cleaning Q00 and L0	95
	Reassembling the Ion Optics Cage Assembly	96
	Reinstalling the Ion Optics Cage Assembly	97
	Reinstalling the Ion Source Interface Assembly	98
	Reinstalling the Ion Max or Ion Max-S Ion Source Housing	98
	Starting Up the System	98
	Maintaining the Forepump	99
	Cleaning the Fan Filters	99
Chapter 7	Diagnostics and PCB and Assembly Replacement	101
	Running the TSQ System Diagnostics	102
	Replacing a Fuse	103
	Replacing PCBs and Power Supplies	103

Chapter 8	Replaceable Parts	105
MS Accessory Kit	105	
TSQ Vantage Instrument Specific Accessory Kit	106	
TSQ Quantum Ultra, Ultra AM, and Ultra EMR Instrument Specific Accessory Kit	106	
HESI-II Probe Kit	107	
TSQ Quantum Access Instrument Specific Accessory Kit	107	
TSQ Accurate Mass Calibration Compounds Kit	107	
Fittings, Ferrules, and Sample Loops	107	
Index		109

Preface

About This Guide

This *TSQ Series Hardware Manual* contains a description of the modes of operation and principle hardware components of your TSQ system. In addition, this manual provides step-by-step instructions for cleaning and maintaining your mass spectrometer.

Related Documentation

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

- *Preinstallation Requirements Guide*
- *Getting Connected Guide*
- *Getting Started Guide*
- *H-ESI Probe User Guide*
- *HESI-II Probe User Guide*
- *Ion Max and Ion Max-S API Source Hardware Manual*
- Help available from within the software

Safety and Special Notices

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

Safety and special notices include the following:



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

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

Note Highlights information of general interest.

Tip Highlights helpful information that can make a task easier.

Safety Precautions

Observe the following safety precautions when you operate or perform service on the mass spectrometer.



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



CAUTION Shut Down the Mass Spectrometer and Disconnect It From Line Power

Before You Service It. High voltages capable of causing personal injury are used in the instrument. Some maintenance procedures require that the mass spectrometer be shut down and disconnected from line power before service is performed. Do not operate the mass spectrometer with the top or side covers off. Do not remove protective covers from PCBs.



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



CAUTION Place the Mass Spectrometer in Standby (or Off) Before You Open the Atmospheric Pressure Ionization (API) Source. The presence of atmospheric oxygen in the API source when the mass spectrometer is On could be unsafe. (The TSQ automatically turns the mass spectrometer Off when you open the API source; however, it is best to take this added precaution.)



CAUTION Provide and Adequate Fume Exhaust System. It is your responsibility to provide an adequate fume exhaust system. Samples and solvents that are introduced into the TSQ mass spectrometer will eventually be exhausted from the forepump. Therefore, the forepump should be connected to a fume exhaust system. Consult local regulations for the proper method of exhausting the fumes from your system.



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

Solvent and Gas Purity Requirements

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

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

Solvent source	Telephone number
Fisher Global Chemicals	Tel: (800) 766-7000
Mallinckrodt/Baker, Inc.	Tel: (800) 582-2537 Fax: (908) 859-9370
Burdick & Jackson, Inc.	Tel: (800) 368-0050 Fax: (616) 725-6216

The TSQ mass spectrometer uses argon as a collision gas. The argon must be high purity (99.995%). The required gas pressure is 135 ± 70 kPa (20 ± 10 psig). Thermo Fisher Scientific has found that particulate filters are often contaminated and are therefore not recommended.

Service Philosophy

Servicing the TSQ system consists of performing procedures required to maintain system performance standards, prevent system failure, restore the system to an operating condition, or all of the above. Routine and preventive maintenance procedures are documented in this manual.

The user is responsible for routine and preventive maintenance during and after the warranty period. Regular maintenance increases the life of the system, maximizes the up-time of your system, and allows you to achieve optimum system performance.

Only a Thermo Fisher Scientific customer support engineer can perform services not described in this manual.

Level of Repair

Thermo Fisher Scientific's service philosophy for the TSQ system calls for troubleshooting to the lowest part, assembly, or module listed in [Chapter 8, "Replaceable Parts."](#)

For mechanical failures: A mechanical assembly typically is to be repaired to the level of the smallest item listed in [Chapter 8, "Replaceable Parts."](#)

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

- Complete a brief survey about this document by clicking the link below. Thank you in advance for your help.



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

Introduction

TSQ™ Series mass spectrometers are members of the Thermo Scientific family of mass spectrometers. The TSQ Series mass spectrometer is an advanced analytical instrument that includes a syringe pump, a divert/inject valve, a mass spectrometer, and the Xcalibur™ data system.

Contents

- [Ionization Modes](#)
- [Ion Polarity Modes](#)
- [Scan Modes](#)
- [Scan Types](#)
- [Data Types](#)
- [Mass/Charge Range](#)

In a typical analysis, a sample can be introduced in the following ways:

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

In a typical analysis, a liquid chromatograph (LC) introduces a sample. The LC separates the sample into its various components. The components elute from the LC and pass into the mass spectrometer where they are analyzed.

Analysis by direct infusion or flow injection provides no chromatographic separation of components in the sample before they pass into the mass spectrometer. The data from the mass spectrometer is then stored and processed by the data system.

The TSQ mass spectrometer consists of an atmospheric pressure ionization (API) source, ion optics, triple-stage mass analyzer, and ion detection system. A vacuum manifold encloses the ion optics, mass analyzer, ion detection system, and part of the API source. Ionization of the sample takes place in the API source. The specific process used to ionize the sample is known as the ionization mode. The ion optics transmit the ions produced in the ion source into the mass analyzer, where they are separated according to their mass-to-charge ratio. The polarity

of the potentials applied to the lenses in the ion source and ion optics determines whether they transmit positively charged ions or negatively charged ions to the mass analyzer. You can configure the TSQ mass spectrometer to analyze positively or negatively charged ions (called the positive or negative ion polarity mode).

The TSQ instrument's triple-stage mass analyzer performs either one or two stages of mass analysis:

- The TSQ system is operated as a conventional mass spectrometer with one stage of mass analysis. The ion source ionizes the sample and the ion products are subjected to mass analysis in the first rod assembly. The second and third rod assemblies transmit the resulting mass-selected ions to the ion detection system.¹
- The TSQ system is operated as a tandem mass spectrometer with two stages of mass analysis. The ion source ionizes the sample and the ion products are mass analyzed by the first rod assembly. In this case, however, mass-selected ions exiting the first rod assembly collide with an inert gas in the second rod assembly and fragment to produce a set of ions known as product ions. (A chamber called the collision cell surrounds the second rod assembly. The collision cell can be pressurized with an inert gas.) The product ions undergo further mass analysis in the third rod assembly to detect selected ions. Two stages of mass analysis yield far greater chemical specificity than a single stage can achieve, because of the system's ability to select and determine two discrete but directly related sets of masses.

In a first stage of mass analysis the TSQ systems can be used to elucidate the structures of pure organic compounds and the structures of the components within mixtures. Furthermore, in a second stage of mass analysis, the mass spectrometer can fragment and separate each ionic fragment of a molecule formed in the ion source to build up an entire structure for the molecule, piece by piece. Thus, TSQ systems make investigating all pathways for the formation and fragmentation of each ion in the mass spectrum possible.

The two stages of mass analysis, with resultant reduction of chemical noise in the final mass spectrum, allow for very selective and sensitive analysis.

Each sequence of single- or triple-stage mass analysis of the ions is called a scan. The TSQ mass spectrometer uses several different scan modes and different scan types to filter, fragment, or transmit ions in the mass analyzer. Along with the ionization and ion polarity modes, the ability to vary the scan mode and scan type affords the user great flexibility in the instrumentation for solving complex analytical problems.

¹ The instrument can also be used as a single-stage mass spectrometer by transmitting the ions through the first and second rod assemblies followed by mass analysis in the third rod assembly.

Ionization Modes

The atmospheric pressure ionization (API) source forms gas phase sample ions from sample molecules that elute from the LC or are introduced by the syringe pump. You can operate the API source in the electrospray ionization (ESI) mode or, optionally, the heated electrospray ionization (H-ESI), nanospray ionization (NSI), atmospheric pressure photo ionization (APPI), or atmospheric pressure chemical ionization (APCI) mode. Refer to the *Ion MAX and Ion MAX-S API Source Hardware Manual*, *HESI-II Probe User Guide*, *H-ESI Probe User Guide*, *Ion MAX APPI Source Operator's Manual*, or *Nanospray Ion Source Operator's Manual* for more information regarding the ionization modes.

Ion Polarity Modes

You can operate the TSQ mass spectrometer in either of two ion polarity modes: positive or negative. Both positively charged and negatively charged ions form in the ion source of the mass spectrometer. The TSQ mass spectrometer can control whether positive ions or negative ions are transmitted to the mass analyzer for mass analysis by changing the polarity of the potentials applied to the ion source and ion optics. The ion optics deliver the ions produced in the ion source, in a collimated beam, to the mass analyzer.

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

Scan Modes

You can operate the TSQ mass spectrometer in a variety of scan modes. The most commonly used scan modes can be divided into two categories: single mass spectrometry (MS) scan modes and MS/MS scan modes. The scan modes in each category are as follows:

- MS scan modes: Q1MS and Q3MS scan modes
- MS/MS scan modes product scan mode, parent scan mode, neutral loss scan mode
- Data-dependent scan mode

The scan modes that can be employed depend on the number and type of rod assemblies and the voltages applied to the rod assemblies.

1 Introduction

Scan Modes

The TSQ system mass analyzer has three rod assemblies.² The first and third rod assemblies, Q1 and Q3, are quadrupoles, and the second rod assembly, Q2, is a square-profile quadrupole.

Rod assemblies can operate in either of two capacities:

- As ion transmission devices
- As mass analyzers

If only RF voltage is applied, a rod assembly serves as an ion transmission device that passes all ions within a large range of mass-to-charge ratios (that is, virtually all ions present).

When you apply both RF and dc voltages to a rod assembly, the separation of ions of different mass-to-charge ratios occurs. This separation allows the rod assembly to serve as a mass analyzer.

On the TSQ mass spectrometer, the quadrupole rod assemblies can operate with RF and dc voltages or with only RF voltage. That is, Q1 and Q3 can act either as mass analyzers or ion transmission devices. The Q2 rod assembly operates exclusively with RF voltage. Thus, Q2 is always an ion transmission device. For a summary of how the rod assemblies function in several of the major scan modes, see [Table 1](#).

Table 1. Summary of scan modes

Scan mode	Q1 quadrupole	Q2 collision cell	Q3 quadrupole
Q1MS	Scan ^a	Pass all ions ^b	Pass all ions
Q3MS	Pass all ions	Pass all ions	Scan
Product	Set ^c	Fragment ions ^d , then pass all fragments	Scan
Parent	Scan	Fragment ions, then pass all fragments	Set
Neutral Loss	Scan	Fragment ions, then pass all fragments	Scan

^a Scan = full scan or transmission of selected ions

^b Pass all ions or fragments = pass ions or fragments within a wide range of mass-to-charge ratios

^c Set = set to pass ions of a single mass-to-charge ratio or a set of mass-to-charge ratios

^d Fragment ions = collisions with argon gas cause ions to fragment

² A rod assembly is a regular array of metal rods. See “[Mass Analyzer](#)” on [page 28](#) for a discussion of the rod assemblies used on the TSQ Series instrument.

Q1MS and Q3MS Scan Modes

The Q1MS and Q3MS scan modes perform only one stage of mass analysis. The mass spectrum obtained is equivalent to the mass spectrum obtained from an instrument with a single mass analyzer. In the one stage of analysis, ions formed in the ion source enter the analyzer assembly. One of the mass analyzers (Q1 or Q3) is scanned to obtain a complete mass spectrum. The other rod assemblies (Q2 and Q3, or Q1 and Q2, respectively) act as ion transmission devices. In the Q1MS scan mode, Q1 is used as the mass analyzer; in the Q3MS scan mode, Q3 is used as the mass analyzer.

Product Scan Mode

Product scan mode performs two stages of analysis. In the first stage, ions formed in the ion source enter Q1, which is set to transmit ions of one mass-to-charge ratio. Ions selected by this first stage of mass analysis are called parent ions. (As a result, Q1 is referred to as the parent mass analyzer, and the mass-to-charge ratio of ions transmitted by the parent mass analyzer is referred to as the parent set mass.) Parent ions selected by Q1 then enter Q2, which is surrounded by the collision cell.

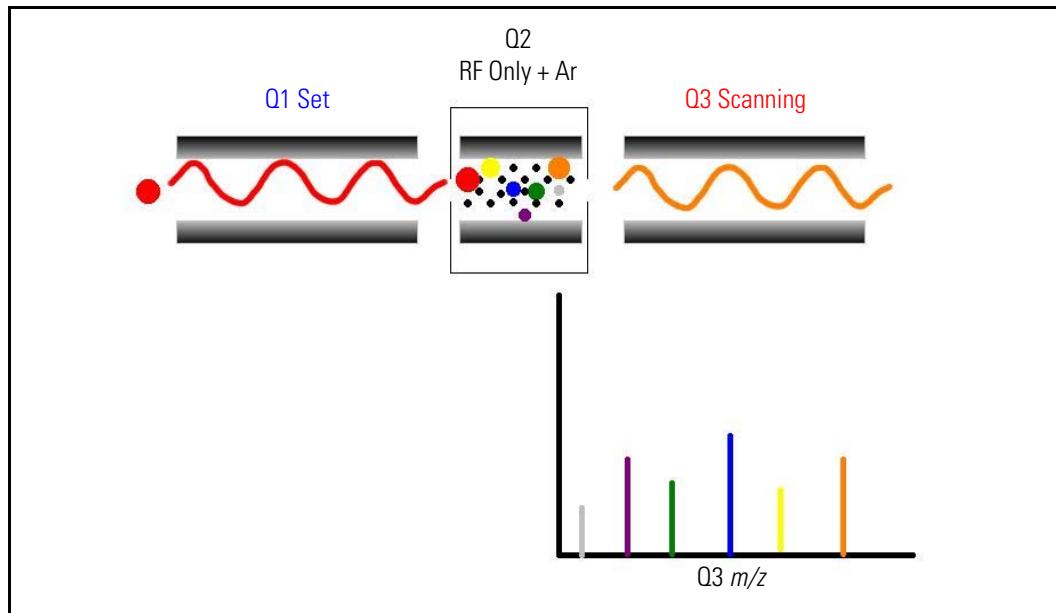
Note For convenience, when referring to the first, second, and third rod assemblies as pieces of hardware, you can call them Q1, Q2, and Q3, respectively. However, for clarity when discussing their function in MS/MS scan modes, you can refer to them as the parent mass analyzer, collision cell (ion transmission device surrounded by the collision cell), and product mass analyzer, respectively.

In the second stage of analysis, ions in the collision cell can fragment further to produce product ions. Two processes produce product ions: by unimolecular decomposition of metastable ions or by interaction with argon collision gas present in the collision cell. This latter step is known as collision-induced dissociation (CID). Ions formed in the collision cell enter Q3 (the product mass analyzer) for the second stage of mass analysis. Q3 is scanned to obtain a mass spectrum that shows the product ions produced from the fragmentation of the selected parent ion.

A mass spectrum obtained in the product scan mode (product mass spectrum) is the mass spectrum of a selected parent ion.

Figure 1 illustrates the product scan mode.

Figure 1. Illustration of product scan mode



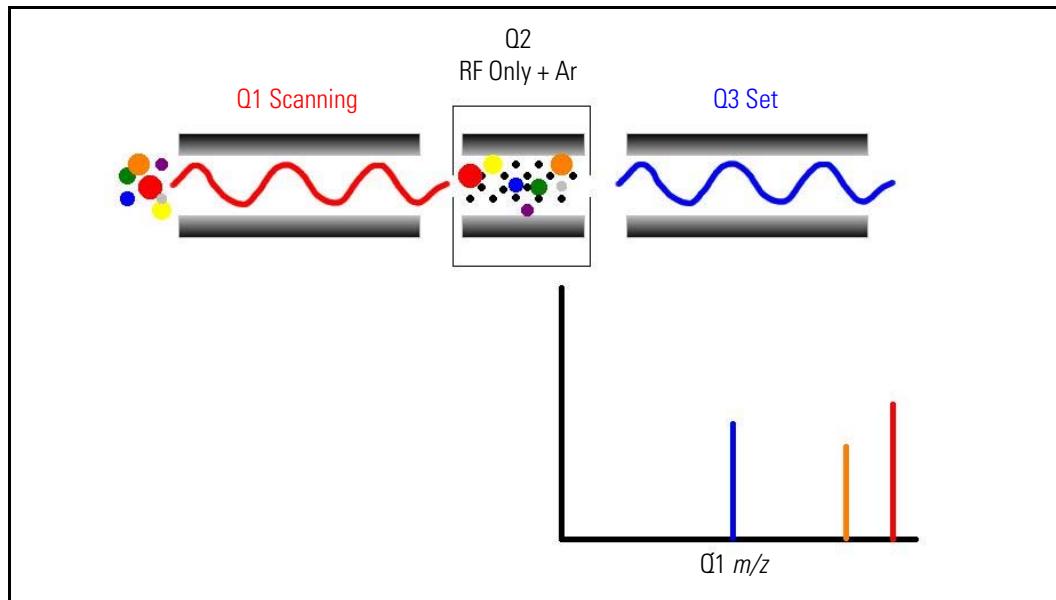
Parent Scan Mode

The parent scan mode also uses two stages of analysis. In the first stage, ions formed in the ion source are introduced into the parent mass analyzer, which is scanned to transmit parent ions sequentially into the collision cell.

In the second stage of analysis, in the collision cell, parent ions can fragment to produce product ions by unimolecular decomposition of metastable ions or by collision-induced dissociation. Ions formed in the collision cell enter the product mass analyzer, which transmits a selected product ion. (The product set mass is the mass-to-charge ratio of ions transmitted by the product mass analyzer.)

The resultant spectrum shows all the parent ions that fragment to produce the selected product ion. Note that for a mass spectrum obtained in the parent scan mode (parent mass spectrum), data for the mass-to-charge ratio axis is obtained from Q1 (the parent ions), whereas data for the ion intensity axis is obtained from Q3 (from monitoring the product ion).

[Figure 2](#) illustrates the parent scan mode.

Figure 2. Illustration of the parent scan mode

Experiments that employ the parent scan mode (parent experiments) can be used in structure and fragmentation studies as well as in survey analyses of mixtures. In general, parent experiments detect all compounds that decompose to a common fragment. The experiments are useful for the rapid detection of a series of structural homologs (for example, substituted aromatics, phthalates, steroids, or fatty acids) that have a common fragment ion (for example, m/z 149 for the phthalates).

Neutral Loss Scan Modes

In the neutral loss scan mode, the two mass analyzers (Q1 and Q3) are linked together so that they are scanned at the same rate over mass ranges of the same width. The respective mass ranges, however, are offset by a selected mass so that the product mass analyzer scans a selected number of mass units lower than the parent mass analyzer.

As a result, in the neutral loss scan mode, there are two stages of mass analysis. In the first stage, the parent mass analyzer separates ions formed in the ion source by mass-to-charge ratio. Then the ions are introduced sequentially into the collision cell.

In the second stage of analysis, ions admitted to the collision cell can fragment further by metastable ion decomposition or by CID to produce product ions. The product mass analyzer then separates these product ions by their mass-to-charge ratio. [Figure 3](#) illustrates the neutral loss scan mode. Examples of compounds with a common neutral loss fragment appear in [Figure 4](#).

For an ion to be detected, between the time the ion leaves Q1 and enters Q3, it must lose a neutral moiety whose mass (the neutral loss mass) is equal to the difference in the mass ranges being scanned by the two mass analyzers. Thus, a neutral loss mass spectrum is a spectrum that shows all the parent ions that lose a neutral species of a selected mass.

Note that a neutral gain (or association) experiment can also be performed in which the mass range scanned by Q3 is offset by a selected mass above the mass range scanned by Q1.

For a neutral loss (or neutral gain) mass spectrum, as for a parent mass spectrum, Q1 (the parent ion) provides data for the mass-to-charge ratio axis, whereas Q3 (the product ion being monitored) provides data for the ion intensity axis.

Experiments that use the neutral loss scan mode (neutral loss experiments) are useful when a large number of compounds are being surveyed for common functionality. Neutral moieties are frequently lost from substituent functional groups (for example, CO₂ from carboxylic acids, CO from aldehydes, HX from halides, and H₂O from alcohols).

Figure 3. Illustration of the neutral loss scan mode

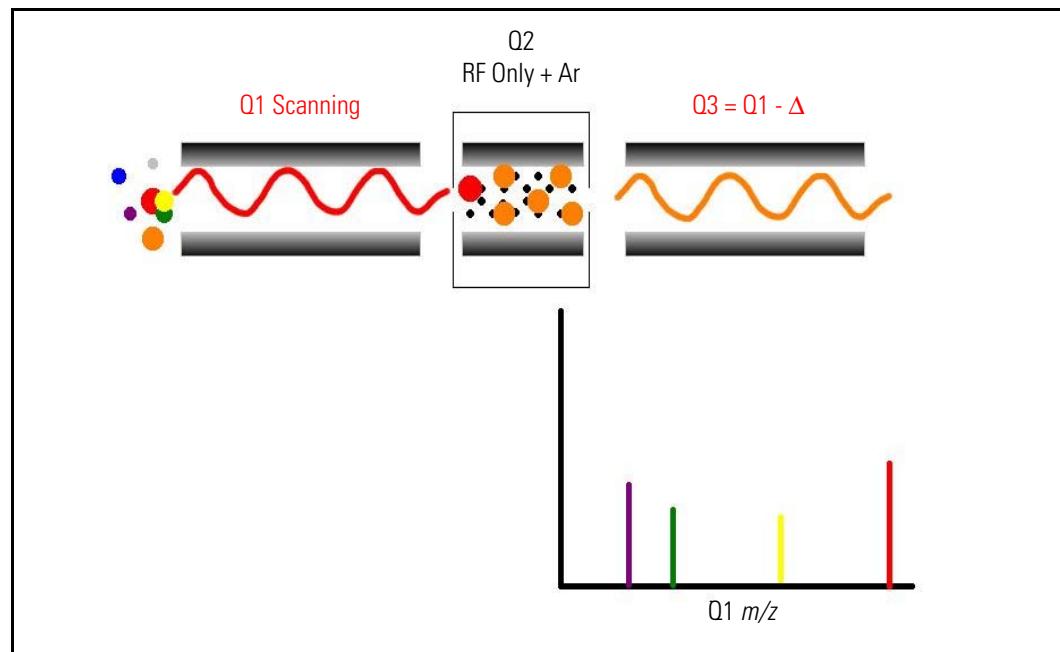
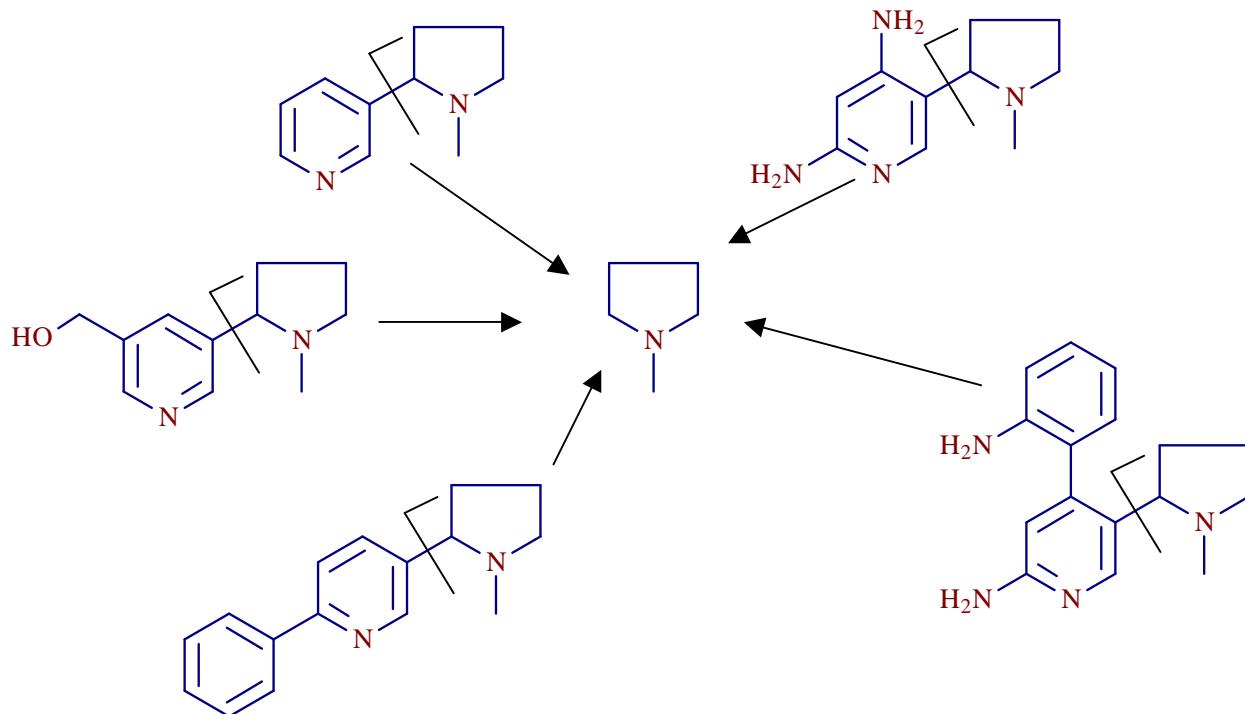


Figure 4. Examples of compounds with a common neutral-loss fragment

Data Dependent Scan Mode

The TSQ mass spectrometer uses the information in a data-dependent scan mode experiment to make automatic decisions about the next step of the experiment without input from a user. In data-dependent scan mode you specify criteria to select one or more ions of interest on which to perform subsequent scans, such as MS/MS. You can approach the setup of data-dependent experiments in either of two ways:

- If you have some idea of what the parent ion is, or if you expect a certain kind of parent, you can 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 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 TSQ system generates product spectra. Later, you can decide if the information is useful.

Because a data-dependent scan needs to use a target ion from a previous scan, the first scan event cannot be a data-dependent scan.

Scan Types

TSQ systems can be operated with a variety of scan types. The most common scan types are as follows:

- [Full Scan](#)
- [Selected Ion Monitoring \(SIM\)](#)
- [Selected Reaction Monitoring \(SRM\)](#)
- [AutoSIM](#)

Full Scan

The full-scan scan type provides a full mass spectrum of each analyte. With full scan, the scanning mass analyzer is scanned from the first mass to the last mass, without interruption, in a given scan time.

Full-scan experiments are used to determine or confirm the identity of unknown compounds or the identity of each component in a mixture of unknown compounds. (Generally, a full mass spectrum is needed to determine the identity of an unknown compound.)

The full-scan scan type gives you more information about an analyte than does SIM, but a full scan does not yield the sensitivity that the other two scan types can achieve. With full scan, you spend less time monitoring the signal for each ion than you do in SIM or SRM. Full scan provides greater information but lower sensitivity than the other two scan types.

To use the SIM or SRM, you need to know what ions or reactions you are looking for before you can perform an experiment with these scan types. Thus, you might use a full scan for SIM to determine the identity of an analyte and to obtain its mass spectrum and a full scan for SRM to determine the mass spectrum and product mass spectra for parent ions of interest. Then, you might use SIM or SRM to do routine quantitative analysis of the compound.

Selected Ion Monitoring

Selected ion monitoring (SIM) monitors a particular ion or set of ions. SIM experiments are useful in detecting small quantities of a target compound in a complex mixture when you know the mass spectrum of the target compound. Thus, SIM is useful in trace analysis and in the rapid screening of a large number of samples for a target compound.

Because SIM monitors only a few ions, it can provide lower detection limits and greater speed than the full-scan modes. 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 analyte. SIM can achieve greater speed because it monitors only a few ions of interest; SIM does not monitor 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 specificity. Because SIM monitors only specific ions, any compound that fragments to produce those ions will appear to be the target compound. The result can be a false positive.

Selected Reaction Monitoring

Selected reaction monitoring (SRM) monitors a particular reaction or set of reactions, such as the fragmentation of an ion or the loss of a neutral moiety.

SRM monitors a limited number of parent or product ion pairs. In product-type experiments, a parent ion is selected as usual, but generally only one product ion is monitored. SRM experiments are normally conducted with the product scan mode.

As does SIM, SRM provides for the very rapid analysis of trace components in complex mixtures. However, because SRM selects two sets of ions, it obtains specificity that is much greater than what SIM can obtain. Any interfering compound would not only have to form an ion source product (parent ion) of the same mass-to-charge ratio as the selected parent ion from the target compound, but that parent ion would also have to fragment to form a product ion of the same mass-to-charge ratio as the selected product ion from the target compound.

AutoSIM

In the scan type known as AutoSIM, the mass spectrometer automatically selects the most intense masses (m/z values) in a survey scan, builds a SIM scan list for them, and then acquires and records ion current at only these selected masses. AutoSIM scans can be performed on any full scan in any scan mode but not on data-dependent scans.

There might be times when the scan ranges of two (or more) selected masses overlap. If this happens, both masses are placed in one SIM window. In EZ Tune, the SIM table in the Define Scan dialog box displays the center mass for this new scan window, not each selected mass.

Data Types

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

- [Profile Data Type](#)
- [Centroid Data Type](#)

1 Introduction

Mass/Charge Range

Profile Data Type

In the profile data type, you can see the shape of the peaks in the mass spectrum. Each atomic mass unit is divided into many sampling intervals. The intensity of the ion current is determined at each of the sampling intervals. The profile data type displays the intensity at each sampling interval 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 Type

The centroid data type displays the mass spectrum as a bar graph and sums the intensities of each set of multiple sampling intervals. This sum is displayed versus the integral center of mass of the sampling intervals. In general, use the centroid scan data type for data acquisition for faster scan speed. Data processing is also much faster for centroid data.

Mass/Charge Range

The TSQ mass spectrometer can operate in a mass/charge range of 10 to 3000 Da (TSQ Quantum™ Access™, TSQ Quantum Access MAX, TSQ Vantage EMR™, and TSQ Quantum Ultra EMR™) or 10 to 1500 Da (TSQ Vantage™, TSQ Vantage AM, TSQ Quantum Ultra™ and TSQ Quantum Ultra AM).

Functional Description

This chapter describes the principal components of the TSQ system and their respective functions.

Contents

- [Autosampler](#) (optional)
- [Liquid Chromatograph](#) (optional)
- [Mass Spectrometer](#)
- [Data System](#)

A functional block diagram of the TSQ mass spectrometer is shown in [Figure 5](#). A sample transfer line connects the LC to the mass spectrometer. The autosampler and LC are usually installed on the left of the mass spectrometer. The syringe pump and divert/inject valve are integrated into the mass spectrometer cabinet.

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

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

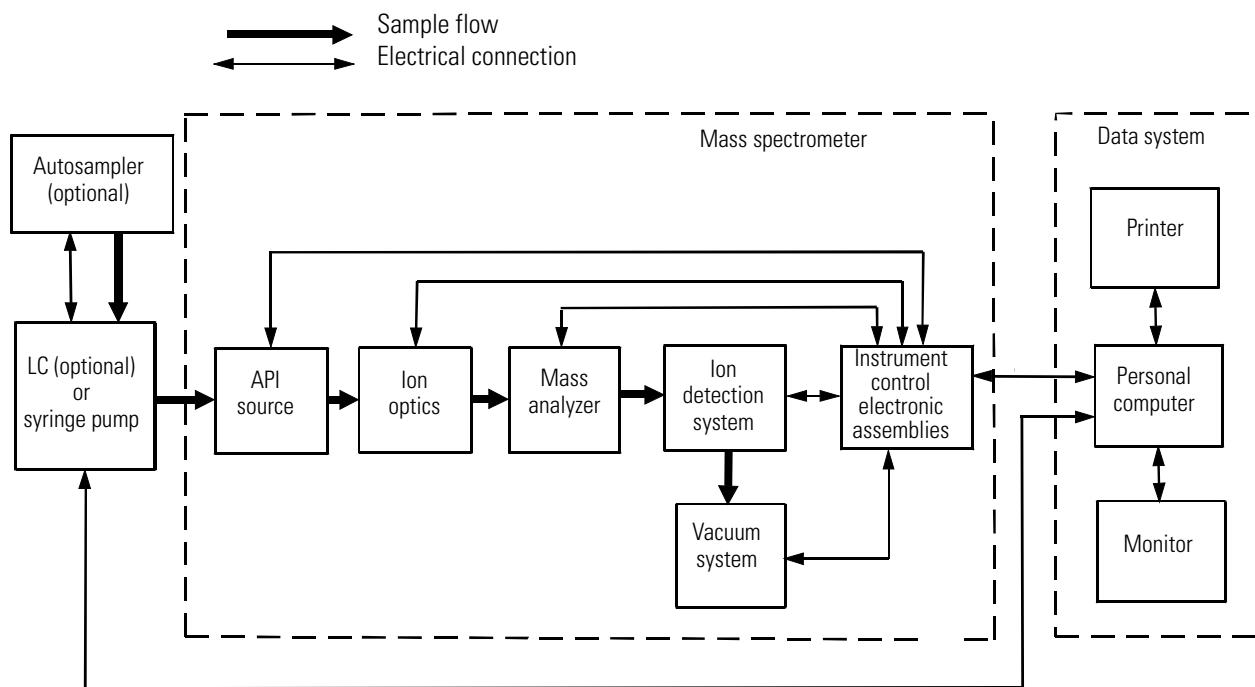
In analysis by LC/MS, a sample is injected onto an LC column. The sample then separates into its various components. The components elute from the LC column and pass into the mass spectrometer where they are analyzed.

Electrospray ionization (ESI), heated electrospray ionization (H-ESI), nanospray ionization (NSI), atmospheric pressure photo ionization (APPI), or atmospheric pressure chemical ionization (APCI) ionize sample molecules at atmospheric pressure. The ion optics focus and accelerate the resulting sample ions into the mass analyzer where they are analyzed according to their mass-to-charge ratios. An ion detection system then produces a signal proportional to the number of ions detected. The system electronics receive and amplify the ion current signal from the ion detection system. That signal is then passed on to the data system for further processing, storage, and display. The data system provides the primary TSQ mass spectrometer user interface.

2 Functional Description

Autosampler

Figure 5. Functional block diagram of the TSQ system



Autosampler

The (optional) autosampler injects samples automatically into the liquid chromatograph (LC) inlet. The TSQ data system computer can control most autosamplers. With an autosampler, you can automate your LC/MS analyses.

Autosampler Start/Stop signals with the TSQ mass spectrometer are provided by contact closure. Refer to the *TSQ Series Getting Connected Guide* for information on connecting an autosampler to the TSQ mass spectrometer by contact closure.

You configure the autosampler from the data system computer. Select the appropriate autosampler button in the Instrument Configuration window, which is available by choosing **Start > All Programs > Thermo Foundation > Instrument Configuration**. See Instrument Configuration Help for a description of autosampler configuration options.

You also use the data system to set up the autosampler to inject samples. Choose **Start > All Programs > Thermo Xcalibur > Xcalibur** and click **Instrument Setup** to open the Instrument Setup window. Then, click the appropriate autosampler icon to open the Autosampler page. For instructions on running your autosampler, refer to the Help.

For front-panel (keypad) operation (if any) and maintenance procedures, refer to the documentation provided with the autosampler.

Liquid Chromatograph

The (optional) 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 in which order each component elutes from the LC and enters the mass spectrometer.

You can control most LCs and the corresponding UV detectors directly from the TSQ data system computer. You can set the flow rate from 0 to 1000 $\mu\text{L}/\text{min}$ or more. Refer to the *TSQ Series Getting Connected Guide* for information on connecting an LC to the TSQ mass spectrometer.

You configure the LC from the data system computer. Select the appropriate LC button in the Instrument Configuration window, which is available by choosing **Start > All Programs > Thermo Foundation > Instrument Configuration**. For a description of LC configuration options, refer to Xcalibur Help.

You also use the data system to set up the LC. Choose **Start > All Programs > Thermo Xcalibur > Xcalibur** and click **Instrument Setup** to open the Instrument Setup window. Then, click the appropriate LC icon to open the LC page. For instructions on running your LC, refer to the Help.

For front-panel (keypad) operation (if any) and maintenance procedures, refer to the documentation provided with the LC.

Syringe Pump

The TSQ mass spectrometer includes an electronically-controlled, integrated syringe pump. See [Figure 6](#). The syringe pump delivers sample solution from the syringe into the atmospheric pressure ionization (API) source. When the syringe pump is operating, a motor drives a pusher block that depresses the plunger of the syringe at a rate of one percent of the syringe volume per minute. Liquid flows out of the syringe needle and into the sample transfer line as the plunger is depressed. A syringe holder holds the syringe in place. Refer to the *TSQ Series Getting Started Guide* or the *TSQ Series Getting Connected Guide* for instructions on setting up the syringe pump.

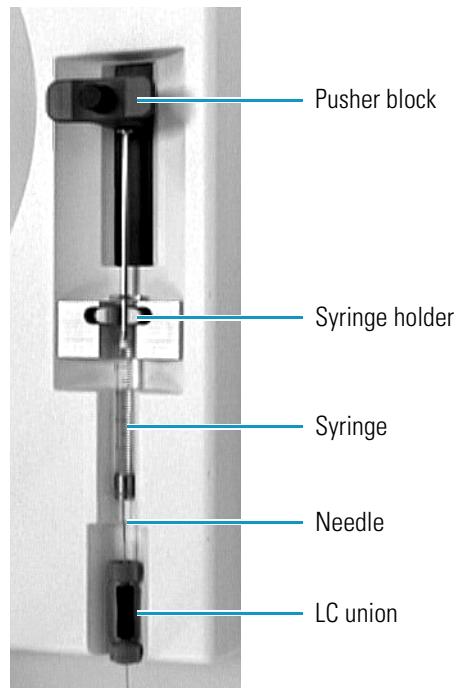
You can start and stop the syringe pump from the EZ Tune window, which is available by choosing **Start > All Programs > Thermo Instruments > TSQ > TSQ Tune**. Refer to EZ Tune Help for instructions on operating the syringe pump from the data system. You can also start and stop the syringe pump by pressing the syringe pump button. By holding down the button, you can run the syringe pump in Purge mode, where the flow rate is five percent of the syringe volume per second.

2 Functional Description

Divert/Inject Valve

The syringe pump light-emitting diode (LED) (see [Figure 9](#) and [Figure 10](#)) illuminates green whenever the syringe pump is pumping. The LED illuminates yellow if the syringe pump is at the end of its travel.

Figure 6. Syringe pump

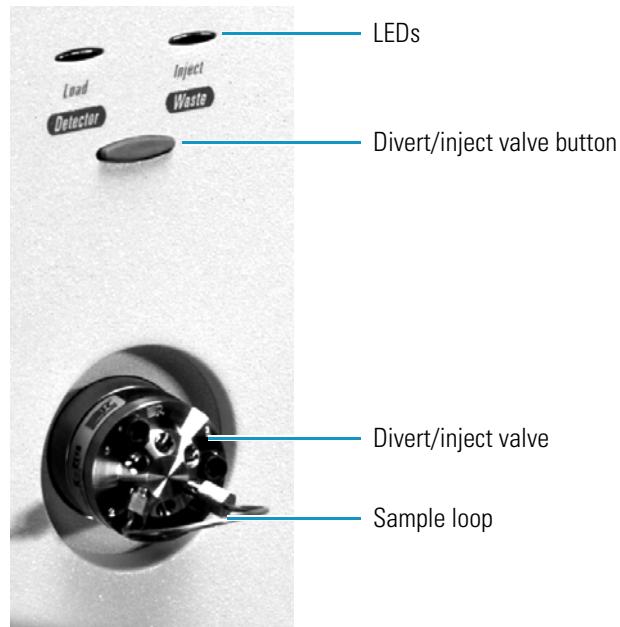
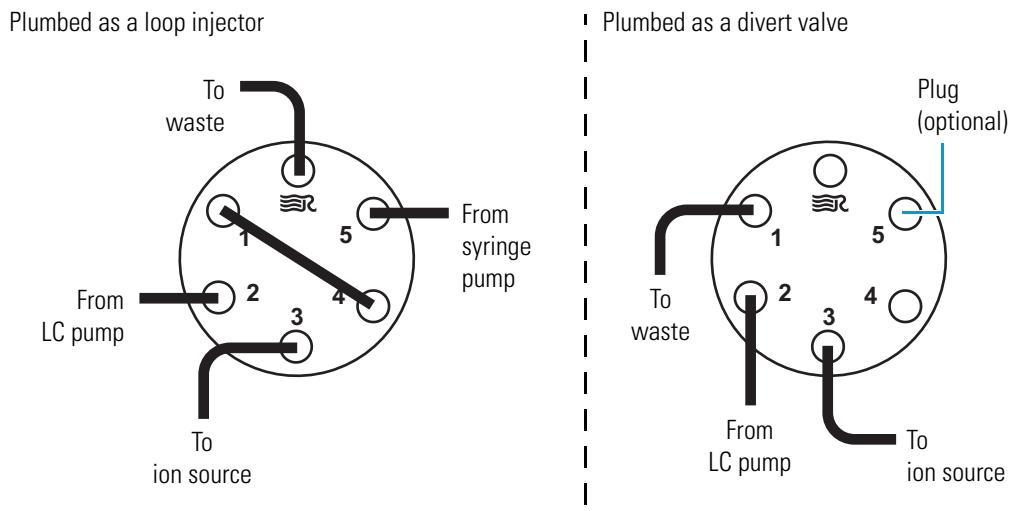


Divert/Inject Valve

The Rheodyne™ 7750E-185 divert/inject valve is a motorized, stainless steel, six-port valve that switches between two positions: Load and Inject. The divert/inject valve is located on the front of the TSQ mass spectrometer above the API source. See [Figure 7](#). You can configure (plumb) the divert/inject valve as a loop injector (for flow injection analysis) or as a divert valve. See [Figure 8](#). The divert valve enables switching the solvent front, gradient endpoint, or any portion of the LC run to waste. The *TSQ Series Getting Started Guide* provides procedures for plumbing the valve in the loop injector or divert valve configuration.

You can control the divert/inject valve from the data system. You specify the parameters of the divert/inject valve on the Divert Valve page, accessible from the Instrument Setup window. For instructions on operating the divert/inject valve from the data system, refer to the Help.

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

Figure 7. Divert/inject valve**Figure 8.** Divert/inject valve plumbed as a loop injector and as a divert valve

2 Functional Description

Mass Spectrometer

Mass Spectrometer

The mass spectrometer provides sample ionization and mass analysis of injected samples or samples eluted from a liquid chromatograph. The TSQ mass spectrometer uses a triple-quadrupole mass analyzer with an ion source external to the mass analyzer. Several important features of the TSQ mass spectrometer are as follows:

- High sensitivity and resolution
- m/z 10 to 3000 mass range for TSQ Quantum Access, TSQ Quantum Access MAX, and TSQ Vantage and TSQ Quantum Ultra with extended mass range (EMR) electronic assemblies installed; and m/z 10 to 1500 mass range for TSQ Vantage, TSQ Vantage AM, TSQ Quantum Ultra, and TSQ Quantum Ultra AM without extended mass range electronic assemblies
- ESI, H-ESI, NSI, APPI, and APCI ionization modes
- Positive and negative ion polarity modes
- MS and MS/MS scan modes
- Full-scan, SIM, SRM, AutoSIM, and data-dependent scan types

The mass spectrometer includes the following components:

- [Controls and Indicators](#)
- [API Source](#)
- [Ion Source Interface](#)
- [Ion Optics](#)
- [Mass Analyzer](#)
- [Ion Detection System](#)
- [Vacuum System and Inlet Gases Hardware](#)
- [Electronic Assemblies](#)

Controls and Indicators

Six LEDs are located at the upper right side of the front panel of the mass spectrometer. See [Figure 9](#) (TSQ Vantage, TSQ Quantum Access, or TSQ Quantum Access MAX) and [Figure 10](#) (TSQ Quantum Ultra).

Figure 9. Front panel LEDs of the TSQ Vantage, TSQ Quantum Access, or TSQ Quantum Access MAX mass spectrometer

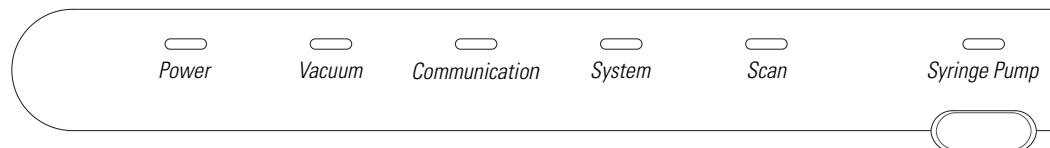
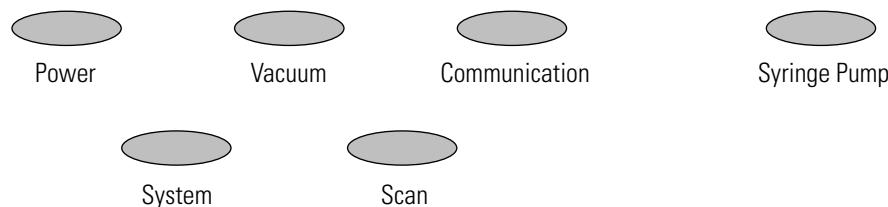


Figure 10. Front panel LEDs of the TSQ Quantum Ultra mass spectrometer



The Power LED illuminates green whenever power is supplied to the vacuum system and electronic assemblies of the mass spectrometer.

The Vacuum LED illuminates yellow when the turbomolecular pump is nearly at speed (80 percent of its operating speed of 750 MHz) and it is safe to turn on the ion gauge. The Vacuum LED is off if the turbomolecular pump is not at speed. The Vacuum LED illuminates green whenever the pressure in the analyzer chamber is at or below the value required to enable high voltages to the mass analyzer (7×10^{-4} Torr).

The Communication LED illuminates yellow when the mass spectrometer and the data system are trying to establish a communication link. The Communication LED illuminates green when the Ethernet communication link between the mass spectrometer and the data system has been made.

The System LED illuminates yellow whenever the mass spectrometer is in standby—that is, high voltage is not supplied to the ion source, mass analyzer, or ion detection system, but the mass spectrometer power is on. The System LED illuminates green whenever the high voltage is enabled and the system is in the On state. High voltage is enabled if the analyzer chamber is below 7×10^{-4} Torr.

The Scan LED flashes blue whenever the mass spectrometer is on and is scanning ions.

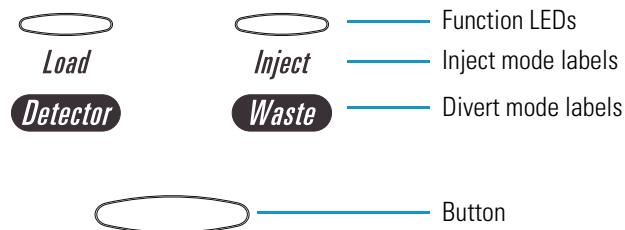
The syringe pump LED illuminates green whenever the syringe pump is pumping. The LED illuminates yellow if the syringe pump is at the end of its travel.

2 Functional Description

Mass Spectrometer

Two additional LEDs and a push-button switch are located on the front panel above the divert/inject valve. See [Figure 11](#). When the divert/inject valve is set up for loop injections, the divert/inject valve button switches the valve between load and inject modes and the labels *Load* and *Inject* apply.

Figure 11. Divert/inject valve button and LEDs



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

The main power circuit breaker switch (labeled Main Power) is located on the power panel at the lower right corner of the right side panel of the mass spectrometer. See [Figure 12](#) and [Figure 13](#). In the Off (O) position, the circuit breaker removes all power to the mass spectrometer, including the vacuum pumps. 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.

Figure 12. Power panel of the TSQ Vantage or TSQ Quantum Ultra

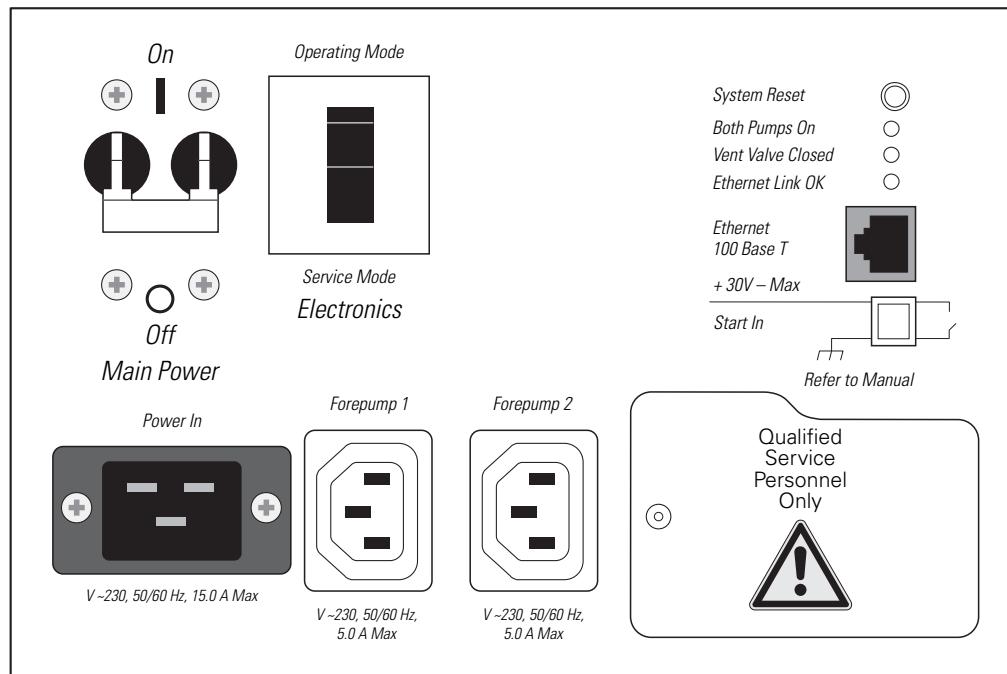
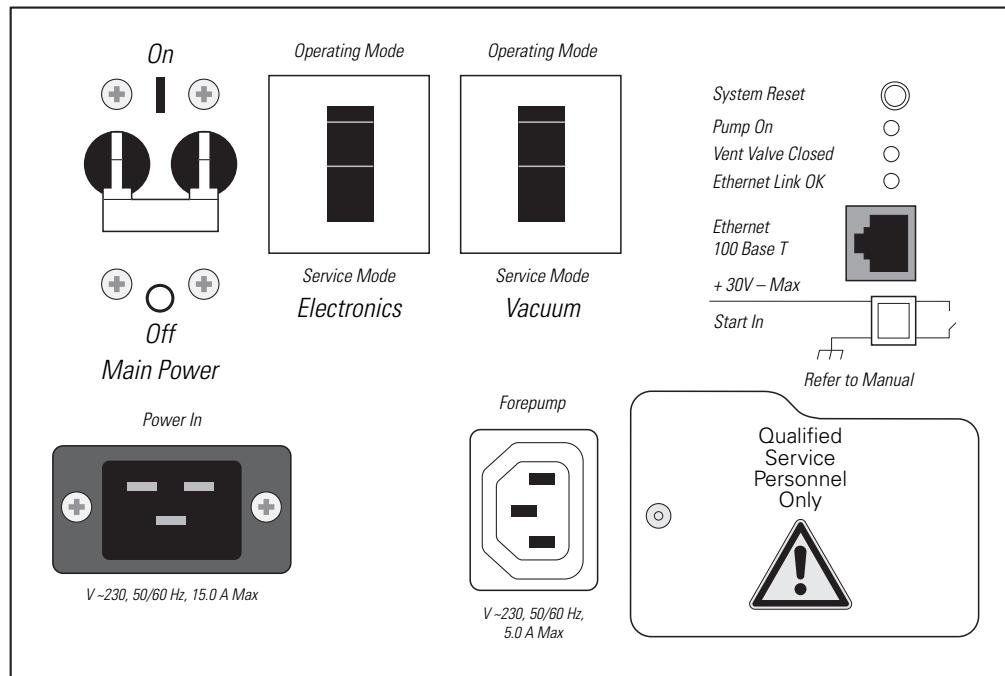


Figure 13. Power panel of the TSQ Quantum Access or TSQ Quantum Access MAX, showing switches and LEDs



The electronics service switch (labeled Electronics) is located next to the main power circuit breaker on the mass spectrometer power panel (Figure 12 and Figure 13). In the Service Mode position the switch removes power to all components of the mass spectrometer other than the vacuum system. The Operating Mode position supplies power to all non-vacuum system components of the mass spectrometer.

On the TSQ Quantum Access and TSQ Quantum Access MAX, a vacuum service switch (labeled Vacuum) is located next to the Electronics service switch on the mass spectrometer power panel (Figure 13). In the Service Mode position the switch removes power to all components of the vacuum system, including the forepump, turbomolecular pump, and turbomolecular pump controller. The switch in the Operating Mode position supplies power to all vacuum system components of the mass spectrometer.

The System Reset button is also located on the mass spectrometer power panel. Pressing the System Reset button causes the embedded computer on the System Control PCB to reboot. The TSQ mass spectrometer software is then reloaded from the data system. See “[Resetting the Mass Spectrometer](#)” on page 55 for information on how to reset the mass spectrometer.

Three LEDs are located on the power panel:

- The Pump On LED illuminates green when the forepump current sensor detects current to the forepump. The LED is off when the forepump current sensor does not detect current to the forepump. If the current sensor detects a loss of current when the TSQ is on, high voltage turns off and the vacuum system vents.

2 Functional Description

Mass Spectrometer

- The Vent Valve Closed LED illuminates green whenever the vent valve current sensor detects current through the vent valve and the vent valve is closed. The LED is off when the vent valve is open.
- The Ethernet Link OK LED illuminates green when the System Control PCB is communicating with the data system PC. The LED is off when there is no communication between the System Control PCB and the data system PC.



CAUTION In an emergency, to shut off all power to the mass spectrometer, place the Main Power circuit breaker switch (labeled Main Power) in the Off (O) position.

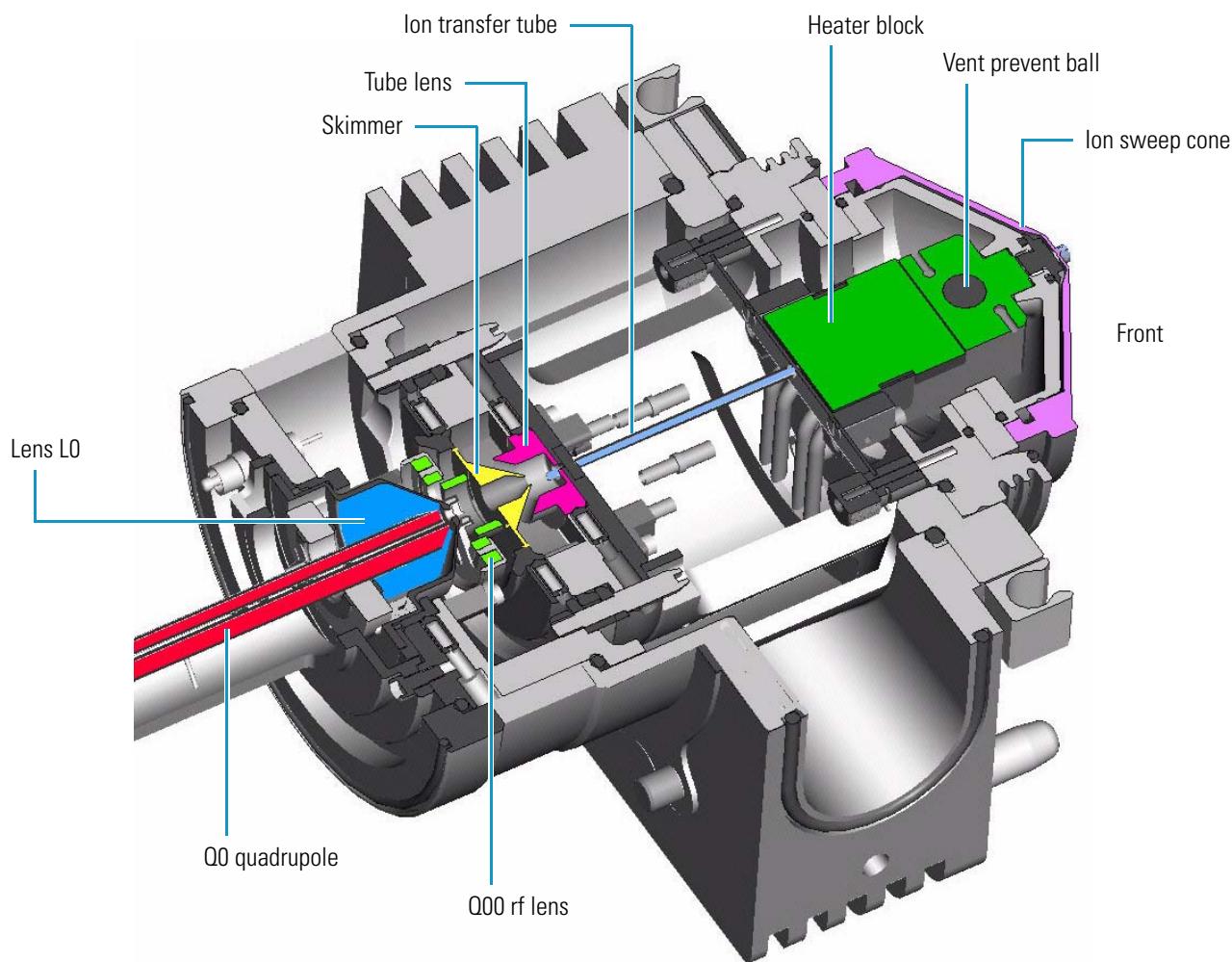
API Source

The atmospheric pressure ionization (API) source forms gas phase sample ions from sample molecules that elute from the LC or are introduced by the syringe pump. 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. For more information regarding the API source, refer to the *Ion Max and Ion Max-S API Source Hardware Manual*, *HESI-II Probe User Guide*, *H-ESI Probe User Guide*, *Ion Max APPI Source Operator's Manual*, or *Nanospray Ion Source Operator's Manual*.

Ion Source Interface

The ion source interface consists of the components of the API source that are held under vacuum (except for the atmospheric pressure side of the ion sweep cone). The ion source interface includes an ion transfer tube, two cartridge heaters, a heater block, a platinum probe sensor, a vent prevent ball, and an ion sweep cone. See [Figure 14](#).

Figure 14. Cross-sectional view of the ion source interface, Q00 ion optics, and Q0 ion optics of the TSQ Quantum Access, TSQ Quantum Access MAX, or TSQ Quantum Ultra



The ion transfer tube assists in desolvating ions that are produced by the API probe. The tube is an elongated, 4 in. (on the TSQ Quantum Access, TSQ Quantum Access MAX, and TSQ Quantum Ultra) or 2.3 in. (on the TSQ Vantage) cylindrical metal tube. See [Figure 15](#). Two heater cartridges are embedded in the heater block. The heater block surrounds the ion transfer tube and heats it to temperatures up to 400 °C. A platinum probe sensor measures the temperature of the heater block. Typical temperatures of the ion transfer tube are 270 °C for ESI and 250 °C for APCI, but these temperatures vary with flow rate and mobile phase composition. A decreasing pressure gradient draws ions into the ion transfer tube in the atmospheric pressure region and transports them to the ion transfer tube-skimmer region of the vacuum manifold. A potential of typically ± 35 V (positive for positive ions and negative for negative ions) assists in repelling ions from the ion transfer tube to the skimmer. The vent prevent ball falls into the space occupied by the ion transfer tube when the tube is removed, thus preventing air from entering the vacuum manifold. The vent prevent ball allows you to remove the ion transfer tube for cleaning without venting the system.

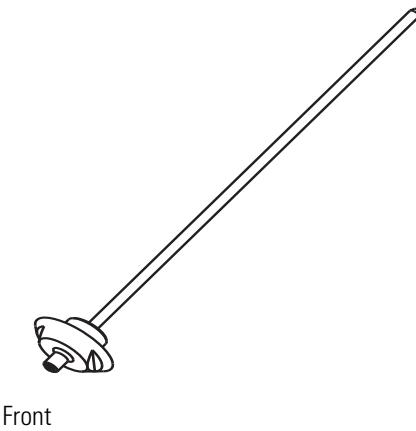
2 Functional Description

Mass Spectrometer

The ion sweep cone is a metallic cone over the ion transfer tube. The ion sweep cone channels the sweep gas towards the entrance of the tube.

The ion source interface is enclosed in a vacuum chamber that is evacuated by the forepump to a pressure of approximately 1.5 Torr.

Figure 15. Ion transfer tube



Ion Optics

The ion optics focus the ions produced in the API source and transmit them to the mass analyzer. The TSQ mass spectrometer uses two ion optics elements:

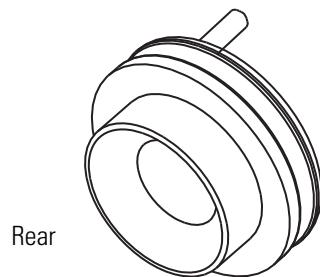
- Q00 ion optics
- Q0 ion optics

Q00 Ion Optics

The Q00 ion optics are the ion optics that are located closest to the API source. Q00 ion optics include either the tube lens and skimmer or the S-lens and exit lens, the Q00 rf lens, the ion source interface cage, and the lens L0. See [Figure 14](#).

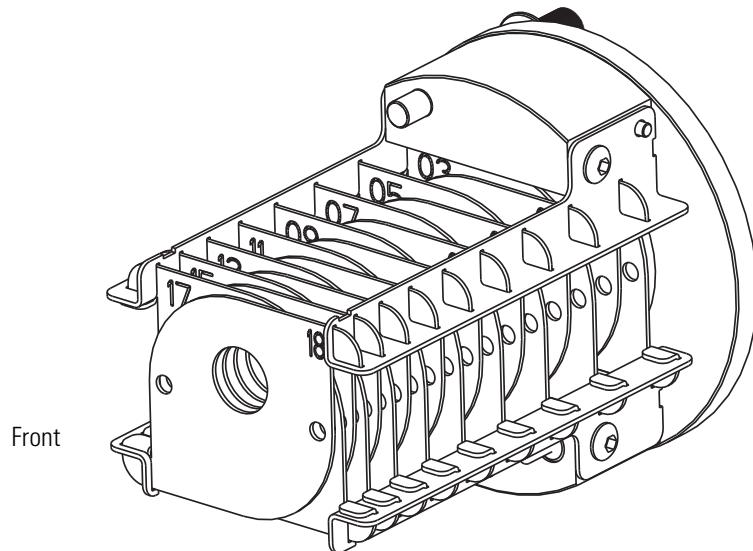
On the TSQ Quantum Access, TSQ Quantum Access MAX, and TSQ Quantum Ultra, ions from the ion transfer tube enter the tube lens. See [Figure 16](#). The tube lens has a mass-dependent potential applied to it to focus the ions toward the opening of the skimmer. An additional potential of between 0 and ± 250 V (positive for positive ions and negative for negative ions), 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 TSQ mass spectrometer, you adjust the tube lens offset voltage to maximize sensitivity by balancing desolvation with fragmentation.

Figure 16. Tube lens of the TSQ Quantum Access, TSQ Quantum Access MAX, or TSQ Quantum Ultra



The TSQ Vantage 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. See [Figure 17](#). A 650 kHz 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 TSQ Vantage determines the mass-dependent rf amplitudes for optimum transmission of ions through the lens. The maximum amplitude is 300 V peak-to-peak.

Figure 17. S-lens of the TSQ Vantage



Ions from the tube lens or S-lens pass through the skimmer ([Figure 18](#)) or exit lens ([Figure 19](#)) and move toward the Q00 rf lens. The skimmer and exit lens act as a vacuum baffle between the higher pressure ion source interface region (at 1.5 Torr) and the lower pressure Q00 ion optics region (at 50 mTorr) of the vacuum manifold. The apertures of the skimmer and exit lens are offset with respect to the bore of the ion transfer tube. This arrangement reduces the number of large, charged particles that pass through the skimmer or exit lens into the mass analyzer, which reduces detector noise. The tube lens and skimmer, or the S-lens and exit lens, mount to the ion source interface cage.

2 Functional Description

Mass Spectrometer

Figure 18. Skimmer of the TSQ Quantum Access, TSQ Quantum Access MAX, or TSQ Quantum Ultra

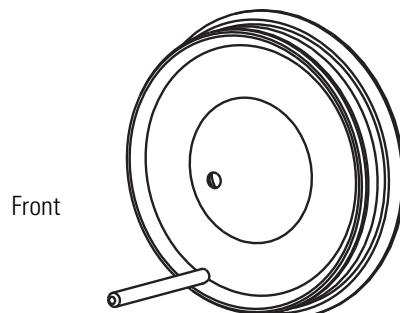
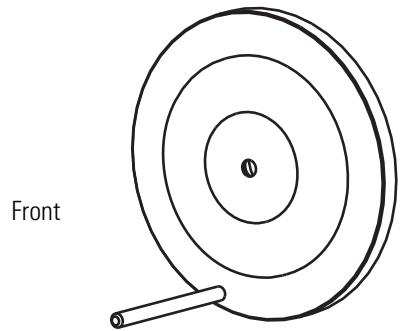
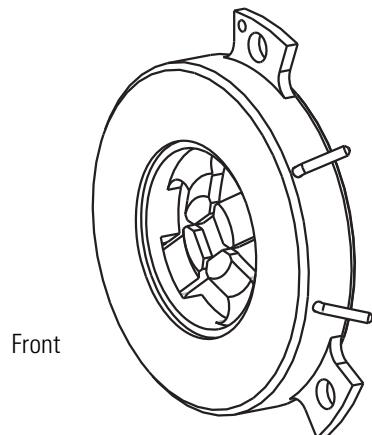


Figure 19. Exit lens of the TSQ Vantage



The Q00 rf lens is a square array of thin metal elements that act as an ion focusing device. See [Figure 20](#). 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. 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. Typical values of the Q00 offset voltage are 0 and ± 4 V (negative for positive ions and positive for negative ions).

Figure 20. Q00 rf lens



Source CID can also be accomplished by increasing the dc voltage offset between the skimmer, which is at ground potential, and the rest of the mass spectrometer beginning with Q00. You use the Source CID parameter in the Tune Master software to adjust this potential.

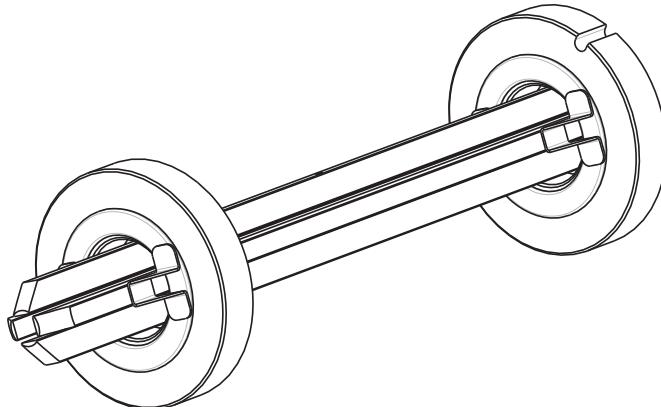
The lens L0 is a metal cylinder with a small hole in one end through which the ion beam can pass. A potential of between 0 and ± 3 V (negative for positive ions and positive for negative ions) is applied to lens L0 to aid in ion transmission. Lens L0 also acts as a vacuum baffle between the Q00 and Q0 ion optics chambers.

Q0 Ion Optics

The Q0 ion optics transmits ions from the Q00 ion optics to the mass analyzer. The Q0 ion optics includes the Q0 quadrupole and lenses L11 and L12.

The Q0 quadrupole is a square array of square-profile rods that act as an ion transmission device. See [Figure 21](#). 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 21. Q0 quadrupole



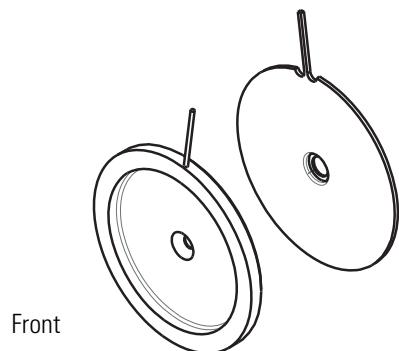
The Q0 offset voltage can also be used to fragment ions. In ion source collision-induced dissociation, the offset voltage (typically -30 V to $+30$ V) imparts enough kinetic energy to the ions so that, when they collide with solvent or air molecules, the ions dissociate to form product ions. The translational kinetic energy imparted to the ions determines the degree of dissociation. At low energies, adduct ions convert to sample ions by collision-induced dissociation without fragmenting. At higher energies, molecular ions can fragment and thereby enable primitive MS/MS/MS analysis.

The L11 and L12 lenses are metal disks with a circular hole in the center through which the ion beam can pass. See [Figure 22](#). Together they act as a two-element cone lens. An electrical potential applied to the lens accelerates (or decelerates) ions as they approach the lens to focus the ion beam as it passes through the lens. The value ranges between 0 and ± 300 V. Lenses L11 and L12 also act as a vacuum baffle between the Q0 ion optics chamber and the mass analyzer chamber.

2 Functional Description

Mass Spectrometer

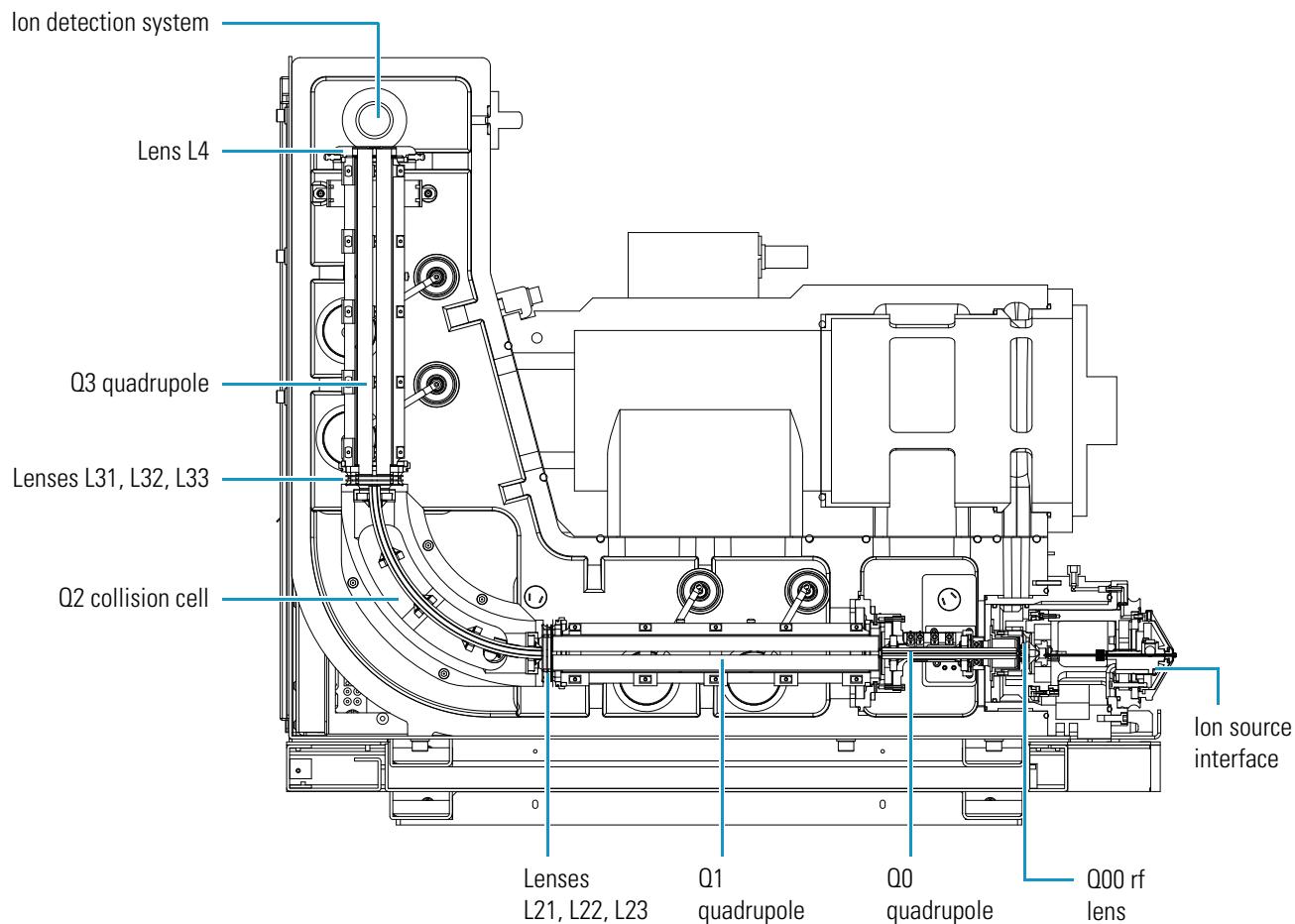
Figure 22. Lenses L11 (left) and L12 (right)



Mass Analyzer

The mass analyzer separates ions according to their mass-to-charge ratio and then passes them to the ion detection system. The mass analyzer on the TSQ consists of three quadrupole rod assemblies (Q1, Q2, and Q3) and three lens sets. See [Figure 23](#).

Figure 23. Mass analyzer, ion detection system, and ion optics



The following subtopics discuss the mass analyzer in detail:

- [Quadrupole Rod Assemblies](#)
- [RF and DC Fields Applied to the Quadrupoles](#)
- [Mass Analysis](#)
- [Collision Cell and CID Efficiency](#)
- [Quadrupole Offset Voltage](#)
- [Mass Analyzer Lenses](#)

Quadrupole Rod Assemblies

The three rod assemblies used in the TSQ mass spectrometer are numbered from the ion source end of the manifold and are designated Q1, Q2, and Q3. Q1 and Q3 are quadrupoles that enable high-resolution scans without signal loss.

Q1 and Q3 are square arrays of precision-machined and precision-aligned, true hyperbolic quadrupoles, called hyperquads (TSQ Vantage and TSQ Quantum Ultra) or hyperbolic-profile round rods (TSQ Quantum Access and TSQ Quantum Access MAX). See [Figure 24](#) and [Figure 25](#). Quartz spacers act as electrical insulators between adjacent rods.

Figure 24. Q1 or Q3 hyperquad of the TSQ Vantage or TSQ Quantum Ultra

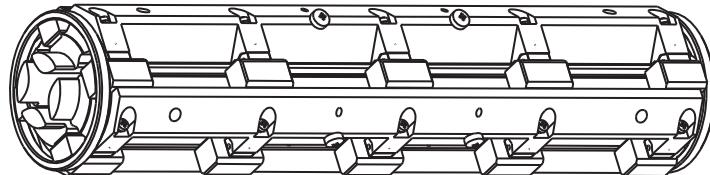


Figure 25. Q1 or Q3 quadrupole of the TSQ Quantum Access, or TSQ Quantum Access MAX

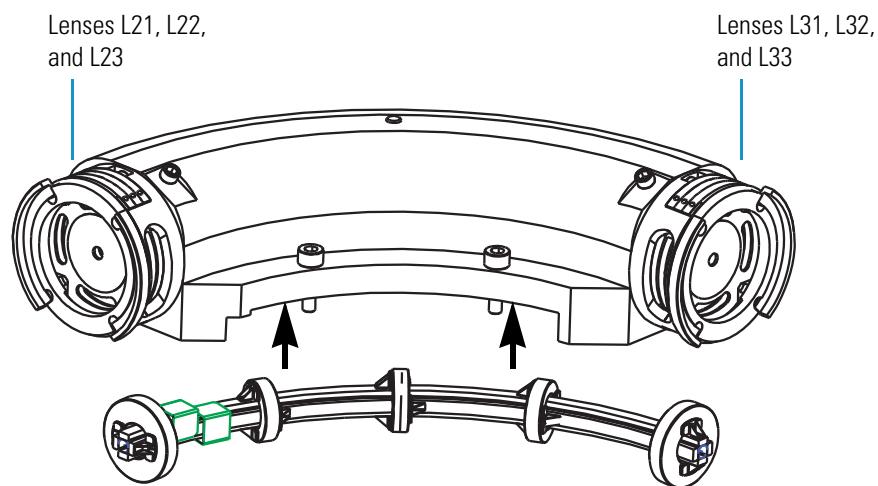


Q2 is a square-profile quadrupole rod assembly. Q2 always acts as an ion transmission device. The Q2 quadrupole rods are bent through a 90-degree arc. In addition to reducing the footprint of the instrument, this bending of the rods prevents the transmission of unwanted neutral species to the detector and dramatically lowers the noise level in the data. Q2 has become synonymous with the term *collision cell*. Technically, the collision cell is the chamber that encloses Q2 where collision-induced dissociation can take place if the argon collision gas is present. See [Figure 26](#).

2 Functional Description

Mass Spectrometer

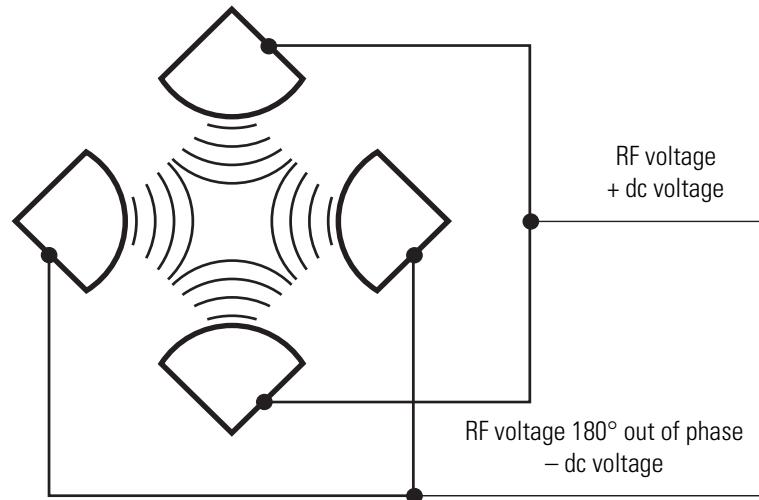
Figure 26. Collision cell (top), Q2 quadrupole (bottom), and lenses



RF and DC Fields Applied to the Quadrupoles

In a quadrupole rod assembly, because rods opposite each other in the array connect electrically, the four rods can be considered as two pairs of two rods each. Ac and dc voltages are applied to the rods and these voltages are ramped during the scan. Voltages of the same amplitude and sign are applied to the rods of each pair. However, the voltages applied to the different rod pairs are equal in amplitude but opposite in sign. See [Figure 27](#).

Figure 27. Polarity of the rf and dc voltages applied to the rods of the Q1 and Q3 mass analyzers



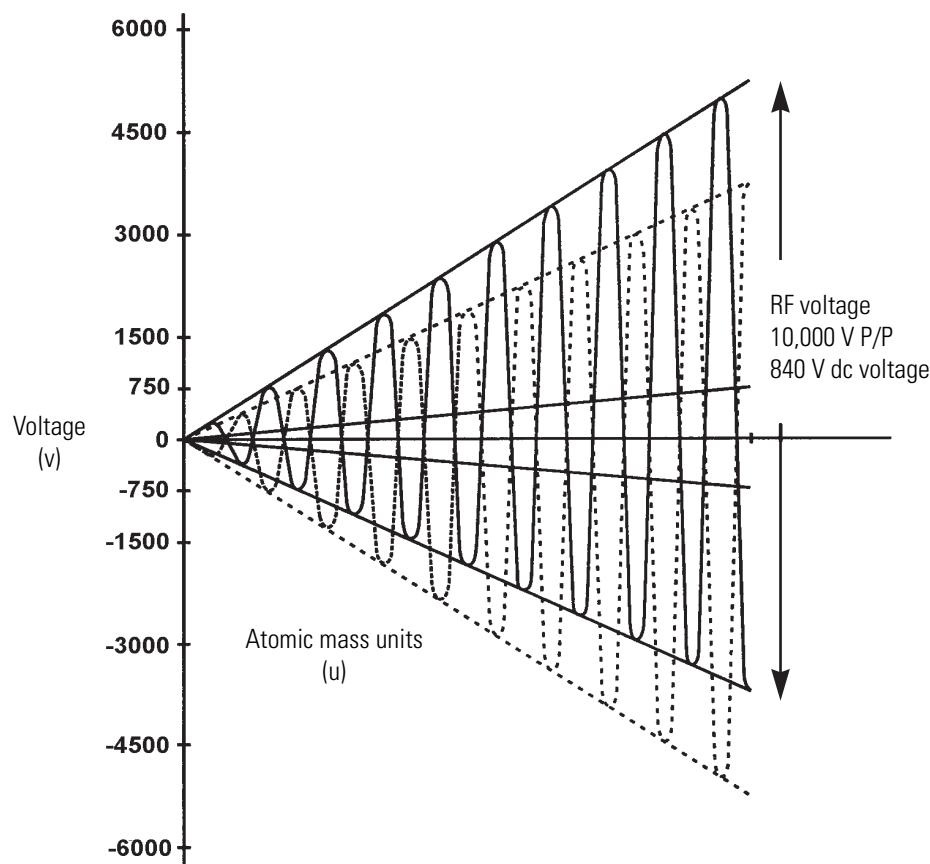
The ac voltage applied to the quadrupole rods is of constant frequency (1.123 MHz). The rf voltage applied to the rods varies from 0 to 10 000 V peak-to-peak, and the dc voltage varies from 0 to ± 840 V. Voltages of the same amplitude and sign are applied to each rod pair. However, the voltages applied to the other rod pair are equal in amplitude but opposite in sign.

Because the frequency of this ac voltage is in the radio frequency range, it is referred to as rf voltage. In Figure 28, the solid line represents the combined rf and dc voltage applied to one rod pair, and the dashed line represents the combined rf and dc voltage applied to the other rod pair. The ratio of rf voltage to dc voltage determines the ability of the mass spectrometer to separate ions of different mass-to-charge ratios.

The first and third quadrupole rod assemblies (Q1 and Q3 quadrupoles) can act as mass analyzers or as ion transmission devices. When both rf and dc voltages are applied, Q1 and Q3 function as mass analyzers. When only rf voltage is applied, they act as ion transmission devices. In the ion transmission mode, the quadrupole rod assemblies allow ions in a wide window of mass-to-charge ratios to pass.

The square quadrupole rod assembly (Q2) operates in the ion transmission mode only. Surrounding Q2 is a collision cell where collision-induced dissociation (CID) can take place if the argon collision gas is present in the cell.

Figure 28. Magnitude of the rf and dc voltages applied to the rods of the Q1 and Q3 mass analyzers



2 Functional Description

Mass Spectrometer

Mass Analysis

The mass analyzers (Q1 and Q3) are square arrays of precision-machined and precision-aligned hyperbolic or round-profile rods. The rods are charged with a variable ratio of rf voltage and dc voltage (Figure 28). These potentials give rise to an electrostatic field that gives stable oscillations to ions with a specific mass-to-charge ratio and unstable oscillations to all others.

At any given instant, one particular set of rf and dc voltage values is being applied to the mass analyzer rods. Under these conditions, only ions of one mass-to-charge ratio (for example, m/z 180) are maintained within bounded oscillations as their velocity carries them through the mass analyzer. At the same time, all other ions undergo unbounded oscillations. These ions strike one of the rod surfaces, become neutralized, and are pumped away, or they are ejected from the rod assembly.

Then, at a later time, both rf and dc voltages change, and ions of the next mass-to-charge ratio (for example, m/z 181) are allowed to pass, while all other ions (including m/z 180) become unstable and undergo unbounded oscillations. This process continues, with ions of one mass-to-charge ratio after another being transmitted, as the rf and dc voltages change in value. At the end of the scan, the rf and dc voltages are discharged to zero, and the process repeats.

The TSQ system can rapidly and precisely change the potentials on the quadrupole rods. The rf and dc voltages in the TSQ mass spectrometer can be scanned over the full mass range of the system, m/z 10 to 3000, in 0.85 seconds.

The more closely the electrostatic field generated by a set of quadrupole rods approximates a hyperbolic geometry, the better their operating characteristics are. As a result, the precision quadrupole rods of the TSQ mass spectrometer provide excellent sensitivity, peak shape, resolution, and high mass transmission.

Collision Cell and CID Efficiency

In the MS/MS scan modes, the TSQ applies a large voltage of opposite polarity to the rod pairs between scans, which empties the collision cell. This process ensures that no ions remain in the collision cell from scan to scan.

The collision cell quadrupole rod assembly (Q2), which always acts as an ion transmission device, is a quadrupole array of square-profile rods. A variable rf voltage charges the rods, which creates an electrostatic field that gives stable oscillations to ions in a wide window of mass-to-charge ratios.

The collision cell surrounds Q2 and is usually pressurized from about 1×10^{-3} to 4×10^{-3} Torr with argon collision gas. The collision cell is where collision-induced dissociation takes place.

CID is a process in which an ion collides with a neutral atom or molecule and then, because of the collision, dissociates into smaller fragments. The mechanism of dissociation involves converting some of the translational kinetic energy (TKE) of the ion into internal energy. This collision places the ion in an excited state. If the internal energy is sufficient, the ion fragments.

Three expressions convey the efficiency of the CID process:

- Collection efficiency
- Fragmentation efficiency
- Overall CID efficiency

Collection efficiency: The ion flux ratio measured at the exit of the collision cell and at its entrance. With no collision gas present, the TSQ obtains virtually 100 percent collection efficiency. Collection efficiency is a mass-dependent parameter. For example, with mid-range collision gas pressure, the collection efficiency might vary from about 50 percent for comparatively less massive ions (which are more prone to scatter) up to 75 percent for comparatively more massive ions (which are less prone to scatter).

Fragmentation efficiency: The fraction of the ion flux at the exit of the collision cell that results from fragmented ions. Fragmentation efficiency depends directly on the stability of the ion and indirectly on the mass of the ion. The more stable the ion, the less likely a given collision will fragment the ion. The more massive the ion, the greater its ability to distribute the vibrational energy imparted by a collision. As a result, ion fragmentation might decrease.

With mid-range collision gas pressure, fragmentation efficiency might vary from 15 percent to 65 percent for various compounds. As the collision gas pressure increases, the fragmentation efficiency for all compounds approaches 100 percent due to multiple collisions. The collection efficiency decreases, however, due to scattering.

Overall CID efficiency: The product of the collection efficiency and the fragmentation efficiency. The overall CID efficiency exhibits a maximum with intermediate pressure. As the pressure increases beyond the optimum value, more and more collisions take place, the probability of scattering increases, and fewer and fewer ions pass through the collision cell. Scattering results in the collection efficiency decreasing. The fragmentation efficiency also decreases as the pressure is decreased from its optimum value, because fewer and fewer collisions take place.

Quadrupole Offset Voltage

The quadrupole offset voltage is a dc potential applied to the quadrupole rods in addition to the ramping dc voltage. The offset voltage applied to the two rod pairs of the assemblies is equal in amplitude and equal in sign. The quadrupole offset voltage accelerates or decelerates ions and, therefore, sets the TKE of the ions as they enter the quadrupole rod assembly.

In general, for a given experiment, the TSQ has fixed offset voltages for Q1 and Q2. However, in MS/MS experiments, the quadrupole offset voltage applied to Q3 usually varies as a scan proceeds. The TSQ automatically computes the Q3 quadrupole offset voltage necessary and then varies the voltage, as appropriate, as each scan proceeds.

2 Functional Description

Mass Spectrometer

The offset voltage applied to Q2 (which contains the collision cell) is responsible for the collision energy. The collision energy is the difference in potential between the ion source (where parent ions are formed) and Q2 (where they collide with collision gas). As the offset voltage on Q2 increases, the TKE of the parent ions also increases. As a result, increases in the Q2 offset voltage increase the energy of ion/Ar collisions. The collision energy is generally set to one value for an entire scan and can be set from 0 to ± 200 V.

Before obtaining any mass spectra, the TSQ tunes Q1 in the Q1MS scan mode (Q2 and Q3 rf voltage only), and tunes Q3 in the Q3MS scan mode (Q1 and Q2 rf voltage only). During tuning, the TSQ determines the optimum quadrupole offset voltage for Q1 and for Q3.

Mass Analyzer Lenses

The TSQ system mass analyzer has three lens sets. See [Figure 26 on page 30](#). Those between Q1 and Q2 are designated L21, L22, L23; those between Q2 and Q3 are designated L31, L32, L33; and the lens between Q3 and the ion detection system is designated as L4 (or the exit lens). All of the lenses have circular holes in their centers through which the ion beam passes.

The lens assemblies also retain the three rod assemblies to ensure accurate and automatic axial alignment of the rod assemblies.

The L2x lens set (between Q1 and Q2) and the L3x lens set (between Q2 and Q3) serve these functions:

- To minimize the amount of collision gas that enters the mass analyzers (Q1 and Q3) from the collision cell (Q2). (For high-mass transmission, it is important to maintain a low pressure in the mass analyzers.)
- To retain the collision gas. Lenses L23 and L31 form two of the walls of the collision cell, so they tend to hold the collision gas in the collision cell. The collision gas escapes, however, through the same lens holes through which the ion beam passes.
- To prevent gas from entering the mass analyzers. Lenses L22 and L21 on one side of Q2 and lenses L32 and L33 on the other side of Q2 act as baffles to help prevent the gas that escapes from the collision cell from entering the mass analyzers.
- To shield Q1 from the rf voltage applied to Q2 and vice versa (L2x lens set) and to shield Q3 from the rf voltage applied to Q2 and vice versa (L3x lens set).
- To focus the ion beam. The three lenses between Q1 and Q2 (and those between Q2 and Q3) together form a three-element aperture lens. The first and third lenses are generally set to similar or identical values and the central lens is set to a value different (either higher or lower) from the other two.

The voltage applied to each of the lenses can vary from about -300 to $+300$ V. Typically, however, the voltage applied to the first and third elements of the L2x lens set is somewhat greater than the quadrupole offset voltage applied to Q1. Because the Q1 quadrupole offset voltage is generally set to about ± 5 V (depending on the charge of the ions of interest), the voltage applied to lenses L21 and L23 is typically about -10 V for positive ions and $+10$ V for negative ions. The voltage applied to the central lens of the L2x lens set is typically about ± 225 V.

In the Q3MS scan mode, the voltage applied to the lenses of the L3x lens set is about the same as that applied to the corresponding lens in the L2x lens set. Note, however, that in the MS/MS scan modes, the voltage applied to the L3x lens set automatically varies with the quadrupole offset voltage applied to Q3. As the Q3 quadrupole offset voltage ramps, the voltages applied to the lenses ramp correspondingly.

Lens L4 is located between Q3 and the ion detection system. L4 is held at ground potential. Its purpose is to shield Q3 from the high voltage applied to the ion detection system and to shield the ion detection system from the high rf voltages applied to Q3.

Ion Detection System

The TSQ mass spectrometer is equipped with a high-sensitivity, off-axis ion detection system. This system produces a high signal-to-noise ratio and allows for voltage polarity switching between positive ion and negative ion modes of operation. The ion detection system includes a 15 kV conversion dynode and a channel electron multiplier. See [Figure 29](#). The ion detection system is located at the rear of the vacuum manifold behind the mass analyzer.

The conversion dynode is a concave metal surface located at a right angle to the ion beam. The TSQ applies to the conversion dynode a potential of $+15$ kV for negative ion detection or -15 kV for positive ion detection. When an ion strikes the surface of the conversion dynode, one or more secondary particles are produced. These secondary particles can include positive ions, negative ions, electrons, and neutrals. When positive ions strike a negatively charged conversion dynode, the secondary particles of interest are negative ions and electrons. When negative ions strike a positively charged conversion dynode, the secondary particles of interest are positive ions. The curved surface of the conversion dynode focuses these secondary particles and a voltage gradient accelerates the particles into the electron multiplier.

The electron multiplier includes a cathode and an anode. The cathode of the electron multiplier is a lead-oxide, funnel-like resistor. The high voltage ring applies a potential of up to -2.5 kV to the cathode. The exit end of the cathode (at the anode) is near ground potential.

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

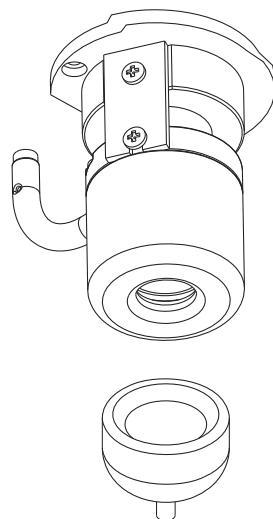
Secondary particles from the conversion dynode strike the inner walls of the electron multiplier cathode with sufficient energy to eject electrons. The ejected electrons are accelerated farther into the cathode, drawn by the increasingly positive potential gradient.

2 Functional Description

Mass Spectrometer

The funnel shape of the cathode causes the ejected electrons not to travel far before they again strike the inner surface of the cathode, which causes the emission of more electrons. A cascade of electrons is then created that finally results in a measurable current at the end of the cathode where the anode collects the electrons. The current collected by the anode is proportional to the number of secondary particles striking the cathode.

Figure 29. Ion detection system, showing the electron multiplier (top) and conversion dynode (bottom)



Typically, the electron multiplier is set to a gain of about 3×10^5 (that is, for each ion or electron that enters, 3×10^5 electrons exit) in MS mode and 2×10^6 in MS/MS mode. The electrometer circuit converts the current that leaves the electron multiplier via the anode to a voltage and the data system records the voltage.

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

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

Vacuum System and Inlet Gases Hardware

The vacuum system evacuates the region around the ion source interface, ion optics, mass analyzer, and ion detection system. The principal components of the vacuum system include the following:

- Vacuum manifold
- Turbomolecular pump

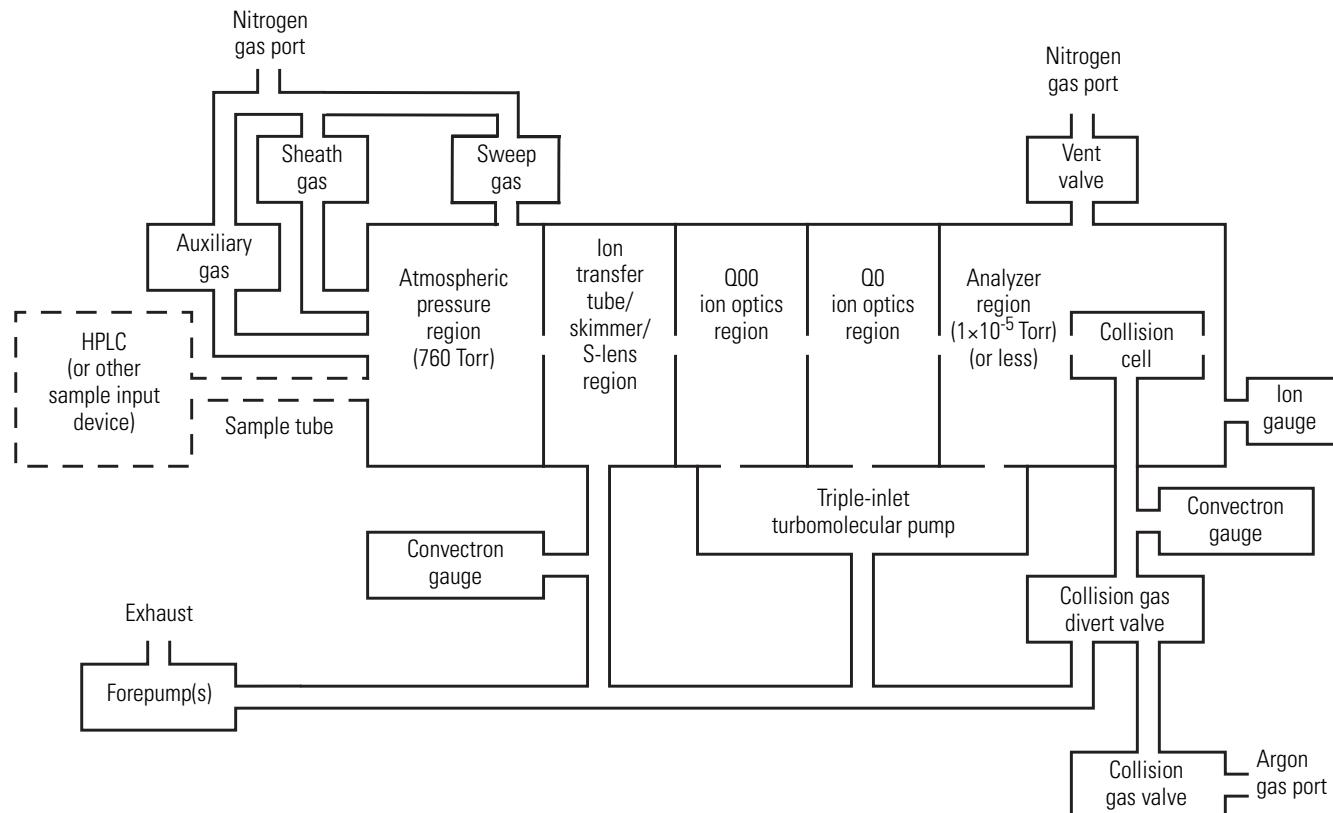
- Forepump
- Convectron™ gauges
- Ion gauges

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

- Vent valve
- Collision gas flow control valves
- Sheath gas valve
- Auxiliary gas valve

A functional block diagram of the vacuum system and inlet gasses hardware is shown in [Figure 30](#).

Figure 30. Functional block diagram of the vacuum system and inlet gasses hardware

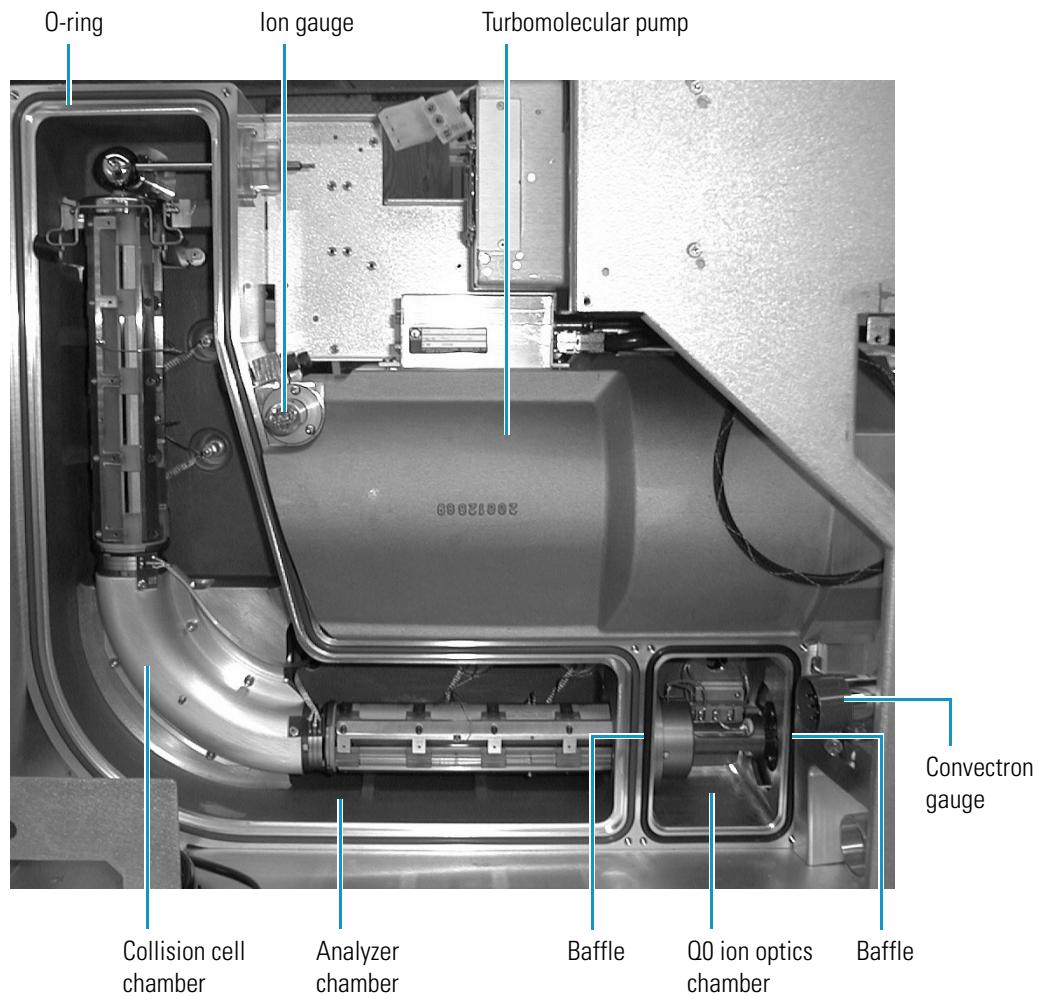


Vacuum Manifold

The vacuum manifold encloses the ion source interface, ion optics, mass analyzer, and ion detection system assemblies. The vacuum manifold is a thick-walled, aluminum chamber with two removable side cover plates, with openings on the front, sides, and top, and various electrical feedthroughs and gas inlets.

The vacuum manifold is divided into four chambers by three baffles. See [Figure 31](#). The forepump evacuates the region inside the first chamber, called the ion transfer tube/skimmer region. The third inlet in the molecular drag section of the triple-inlet turbomolecular vacuum pump evacuates the region inside the second chamber, called the Q00 ion optics region. The interstage port of the turbomolecular vacuum pump evacuates the region inside the third chamber, called the Q0 ion optics region. The high vacuum port of the turbomolecular pump evacuates the region inside the fourth chamber, called the analyzer region, to less than 10^{-5} Torr. The turbomolecular pump in turn discharges into the forepump through the foreline.

Figure 31. Vacuum manifold (interior)



The collision cell chamber, inside the analyzer chamber, has a user controlled argon pressure of between one and four mTorr when CID is turned on. Argon in the collision cell is evacuated by the forepump when CID is turned off.

The vacuum manifold has the following feedthroughs and inlets:

- A feedthrough for the high voltage for the conversion dynode
- A feedthrough for the high voltage for the electron multiplier
- A feedthrough for the ion current signal from the anode of the electron multiplier
- Two feedthroughs for the Q1 quadrupole rf voltage
- Two feedthroughs for the Q3 quadrupole rf voltage
- A feedthrough for the Q2 quadrupole rf voltage
- A feedthrough for lens L21, L22, L23, L31, L32, and L33 voltages
- A feedthrough for lens L0, L11, and L12 voltages
- A feedthrough for the Q00 and Q0 ion optics rf voltages
- A feedthrough for the tube lens offset voltage, ion transfer tube offset voltage, and ion transfer tube heater voltages
- A vacuum connection for measuring the pressure in the analyzer region with the ion gauge
- An argon gas inlet into the collision cell
- A vent gas inlet

Two removable side cover plates on the left side of the vacuum manifold allow access to the Q0 ion optics, mass analyzer, and ion detection system. Two electrically conductive O-rings provide a vacuum-tight seal between the side cover plates and the vacuum manifold.

Turbomolecular Pump

A Leybold TW220/150/15S triple-inlet turbomolecular pump provides the vacuum for the Q00 ion optics region, Q0 ion optics region, and analyzer region of the vacuum manifold. The turbomolecular pump mounts onto the top of the vacuum manifold ([Figure 31](#)).

The turbomolecular pump has three pumping inlets:

- A high-vacuum inlet at the top of the rotor stack, which evacuates the analyzer chamber
- An interstage inlet about halfway down the rotor stack, which evacuates the Q0 ion optics chamber
- A third inlet in the molecular drag section of the pump, which evacuates the Q00 ion optics chamber

2 Functional Description

Mass Spectrometer

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

Power to the turbomolecular pump is shut off if the foreline pressure, as measured by the Convectron gauge, is too high, or if the turbomolecular temperature is too high.

Forepump

One (TSQ Quantum Access and TSQ Quantum Access MAX) or two (TSQ Vantage and TSQ Quantum Ultra) Edwards™ E2M30 forepumps (or roughing pumps) establish the vacuum necessary for the proper operation of the turbomolecular pump. The forepump also evacuates the inlet valve and the collision cell. The pump has a maximum displacement of 650 L/min and maintains a minimum pressure of approximately 1 Pa (0.01 Torr).

The forepump connects to the turbomolecular pump by a section of reinforced PVC tubing. The power cord of the forepump plugs into the outlet labeled *Forepump* on the power panel (see [Figure 13 on page 21](#)). This outlet supplies power to the pump and is controlled by the Main Power circuit breaker switch and Vacuum service switch, not by the Electronics service switch.



CAUTION Always plug the forepump power cord into the outlets labeled *Forepump* on the right-side power panel of the mass spectrometer. Never plug it directly into a wall outlet.

Convectron Gauges

A Convectron gauge measures the pressure in the inlet valve and the foreline, which connects the turbomolecular pump and the forepump. The Convectron gauge uses a Wheatstone bridge with a temperature dependent resistor to measure pressure down to a fraction of a milliTorr. A second Convectron gauge measures the pressure of argon collision gas in the collision cell.

Ion Gauges

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

Vent Valve

The vent valve, located in the area of Q2, allows the vacuum manifold to be vented to dry nitrogen or filtered air. The vent valve is a solenoid-operated valve, which is controlled by the Vent Delay PCB. When the solenoid is energized, the vent valve closes. If the power fails or the main power circuit breaker is placed in the Off (O) position, a 4-farad capacitor, which is located in the Power Entry Module, keeps the solenoid in the closed position for several minutes. If power is not restored in this time, then the solenoid opens and the system is vented with dry nitrogen or filtered air. Dry nitrogen (35 kPa [5 psi], maximum, 99% purity) enters the mass spectrometer through a 1/4 in. port on the left side of the mass spectrometer. See [Figure 32](#). The vent valve closes after power is restored to the mass spectrometer.

Collision Gas Flow Control Valves

The collision gas flow control valves control the flow of argon collision gas into and out of the Q2 collision cell. A solenoid valve acts to shut off argon gas flow to the cell. The collision gas pressure is regulated by a proportional valve that is controlled by the data system. You can set the collision gas pressure (0 to 5 milliTorr) in the Define Scan dialog box of the EZ Tune window.

Ions enter the Q2 collision cell, collide with the argon collision gas, and then, because of the collision, dissociate into smaller fragments. See [“Collision Cell and CID Efficiency” on page 32](#).

Argon (135 ± 70 kPa [20 ± 10 psi], 99.995% minimum purity) enters the mass spectrometer through a 1/8-in. port on the left side of the mass spectrometer. See [Figure 32](#).

A second proportional valve allows the forepump to evacuate the Q2 collision cell of argon and waste gasses when CID is turned off. The TSQ mass spectrometer automatically opens and closes the collision gas evacuation valve, depending on whether Q2 is acting as an ion transmission device or a collision cell.

Sheath Gas Valve

The sheath gas valve controls the flow of sheath gas (nitrogen) into the API source. Dry nitrogen (690 ± 140 kPa [100 ± 20 psi], 99% purity) enters the mass spectrometer through a 1/4 in. port on the left side of the mass spectrometer. See [Figure 32](#). A solenoid shutoff valve starts and stops the flow of nitrogen to the API source. The data system controls a valve that regulates the sheath gas pressure. You can set the sheath gas flow rate (0 to 100 in arbitrary units) in the Ion Source dialog box from the EZ Tune window. The sheath gas enters the API source through 1/8 in. ID tubing.

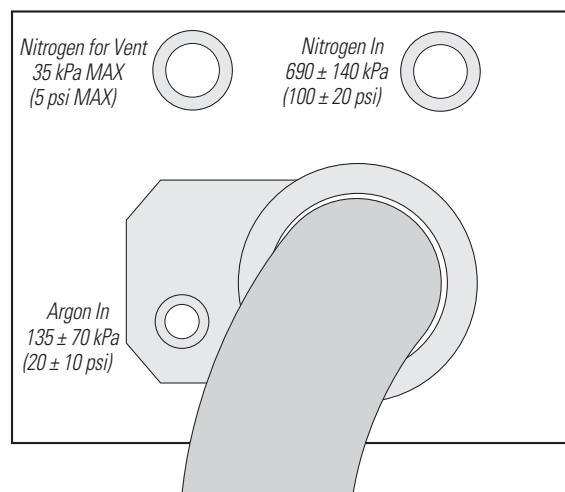
2 Functional Description

Mass Spectrometer

Auxiliary Gas Valve

The auxiliary gas valve controls the flow of auxiliary gas (nitrogen) into the API source. Dry nitrogen (690 ± 140 kPa [100 ± 20 psi], 99% purity) enters the mass spectrometer through a 1/4 in. port on the left side of the mass spectrometer. A solenoid shutoff valve starts and stops the flow of nitrogen to the API source. The auxiliary gas pressure is regulated by a flow valve that is controlled by the data system. You can set the auxiliary gas flow rate (0 to 60 in arbitrary units) in the Ion Source dialog box. The auxiliary gas enters the API source through 1/8 in. ID tubing.

Figure 32. Nitrogen and argon gas inlets



Electronic Assemblies

The electronic assemblies that control the operation of the mass spectrometer are distributed among various PCBs and other modules located in the tower, in the embedded computer, and on or around the vacuum manifold of the mass spectrometer.

The Power Entry Module provides mass spectrometer power control, a contact closure interface, vent valve control, an Ethernet 100 base-T connection from the System Control PCB to the data system PC, a mechanical pump failure protection circuit (linked to vent valve control), a system reset button, status LEDs, and service ports. The right-side power panel, shown in [Figure 13](#) on [page 21](#), is part of the Power Entry Module.

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

- Main power circuit breaker switch
- Surge suppressor
- Line filter
- Electronics service switch
- Vacuum service switch

The “brains” of the TSQ mass spectrometer is the System Control PCB. The System Control PCB and embedded computer include the following:

- PowerPC processor
- Serial Peripheral Interconnect (SPI) bus
- I/O coprocessor
- Super Harvard Architecture Computer (Sharc) bus
- Scan generator DSP
- Acquisition processor DSP
- Interbus bridge
- 100 base-T Ethernet port

The rf voltage generation electronic assemblies produce the S-lens (TSQ Vantage only), Q00, Q0, Q1, Q2, and Q3 rf voltages that enable ion transmission and mass analysis. The Analyzer Control PCB and the System Control PCB control all rf voltages.

The Q1 and Q3 rf voltage amplifier circuits are identical, and the circuits for Q0 and Q2 are similar.

The rf voltage generation electronic assemblies include the following components:

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

The ion detection system electronic assemblies provide high voltage to the electron multiplier and conversion dynode of the ion detection system. They also receive the electron multiplier output current signal, convert it to a voltage (by the electrometer circuit), and pass it to the embedded computer.

The ion detection system electronic assemblies include the following:

- Electron multiplier power supply
- Conversion dynode power supply
- Electrometer PCB
- Acquisition DSP

2 Functional Description

Data System

The Analyzer Control PCB contains circuitry for controlling and monitoring the operation of the ion source, ion optics, mass analyzer, and ion detection system. These circuits are in turn monitored by the PowerPC processor of the System Control PCB via the SPI bus.

The Analyzer Control PCB controls and monitors the rf voltages for Q0, Q1, Q2, and Q3 quadrupoles. It also has lens voltage drivers that convert ± 330 V dc power from the DC Rod Driver PCB to dc voltages that are applied to the lenses.

Data System

The data system controls and monitors the TSQ mass spectrometer. The data system also processes data that the TSQ mass spectrometer acquires. The data system is composed of the following:

- [Computer Hardware](#)
- [Data System / Mass Spectrometer / LC Interface](#)
- [Data System / Local Area Network Interface](#)

Computer Hardware

The data system computer has the following major features:

- Intel™ Pentium™ IV processor
- High capacity hard disk drive
- Recordable/rewriteable CD drive
- Primary Ethernet port (data system to mass spectrometer)
- Secondary Ethernet port (data system to local area network)
- High performance video graphics card
- DVD drive
- 1280×1024 resolution color monitor
- Keyboard and mouse
- Laser printer

For more information about the computer, refer to the appropriate manuals.

Data System / Mass Spectrometer / LC Interface

The data system computer contains a 100 base-T Ethernet adapter (called the primary Ethernet adapter) that is dedicated to data system/mass spectrometer/LC communications. This primary Ethernet adapter communicates with the mass spectrometer, Accela PDA detector, and autosampler via a 10/100 base-T Ethernet switch. The Ethernet adapter on the mass spectrometer resides on the System Control PCB. A twisted pair Ethernet cable connects the primary Ethernet adapter of the data system with the Ethernet connector on the power panel of the mass spectrometer. See [Figure 33](#). The mass spectrometer communicates with the Accela LC pump via a USB connection

Data System / Local Area Network Interface

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

Printer

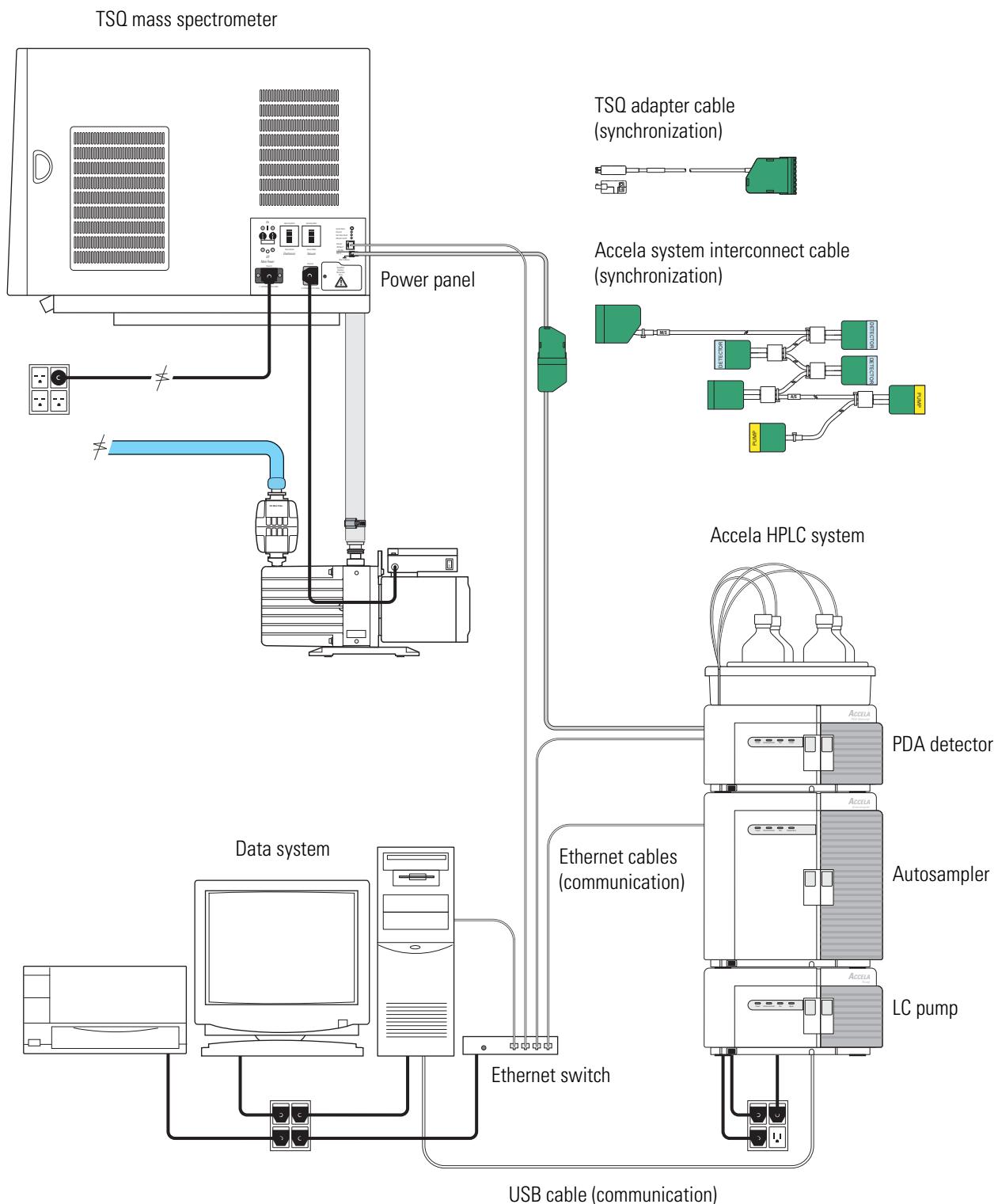
A high-resolution laser printer communicates with the PC via the local area network. Refer to the manual supplied by the manufacturer for details about the printer.

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

2 Functional Description

Data System

Figure 33. TSQ system interconnect diagram, showing the TSQ mass spectrometer, Accela HPLC, and data system



System Shutdown, Startup, and Reset

Many maintenance procedures for the TSQ system require that the mass spectrometer be shut down completely. In addition, you can place the TSQ mass spectrometer in standby mode if the system is not to be used for 12 hours or more.

Contents

- [Shutting Down the System in an Emergency](#)
- [Placing the System in Standby Condition](#)
- [Shutting Down the System Completely](#)
- [Starting Up the System after a Complete Shutdown](#)
- [Resetting the Mass Spectrometer](#)
- [Resetting the Data System](#)
- [Turning Off Selected Mass Spectrometer Components](#)

Shutting Down the System in an Emergency

If you need to turn off the mass spectrometer in an emergency, use the following process.



CAUTION Place the Main Power circuit breaker switch, located on the power panel on the right-side panel of the mass spectrometer, in the Off (O) position. See [Figure 34](#) and [Figure 35](#). This turns off all power to the mass spectrometer, including the vacuum pumps. Although removing power abruptly will not harm any component within the system, under normal conditions do not shut down the system with the main power circuit breaker switch. For the recommended procedure, see “[Shutting Down the System Completely](#)” on page 50.

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

3 System Shutdown, Startup, and Reset

Shutting Down the System in an Emergency

Figure 34. Power panel of the TSQ Vantage or TSQ Quantum Ultra, showing the Main Power circuit breaker switch, Electronics service switch, and System Reset button

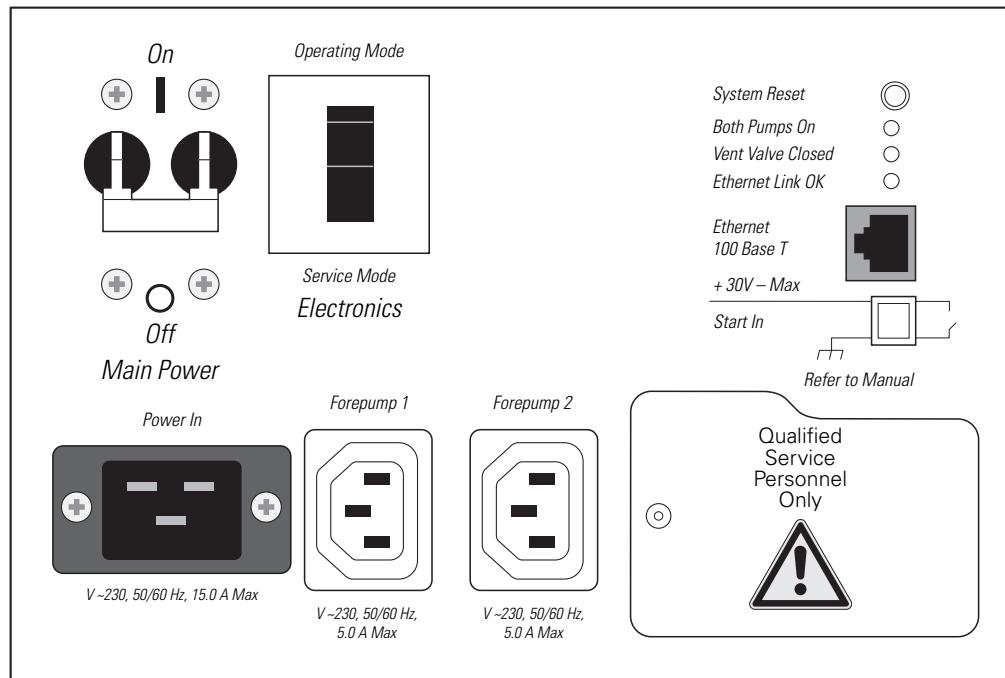
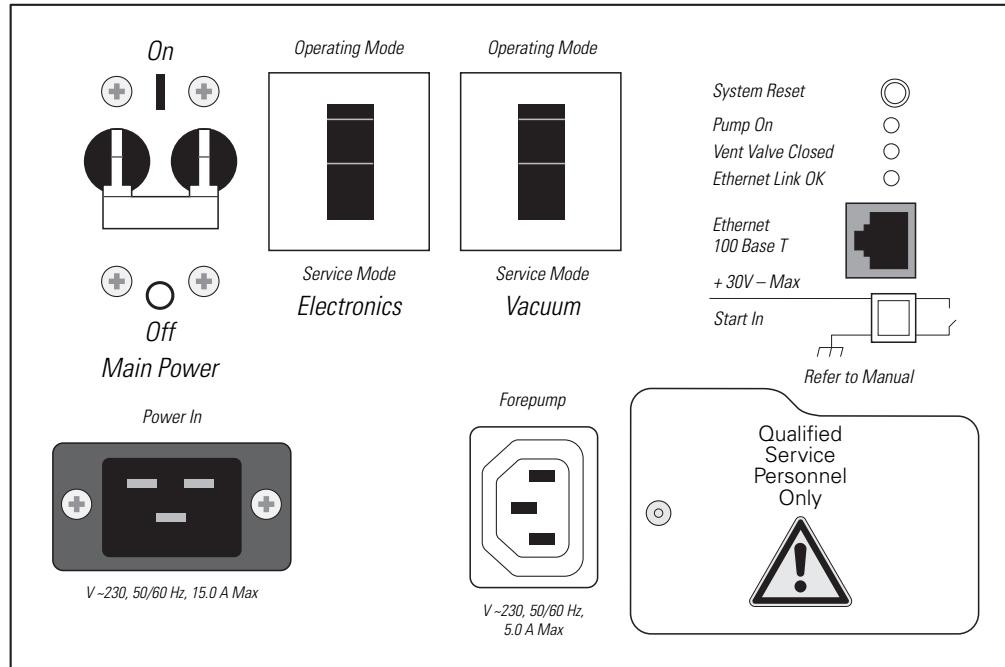


Figure 35. Power panel of the TSQ Quantum Access, or TSQ Quantum Access MAX, showing the Main Power circuit breaker switch, Electronics service switch, Vacuum service switch, and System Reset button



Placing the System in Standby Condition

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

❖ To place the TSQ system in standby mode

1. Wait until data acquisition, if any, is complete.
2. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source:
 - a. Choose **Start > Programs > Thermo Instruments > TSQ > TSQ Tune** to open the EZ Tune window.
 - b. In the EZ Tune window, choose **Setup > Inlet Direct Control**. The Inlet Direct Control view appears.
 - c. Click the **LC** tab and click  (Stop) to stop the LC pump.
3. From the EZ Tune window, choose **Control > Standby** (or click the **On/Standby** button) to put the mass spectrometer in standby.



On



Off



Standby

When you choose Control > Standby, the TSQ system turns off the electron multiplier, conversion dynode, 8 kV power to the API source, and the mass analyzer and ion optics rf voltages. The TSQ system also turns off the auxiliary gas and sets the sheath gas flow to zero units. See [Table 2 on page 58](#) 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 illuminates yellow when the system is in standby.

4. Flush the ion sweep cone and ion transfer tube of the API source as described in the topic [“Cleaning the Ion Sweep Cone and Ion Transfer Tube” on page 66](#).
5. Leave the mass spectrometer power on.
6. Leave the LC power on.
7. Leave the autosampler power on.
8. Leave the data system power on.

3 System Shutdown, Startup, and Reset

Shutting Down the System Completely

Shutting Down the System Completely

Shut down the TSQ system completely if not in use for an extended period only, or if it must be shut down for a maintenance or service procedure. For a short period of time, such as overnight or over weekends, you can place the system in standby. See “[Placing the System in Standby Condition](#).”

❖ To shut down the TSQ system completely

1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source. To turn off the flow of liquid from the LC to the API source, do the following:
 - a. Choose **Start > Programs > Thermo Instruments > TSQ > TSQ Tune** to open the EZ Tune window.
 - b. In the EZ Tune window, choose **Setup > Inlet Direct Control**. The Inlet Direct Control view appears.
 - c. Click the **LC** tab and click  (Stop) to stop the LC pump.
2. From the EZ Tune window, choose **Control > Off** (or click the **On/Standby/Off** button) to turn off the mass spectrometer.



3. Place the Electronics service switch, located on the power panel (see [Figure 34](#) and [Figure 35](#)), in the Service Mode position.
4. On the TSQ Quantum Access or TSQ Quantum Access MAX, place the Vacuum service switch, located on the power panel (see [Figure 35](#) on page 48), in the Service Mode position.
5. Place the Main Power circuit breaker switch, located on the power panel (see [Figure 34](#) and [Figure 35](#)) in the Off (O) position. When you place the Main Power circuit breaker switch in the Off (O) position, the following occurs:
 - All power to the mass spectrometer is turned off. (All LEDs on the front panel of the mass spectrometer are off.)
 - A capacitor on the Vent Delay PCB provides power to the vent valve for two to four minutes (to allow the turbomolecular pump to spin down). After the capacitor discharges, power to the vent valve solenoid shuts off. When power to the vent valve solenoid shuts off, the vent valve opens and the vacuum manifold is vented to filtered air or nitrogen.
 - After about two minutes, the pressure of the vacuum manifold reaches 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, argon and nitrogen gases, data system, or autosampler. In this case, the shutdown procedure is completed. However, if you do not plan to operate your system for an extended period of time, Thermo Fisher Scientific recommends that you turn off the LC, data system, and autosampler as described in the following steps, 7 through 12.

7. Turn off the (optional) LC. Follow the procedure described in the manual that came with the LC.
8. Turn off the argon collision gas supply at the tank.
9. Turn off the nitrogen supply at the tank.
10. Turn off the data system:
 - a. Choose **Start > Shut Down** from the Windows™ taskbar. The Shut Down Windows dialog box appears.
 - b. To start the Windows shutdown procedure, select **Shut down** and click **OK**.
11. Turn off the laser printer by using the on/off switch.
12. Turn off the autosampler by using the Main Power on/off switch.

3 System Shutdown, Startup, and Reset

Starting Up the System after a Complete Shutdown

Starting Up the System after a Complete Shutdown

To start up the TSQ system after it has been shut down completely, do the following procedures:

- [Starting Up the LC \(optional\)](#)
- [Starting Up the Data System](#)
- [Starting Up the Mass Spectrometer](#)
- [Starting Up the Autosampler \(optional\)](#)
- [Setting Up Conditions for Operation](#)

Starting Up the LC

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

Starting Up the Data System

❖ To start up the data system

1. Turn on the monitor, computer, and printer.
2. Observe the Windows XP startup procedure on the monitor and press CTRL+ALT+DEL when you are prompted to do so.
3. In the Logon Information dialog box, click **OK** or enter your password (if you have one).

Starting Up the Mass Spectrometer

❖ To start up the mass spectrometer

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

1. Turn on the flows of argon and nitrogen at the tanks if they are off.
2. Make sure that the Main Power circuit breaker switch is in the Off (O) position and that the Electronics service switch and the Vacuum service switch (TSQ Quantum Access or TSQ Quantum Access MAX) are both in the Service Mode position.
3. Plug in the power cord for the mass spectrometer.

4. Place the Main Power circuit breaker switch in the On (|) position. When you place the Main Power circuit breaker switch in the On (|) position, power is supplied to those mass spectrometer components that are not affected by the Vacuum service switch and the Electronics service switch.
5. On the TSQ Quantum Access or TSQ Quantum Access MAX, place the Vacuum service switch in the Operational position.
6. Place the Electronics service switch in the Operational position. When you place the Electronics service switch in the Operational position, the following occurs:
 - The Power LED on the mass spectrometer front panel illuminates green to indicate that power is provided to the mass spectrometer electronics. (The electron multiplier, conversion dynode, ion source, and mass analyzer and ion optics rf voltages remain off.)
 - The embedded computer reboots. After several seconds the Communication LED on the front panel illuminates 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 illuminates green to indicate that the data system and the mass spectrometer have established a communication link. Software for the operation of the mass spectrometer is then transferred from the data system to the mass spectrometer.
 - After three minutes, the System LED illuminates yellow to indicate that the software transfer from the data system to the mass spectrometer is complete and that the instrument is in standby.
 - The Vacuum LED on the front panel of the mass spectrometer remains off until the turbomolecular pump reaches 80 percent of its operational speed of 750 Hz. At this time the ion gauge is turned on and the Vacuum LED illuminates yellow. The Vacuum LED illuminates green, and the high voltage can be turned on, only if the pressure in the mass analyzer region, as measured by the ion gauge, is below the maximum allowable pressure of 7×10^{-4} Torr.

If you have an autosampler, go to the next topic, “[Starting Up the Autosampler](#).” If you do not have an autosampler, go to the topic “[Setting Up Conditions for Operation](#).”

Starting Up the Autosampler

❖ To start up the autosampler

Place the main power switch on the autosampler in the on position. If necessary, configure the autosampler. For procedures for placing sample vials, preparing solvent and waste bottles, installing syringes, and so on, refer to the manual that came with the autosampler. Refer also to the *TSQ Series Getting Connected Guide*.

3 System Shutdown, Startup, and Reset

Starting Up the System after a Complete Shutdown

Setting Up Conditions for Operation

❖ To set up your TSQ mass spectrometer for operation

1. Before you begin data acquisition with your TSQ system, allow the system to pump down for at least one hour. Operation of the system with excessive air and water in the vacuum manifold can cause reduced sensitivity, tuning problems, and reduced lifetime of the electron multiplier.
2. Ensure that the argon pressure and nitrogen pressure are within the operational limits [argon: 135 ± 70 kPa (20 ± 10 psig), nitrogen: 690 ± 140 kPa (100 ± 20 psig)].

Note Air in the argon line must be purged or given sufficient time to be purged for normal TSQ mass spectrometer performance.

3. In the EZ Tune window, choose **View > Instrument Status** and look at the Instrument Status view. Check that the ion gauge pressure is below about 5×10^{-6} Torr, and that the forepump pressure is below about 50 mTorr (with the ion transfer tube sealed with a septum cap).
4. Remove the septum cap from the orifice of the ion transfer tube.
5. Set up the API source for operation as described in the *Ion Max and Ion Max-S API Source Hardware Manual*, *HESI-II Probe User Guide*, *H-ESI Probe User Guide*, *Nanospray Ion Source Operator's Manual*, and *TSQ Series Getting Started Guide*.

Note You do not need to calibrate and tune the TSQ mass spectrometer each time you restart the TSQ system.

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 TSQ mass spectrometer (that is, optimize the tune and calibration parameters) perhaps once a quarter. Refer to “Automatic Tuning and Calibrating in the ESI/MS Mode” in the *TSQ Series Getting Started Guide* for a procedure for tuning and calibrating the TSQ mass spectrometer.

You must optimize the tune parameters (or change the Tune Method) whenever you change the type of experiment. For procedures on how to optimize the tune parameters for an ESI or APCI experiment, refer to “Optimizing the Mass Spectrometer with Your Compound in ESI/MS/MS Mode” or “Optimizing the Mass Spectrometer with Your Compound in APCI/MS/MS Mode” in the *TSQ Series Getting Started Guide*.

Resetting the Mass Spectrometer

If communication between the mass spectrometer and data system computer is lost, it might be necessary to reset the mass spectrometer using the System Reset button on the right-side power panel. Pressing the System Reset button creates an interrupt in the embedded computer. This causes the embedded computer to restart in a known (default) state. See [Figure 34](#) on [page 48](#) for the location of the System Reset button.

The procedure given here 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, go to [“Starting Up the System after a Complete Shutdown”](#) on [page 52](#).

❖ **To reset the mass spectrometer**

Press the System Reset button located on the right-side power panel. Make sure the Communication LED is extinguished before releasing the System Reset button. When you press the Reset button, the following occurs:

- An interrupt on the embedded computer causes the CPU to reboot. All LEDs on the front panel of the mass spectrometer are off except the Power LED.
- After several seconds, the Communication LED illuminates 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 illuminates green to indicate that the data system and the mass spectrometer have established a communication link. Software for the operation of the mass spectrometer is then transferred from the data system to the mass spectrometer.
- After three minutes the software transfer is complete. The System LED illuminates either green to indicate that the instrument is functional and the high voltages are on, or yellow to indicate that the instrument is functional and is in standby.

Resetting the Data System

There are two ways to reset the data system:

- [Resetting the Data System by Using the Windows Shutdown and Restart Procedure](#)
- [Resetting the Data System by Turning the Personal Computer Off Then On](#)

3 System Shutdown, Startup, and Reset

Resetting the Data System

Resetting the Data System by Using the Windows Shutdown and Restart Procedure

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

❖ To reset the data system by using the Windows shutdown and restart procedure

1. Choose **Start > Shut Down** from the Windows taskbar. The Shut Down Windows dialog box appears.
2. To start the Windows shutdown and restart procedure, select **Restart** and click **OK**.
3. Observe the Windows shutdown and restart procedure on the monitor. Press **CTRL+ALT+DELETE** when you are prompted to do so.
4. To complete the shutdown and restart procedure, click **OK** or enter your password (if you have one) in the Logon Information dialog box.

Note The communications link between the data system and the mass spectrometer should automatically reestablish after you reset the data system. When this occurs the Communication LED on the front panel of the mass spectrometer illuminates yellow and then green. If the system is unable to reestablish the communications link, press the System Reset button on the power panel of the mass spectrometer.

Resetting the Data System by Turning the Personal Computer Off Then On

If you are unable to reset the data system by using the Windows shutdown and restart procedure, proceed as follows:

1. Press the Power button on the personal computer to turn the personal computer off.
2. After several seconds, press the Power button on the personal computer to turn the personal computer on.
3. Observe the Windows XP startup procedure on the monitor and press **CTRL+ALT+DELETE** when you are prompted to do so.
4. To complete the shutdown and restart procedure, click **OK** or enter your password in the Logon Information dialog box.
5. When the shutdown and restart procedure has completed, choose **Start > All Programs > Thermo Instruments > TSQ > TSQ Tune** to display the EZ Tune window.

Note The communications link between the data system and the mass spectrometer should automatically reestablish after you reset the data system. When this occurs the Communication LED on the front panel of the mass spectrometer illuminates yellow and then green. If the system is unable to reestablish the communications link, press the System Reset button on the right-side power panel of the Power Entry Module of the mass spectrometer.

Turning Off Selected Mass Spectrometer Components

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

- Turn off individual mass spectrometer components from the EZ Tune window. Turning off individual mass spectrometer components might be necessary when you are troubleshooting or when you are running certain diagnostic procedures.
- Place the mass spectrometer in standby mode. Standby is the normal condition to leave the mass spectrometer in when it is not in use. Choose **Control > Standby** (or turn the On/Standby button on or off) from the EZ Tune window to place the mass spectrometer in standby.
- Place the mass spectrometer in the off condition. The off condition is similar to standby, except all high voltage components of the mass spectrometer are turned off. Choose **Control > Off** from the EZ Tune window to place the mass spectrometer in the off condition.
- Place the Electronics service switch in the Service Mode position. The Electronics service switch turns off all components in the mass spectrometer other than the +24 V power supply, forepump, turbomolecular pump, Vent Delay PCB, and fans.
- Place the Vacuum service switch on the TSQ Quantum Access or TSQ Quantum Access MAX in the Service Mode position. The Vacuum service switch turns off all vacuum system components, including the +24 V power supply, forepump, turbomolecular pump, Vent Delay PCB, and fans.
- Place the Main Power circuit breaker switch in the Off (O) position. Placing the Main Power circuit breaker switch in the Off (O) position removes all power to the mass spectrometer, including the vacuum system.

3 System Shutdown, Startup, and Reset

Turning Off Selected Mass Spectrometer Components

Table 2 summarizes the on/off status of mass spectrometer components, voltages, and gas flows.

Table 2. On/Off status of mass spectrometer components, voltages, and gas flows (Sheet 1 of 2)

Mass spectrometer component	Standby	Off	Electronics service switch in Service Mode position	Vacuum service switch (TSQ Quantum Access or Access MAX) in Service Mode position	MS Main Power circuit breaker switch in Off position
Electron multiplier	Off	Off	Off	Off	Off
Conversion dynode	Off	Off	Off	Off	Off
Mass analyzer rf voltage	Off	Off	Off	Off	Off
Mass analyzer dc offset voltage	Off	Off	Off	Off	Off
Q00 and Q0 ion optics rf voltage	Off	Off	Off	Off	Off
Q00 and Q0 ion optics dc offset voltage	Off	Off	Off	Off	Off
Tube lens or S-lens	On	Off	Off	Off	Off
Ion transfer tube heater	On	Off	Off	Off	Off
Ion transfer tube dc offset	On	Off	Off	Off	Off
APCI corona discharge needle	Off	Off	Off	Off	Off
APCI vaporizer	Off	Off	Off	Off	Off
ESI needle	Off	Off	Off	Off	Off
Sheath gas	Off	Off	Off	Off	Off
Auxiliary gas	Off	Off	Off	Off	Off
Argon collision gas	Off	Off	Off	Off	Off
Vent valve	Closed	Closed	Closed	Open (after 2 to 4 min)	Open (after 2 to 4 min)
Turbomolecular pump	On	On	On	Off	Off
Forepump	On	On	On	Off	Off
Vent Delay PCB	On	On	On	Off	Off
Embedded computer	On	On	Off	On	Off
Turbomolecular pump controller	On	On	On	Off	Off
Power supply, electron multiplier, and conversion dynode	Off	Off	Off	Off	Off
Power supply, 8 kV	Off	Off	Off	Off	Off
PS1 power supply, +24 V	On	On	On	Off	Off

Table 2. On/Off status of mass spectrometer components, voltages, and gas flows (Sheet 2 of 2)

Mass spectrometer component	Standby	Off	Electronics service switch in Service Mode position	Vacuum service switch (TSQ Quantum Access or Access MAX) in Service Mode position	MS Main Power circuit breaker switch in Off position
PS2 power supply, +5, ±15, ±24 V dc			Off	Off	Off
PS3 power supply, +36, -28 V dc	On	On	Off	Off	Off
Fan, turbomolecular pump	On	On	On	Off	Off
Fan, above manifold	On	On	On	Off	Off
Fan, center wall	On	On	On	Off	Off
Convectron gauge, foreline	On	On	On	On	Off
Convectron gauge, collision cell	On	On	Off	On	Off
Ion gauge	On	On	Off	Off	Off

Daily Operation

To ensure the proper operation of your system, Thermo Fisher Scientific recommends daily performance of these checks and cleaning procedures for the TSQ system.

Contents

- [Things to Do Before Operating the TSQ System](#)
- [Things to Do After Operating the TSQ System](#)

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

Tune parameters are instrument parameters that affect the intensity of the ion signal. Calibration parameters are instrument parameters that affect the mass accuracy and resolution of the mass spectrum. You must tune and calibrate the mass spectrometer (that is, optimize the tune and calibration parameters) perhaps once a quarter. For procedures on how to tune and calibrate your mass spectrometer, refer to “Automatic Tuning and Calibrating in the ESI/MS Mode” in the *TSQ Series Getting Started Guide*.

You must optimize the tune parameters (or change the Tune Method) whenever you change the type of experiment. For procedures on how to optimize the tune parameters for your ESI or APCI experiment, refer to “Optimizing the Mass Spectrometer with Your Compound in ESI/MS/MS Mode” or “Optimizing the Mass Spectrometer with Your Compound in APCI/MS/MS Mode” in the *TSQ Series Getting Started Guide*.

Things to Do Before Operating the TSQ System

Every day before starting analyses, verify that the instrument is ready for operation by doing the following:

- Check the argon and nitrogen supplies.
- Check the ESI fused-silica sample tube for elongation.
- Check the system vacuum levels.

4 Daily Operation

Things to Do Before Operating the TSQ System

Checking the Argon and Nitrogen Supplies

Check the argon 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 argon. Verify that the pressure of argon reaching the mass spectrometer is between 135 ± 70 kPa (20 ± 10 psig). If necessary, adjust the pressure with the tank pressure regulator.

Check the nitrogen supply on the regulator of the nitrogen gas tank or liquid nitrogen boil-off tank. Make sure that you have sufficient gas for your analysis. Based on 24-hour per day operation, typical nitrogen consumption is 2800 liters per day (100 cubic feet per day). If necessary, replace the tank. Verify that the pressure of nitrogen reaching the mass spectrometer is between 690 ± 140 kPa (100 ± 20 psig). If necessary, adjust the pressure with the tank pressure regulator.



CAUTION Before you begin normal operation each day, ensure that you have sufficient nitrogen for your API source. The presence of oxygen in the ion source when the mass spectrometer is on could be unsafe. The TSQ system displays a pop-up message if the nitrogen pressure is too low.

Checking the ESI Fused-Silica Sample Tube for Elongation

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

If you are running in ESI mode with a fused-silica sample tube, verify the sample tube is not elongated past the tip of the ESI spray needle. (This elongation does not occur with a metal needle.)

To cut and reposition the sample tube approximately 0.5 mm (between 0 and 1 mm) inside the end of the ESI needle, refer to the *Ion Max and Ion Max-S API Source Hardware Manual* for more information.

Checking the System Vacuum Levels

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

You can check the current values of the pressures in the ion transfer tube-skimmer region and foreline (labeled *Forepump Pressure*) and in the analyzer region (labeled *Ion Gauge Pressure*) in the Instrument Status view of the EZ Tune window. To display the EZ Tune window, from the Windows taskbar choose **Start > All Programs > Thermo Instruments > TSQ > TSQ Tune**. Choose **View > Instrument Status** to display the Instrument Status view.

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

Table 3. Typical pressure readings for TSQ Vantage and TSQ Quantum Ultra

Conditions	Convection gauge reading (foreline, ion transfer tube- skimmer region)	Ion gauge reading (analyzer region)
Collision gas off, ion transfer tube orifice sealed	less than 0.05 Torr	Less than 3×10^{-6} Torr (after pumping for at least one hour)
Collision gas off, ion transfer tube orifice open	0.9 to 1.2 Torr (110 V at 60 Hz) 1.5 to 2.2 Torr (220 V at 50 Hz)	Less than 5×10^{-6} Torr
Collision gas set to 2 mTorr, ion transfer tube orifice open	0.9 to 1.2 Torr (110 V at 60 Hz) 1.5 to 2.2 Torr (220 V at 50 Hz)	Less than 3×10^{-5} Torr

Table 4. Typical pressure readings for TSQ Quantum Access and TSQ Quantum Access MAX

Conditions	Convection gauge reading (foreline, ion transfer tube- skimmer region)	Ion gauge reading (analyzer region)
Collision gas off, ion transfer tube orifice sealed	less than 0.05 Torr	Less than 3×10^{-6} Torr (after pumping for at least one hour)
Collision gas off, ion transfer tube orifice open	1.2 to 1.8 Torr (110 V at 60 Hz) 1.5 to 2.2 Torr (220 V at 50 Hz)	Less than 5×10^{-6} Torr
Collision gas set to 2 mTorr, ion transfer tube orifice open	1.2 to 1.8 Torr (110 V at 60 Hz) 1.5 to 2.2 Torr (220 V at 50 Hz)	Less than 3×10^{-5} Torr

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

If the pressure remains high, your system might have an air leak. If you suspect an air leak, shut down the system as described in the topic [“Shutting Down the System Completely”](#) on [page 50](#). Make a visual inspection of the vacuum system and vacuum lines for leaks. Check each fitting and flange on the system for tightness, and tighten the fittings or flanges that are loose. Do not tighten fittings indiscriminately. Pay particular attention to fittings that have been changed recently or to fittings that have been subjected to heating and cooling. Make sure that the cover plates of the vacuum manifold are properly seated.

4 Daily Operation

Things to Do After Operating the TSQ System

Things to Do After Operating the TSQ System

After operating the TSQ system, verify the instrument is ready for a period of inactivity by doing the following:

- [Flushing the Sample Transfer Line, Sample Tube, and API Probe](#)
- [Placing the System in Standby Condition](#)
- [Cleaning the Ion Sweep Cone and Ion Transfer Tube](#)
- [Emptying the Solvent Waste Bottle](#)

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

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

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

1. Wait until data acquisition, if any, is complete.
2. To display the EZ Tune window, from the Windows taskbar choose **Start > Programs > Thermo Instruments > TSQ > TSQ Tune**.
3. From the EZ Tune window, choose **Control > On** (or click the On/Standby button) to turn on the voltages and gas flows to the API source.
 - If you are operating in APCI mode, go to step 4.
 - If you are operating in ESI mode, go to step 5.
4. Set up the APCI source:
 - a. In the EZ Tune window, click on the Ion Source button to display the Ion Source Devices dialog box.
 - b. Set the APCI vaporizer temperature to 500 °C:
Select **Vaporizer Temperature** in the device list, and then type **500** in the box and click **Apply**.
 - c. Set the sheath gas flow rate to 30:
Select **Sheath Gas Pressure** in the device list, and then type **30** in the box and click **Apply**.
 - d. Set the auxiliary gas flow rate to 5:
Select **Aux Valve Flow** in the device list, and then type **5** in the box and click **Apply**.
 - e. Set the spray current to 0:
Select **Spray Current** in the device list, and then type **0** in the box and click **Apply**.
5. Go to step 6.

5. Set up the ESI source as follows:
 - a. In the EZ Tune window, click on the Ion Source button to display the Ion Source Devices dialog box.
 - b. Set the sheath gas flow rate to 30:
Select **Sheath Gas Pressure** in the device list, and then type **30** in the box and click **Apply**.
 - c. Set the auxiliary gas flow rate to 5:
Select **Aux Valve Flow** in the device list, and then type **5** in the box and click **Apply**.
 - d. Set the ESI spray voltage to 0:
Select **Spray Voltage** in the device list, and then type **0** in the box and click **Apply**.
6. Set up and start a flow of 50:50 methanol/water solution from the LC to the API source, as follows:
 - a. In the EZ Tune window, choose **Setup > Inlet Direct Control**. The Inlet Direct Control view appears.
 - b. Click the **LC** tab.
 - c. Set the flow rate to a value that is typical for your experiments.
 - d. Set the solvent proportions to 50% methanol and water.
 - e. Click  (Start) to start the LC pump.
7. Let the solution flow through the sample transfer line, sample tube, and API probe for 15 minutes. After 15 minutes, turn off the flow of liquid from the LC to the API source, as follows: Leave the API source (including the APCI vaporizer, sheath gas, and auxiliary gas) on for an additional 5 minutes. Click  (Stop) to stop the LC pump.
8. After 5 minutes, turn off the API source by placing the mass spectrometer in standby:
From the EZ Tune window, choose **Control > Standby** (or click the On/Standby button) to put the mass spectrometer in standby.

Go to the next topic, “[Placing the System in Standby Condition](#).”

Placing the System in Standby Condition

❖ To place the TSQ system in standby condition

1. From the EZ Tune window, choose **Control > Standby** (or click the On/Standby button) to put the mass spectrometer in standby. The System LED on the front panel of the mass spectrometer is illuminated yellow when the system is in standby.
2. Leave the mass spectrometer power on.
3. Leave the LC power on.
4. Leave the autosampler power on.

4 Daily Operation

Things to Do After Operating the TSQ System

5. Leave the data system power on.

Go to the next topic, “[Cleaning the Ion Sweep Cone and Ion Transfer Tube](#).”

Cleaning the Ion Sweep Cone and Ion Transfer Tube

You must clean the ion sweep cone and the ion transfer tube on a regular basis to prevent corrosion and to maintain optimum performance of your API source. If you use nonvolatile buffers in your solvent system or high concentrations of sample, you might need to clean the ion sweep cone and ion transfer tube more often.

See the topic, “[Maintaining the Ion Sweep Cone and Ion Transfer Tube](#)” on [page 77](#).

Go to the next topic, “[Emptying the Solvent Waste Bottle](#).”

Emptying the Solvent Waste Bottle

Thermo Fisher Scientific recommends checking 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 federal regulations.

Removing and Reinstalling the Ion Source Housing

You must remove the Ion Max™ (on the TSQ Quantum Access MAX, TSQ Vantage, or TSQ Quantum Ultra) or Ion Max-S (on the TSQ Quantum Access) ion source housing before performing maintenance on the ion optics or ion source interface, or to access the ion sweep cone.

Contents

- [Removing the Ion Max or Ion Max-S Ion Source Housing](#)
- [Installing the Ion Max or Ion Max-S Ion Source Housing](#)
- [Ion Max and Ion Max-S Housing Maintenance](#)

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

Note If an ion source probe is still installed in the ion source housing, disconnect the external liquid lines to the probe before removing the ion source housing.

❖ To remove the ion source housing

1. Remove the drain tube from the ion source housing drain. See [Figure 36](#) and [Figure 37](#).
2. Rotate the ion source housing locking levers 90 degrees to release the ion source housing from the ion source mount assembly.
3. Remove the ion source housing by pulling it straight off the ion source mount assembly, and place the housing in a safe location for temporary storage.

5 Removing and Reinstalling the Ion Source Housing

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

Figure 36. Ion Max source housing (front)

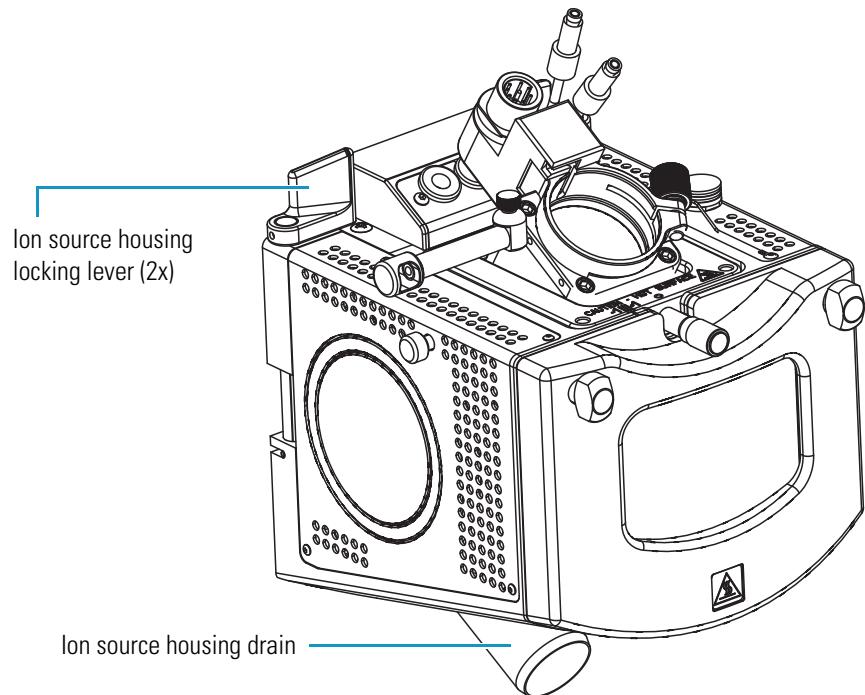
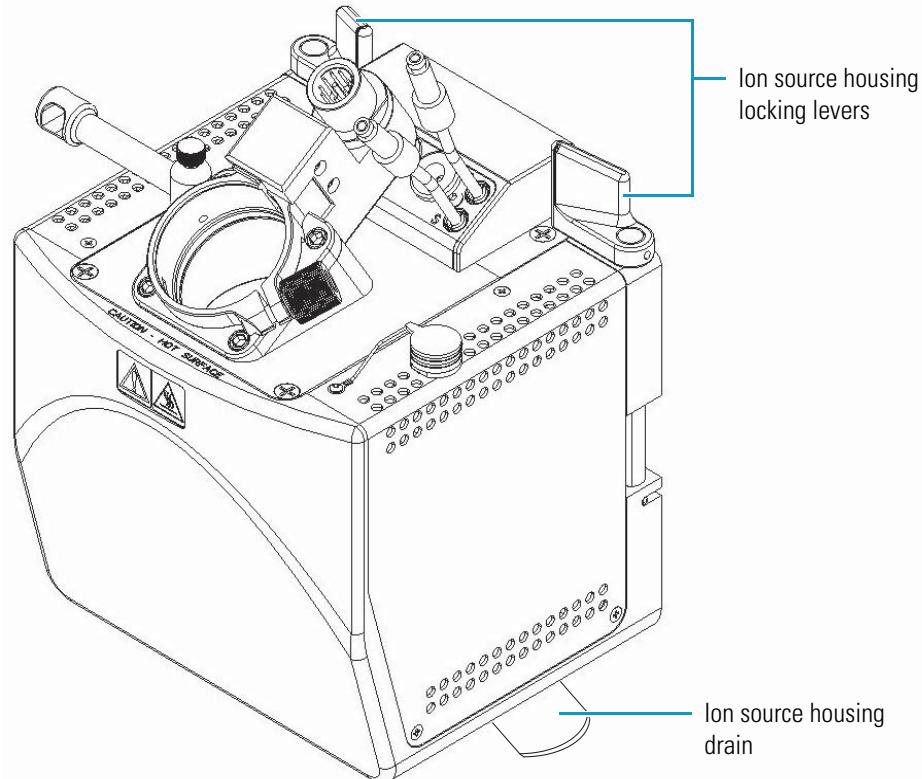


Figure 37. Ion Max-S source housing (front)

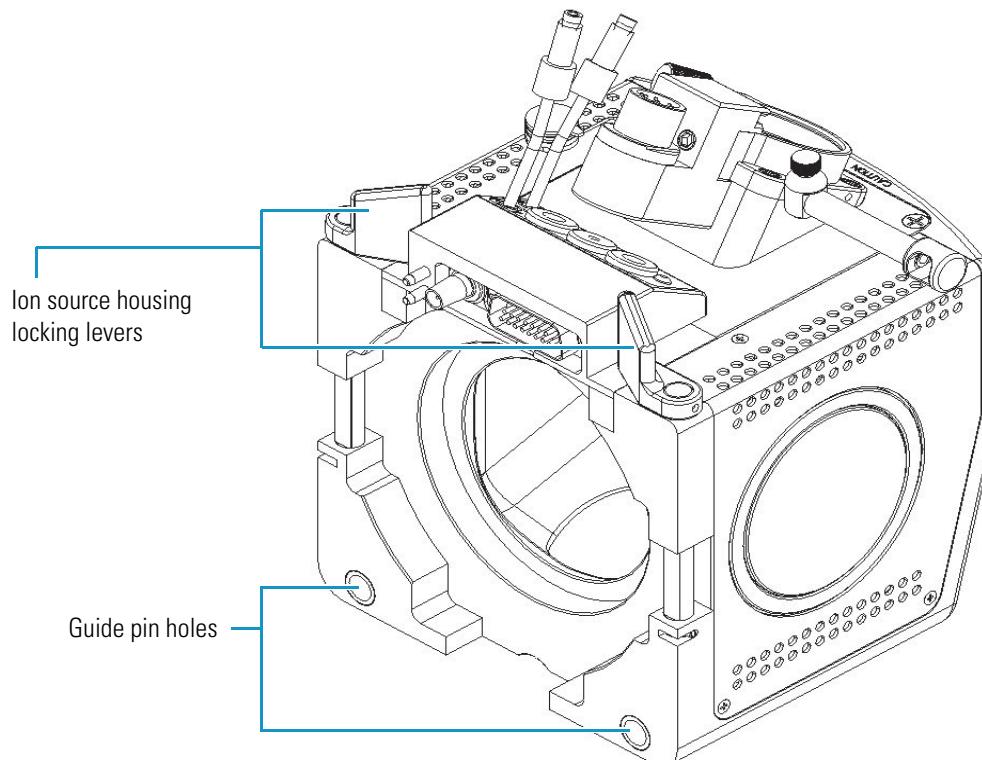


Installing the Ion Max or Ion Max-S Ion Source Housing

❖ To reinstall the Ion Max or Ion Max-S ion source housing

1. Align the two guide pin holes on the rear of the ion source housing with the ion source housing guide pins on the mass spectrometer. Carefully press the ion source housing onto the ion source mount. See [Figure 38](#) and [Figure 39](#).

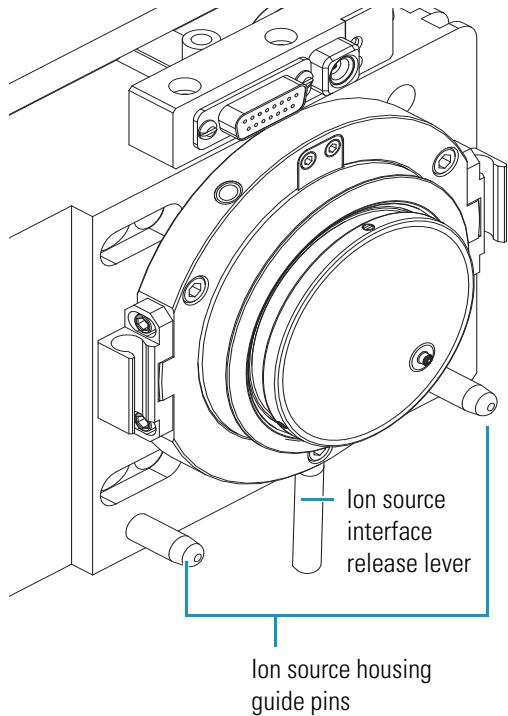
Figure 38. Ion source housing (rear)



5 Removing and Reinstalling the Ion Source Housing

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

Figure 39. Ion source mount, showing the ion source housing guide pins and ion source interface release lever



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



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

3. Reinstall the ion source housing drain tube:



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

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

- a. Connect the 1 in. ID Tygon™ tubing (P/N 00301-22922) to the ion source housing drain fitting.

- b. Attach the free end of the hose to a dedicated drain system. Vent the drain system to a fume exhaust system.

The Ion Max or Ion Max-S ion source is now properly installed on the mass spectrometer.

Ion Max and Ion Max-S Housing Maintenance

The Ion Max and Ion Max-S ion source housings are designed to be serviced by Thermo Fisher Scientific customer support engineers. User maintenance is limited to cleaning the ion source housing as necessary. To clean the housing, remove the housing from the instrument, and in an appropriate fume hood rinse the interior of the housing with methanol. Allow the housing to dry before you install it on the mass spectrometer. Be sure to follow all safety precautions in the sections regarding the installation and removal of the housing. For any additional service that might be required, contact your local Thermo Fisher Scientific service representative.

Maintenance

This chapter describes routine maintenance procedures that you must perform to ensure optimum performance of the instrument. Optimum performance of the TSQ 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.**

Note When you perform maintenance procedures, be methodical; always wear clean, lint-free gloves when handling the components of the ion source; always place the components on a clean, lint-free surface; and never overtighten a screw or use excessive force.

Contents

- [Frequency of Cleaning](#)
- [Maintaining the Ion Sweep Cone and Ion Transfer Tube](#)
- [Maintaining the Ion Source Interface Assembly](#)
- [Cleaning the Q00 Ion Optics](#)
- [Cleaning the Fan Filters](#)

[Table 5](#) lists routine and infrequent mass spectrometer maintenance procedures. Most of the procedures involve cleaning. For example, procedures are provided for cleaning the ion transfer tube, the ion sweep cone, the skimmer and tube lens of the TSQ Quantum Access, TSQ Quantum Access MAX, or TSQ Quantum Ultra, the exit lens and S-lens of the TSQ Vantage, the Q00 rf lens, the lens L0, and the fan filters. Procedures for replacing the ion transfer tube and the capillary heater assembly are also provided. For instructions on maintaining the LC or autosampler, refer to the manual that comes with the LC or autosampler.

6 Maintenance

Table 5. Mass spectrometer maintenance procedures (Sheet 1 of 2)

Mass spectrometer component	Procedure	Frequency	Procedure location
API source	Flush (clean) sample transfer line, sample tube, and API probe	Daily	page 64
	Remove and clean ion transfer tube	Weekly, or if ion transfer tube bore is contaminated or obstructed	page 77
	Remove and clean ion sweep cone	As needed*	page 77
	Clean Ion Max or Ion Max-S housing	As needed*	page 71
	Replace ion transfer tube	If ion transfer tube bore is corroded	page 77
Q00 ion optics	Clean S-lens and exit lens (TSQ Vantage)	As needed*	page 85
	Clean tube lens and skimmer (TSQ Quantum Access, TSQ Quantum Access MAX, and TSQ Quantum Ultra)	As needed*	page 86
	Clean Q00 rf lens and lens L0	Every 3 to 4 months*	page 95
APCI, ESI, or H-ESI probe	Replace fused-silica sample tube	If sample tube is broken or obstructed	<i>Ion Max and Ion Max-S API Source Hardware Manual or H-ESI Probe User Guide</i>
ESI or H-ESI probe	Trim fused-silica sample tube	If polyimide coating on the end of the sample tube has elongated	<i>Ion Max and Ion Max-S API Source Hardware Manual or H-ESI Probe User Guide</i>
HESI-II probe	Replace needle insert	If metal needle is plugged	<i>HESI-II Probe User Guide</i>
Forepump	Purge (decontaminate) oil	If the oil is cloudy or discolored	Manufacturer's documentation
	Add oil	If the oil level is below the MIN mark	Manufacturer's documentation
	Change oil	Every four months, or if oil remains cloudy or discolored after purging	Manufacturer's documentation

Table 5. Mass spectrometer maintenance procedures (Sheet 2 of 2)

Mass spectrometer component	Procedure	Frequency	Procedure location
Q0 ion optics	Clean Q0 quadrupole and lenses L11 and L12 ^{**}	As needed [*]	
Mass analyzer	Clean Q1, Q2, and Q3 quadrupoles and lenses ^{**}	As needed [*]	
Ion detection system	Clean ion detection system (electron multiplier and conversion dynode) ^{**}	Whenever the side cover plate of the vacuum manifold is removed	
Cooling fans	Clean fan filters	Every 4 months	page 99
Ion detection system	Replace electron multiplier assembly ^{**}	If noise in spectrum is excessive or proper electron multiplier gain can not be achieved	
Electronic modules	Replace electronic module ^{**}	If electronic module fails	
PCBs	Replace PCB ^{**}	If PCB fails	

* The frequency of cleaning the components of the mass spectrometer depends on the types and amounts of samples and solvents that are introduced into the instrument. Cleaning of the Q0, Q1, Q2, and Q3 quadrupoles is rarely (if ever) required.

** A Thermo Fisher Scientific field service engineer should perform this maintenance procedure.

Frequency of Cleaning

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

- Clean the sample transfer line, sample tube, and API probe at the end of each operating day to remove any residual salts from buffered mobile phases or other contamination that might accumulate during normal operation. See “[Flushing the Sample Transfer Line, Sample Tube, and API Probe](#)” on [page 64](#).
- Periodically remove and clean the ion transfer tube and ion sweep cone of the API source. See “[Maintaining the Ion Sweep Cone and Ion Transfer Tube](#)” on [page 77](#).
- The S-lens and exit lens (on the TSQ Vantage) or the tube lens and skimmer (on the TSQ Quantum Access, TSQ Quantum Access MAX, and TSQ Quantum Ultra) of the Q00 ion optics become dirty at a slower rate than the API probe, ion sweep cone, and ion transfer tube. See “[Cleaning the S-Lens and Exit Lens \(TSQ Vantage\)](#)” on [page 85](#).
- The rf lens of the Q00 ion optics becomes dirty at a rate significantly slower than the API source, tube lens and skimmer, or S-lens and exit lens. See “[Cleaning the Q00 Ion Optics](#)” on [page 89](#).

6 Maintenance

Frequency of Cleaning

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

- Clean the API probe, ion sweep cone, and ion transfer tube.
- Clean the S-lens and exit lens (on the TSQ Vantage) or the tube lens and skimmer (on the TSQ Quantum Access, TSQ Quantum Access MAX, and TSQ Quantum Ultra).
- Clean the Q00 rf lens and lens L0.

Generally, do not open the vacuum manifold. Cleaning the Q0, Q1, Q2, and Q3 quadrupoles is rarely (if ever) required. (Q0 can be removed and cleaned along with Q00.) If you believe that the Q1, Q2, or Q3 quadrupoles need cleaning, contact Thermo Fisher Scientific and schedule a visit by a Thermo Fisher Scientific field service engineer.

If you open the vacuum manifold, clean the electron multiplier and conversion dynode by blowing them with a clean, dry gas. If you do not open the vacuum manifold, the electron multiplier and conversion dynode do not normally require cleaning, although rarely the electron multiplier might require replacement.



CAUTION As with all chemicals, store and handle solvents and reagents according to standard safety procedures. Dispose of them according to local and federal regulations.

Maintaining the Ion Sweep Cone and Ion Transfer Tube

To prevent corrosion and to maintain optimum performance of the API source, remove and clean the ion sweep cone and the ion transfer tube on a regular basis.

Removing and Cleaning the Ion Transfer Tube

Buffer salts or high concentrations of sample can block the bore of the ion transfer tube. You can easily remove the ion transfer tube for cleaning, however, as it does not require venting the system before removal.

If the pressure in the ion transfer tube-skimmer region (as measured by the Convectron gauge) drops considerably below 1 Torr, a blocked ion transfer tube could be the cause. Check the Convectron gauge pressure by choosing **View > Instrument Status** from the EZ Tune window. The pressure is listed under Forepump Pressure.

❖ To remove and clean the ion transfer tube

1. Place the instrument in standby:
 - a. Choose **Start > Programs > Thermo Instruments > TSQ > TSQ Tune** to open the EZ Tune window.
 - b. From the EZ Tune window, choose **Control > Standby** (or click the **On/Standby** button) to put the mass spectrometer in Standby mode.



On



Off



Standby

2. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source:
 - a. In the EZ Tune window, choose **Setup > Inlet Direct Control**. The Inlet Direct Control dialog box appears.
 - b. Click the **LC** tab and click (Stop) to stop the LC pump.



CAUTION Lower the temperature of the ion transfer tube to 50 °C or less before you remove it. Handling a hot ion transfer tube or ion sweep cone can cause burns.

CAUTION Attempting to remove a hot ion transfer tube might cause it to bind and break in the heater assembly or strip the threads of the ion source interface.

3. Lower the temperature of the ion transfer tube (capillary):
 - a. In the EZ Tune window, click to open the Ion Source Devices dialog box. See [Figure 40](#).

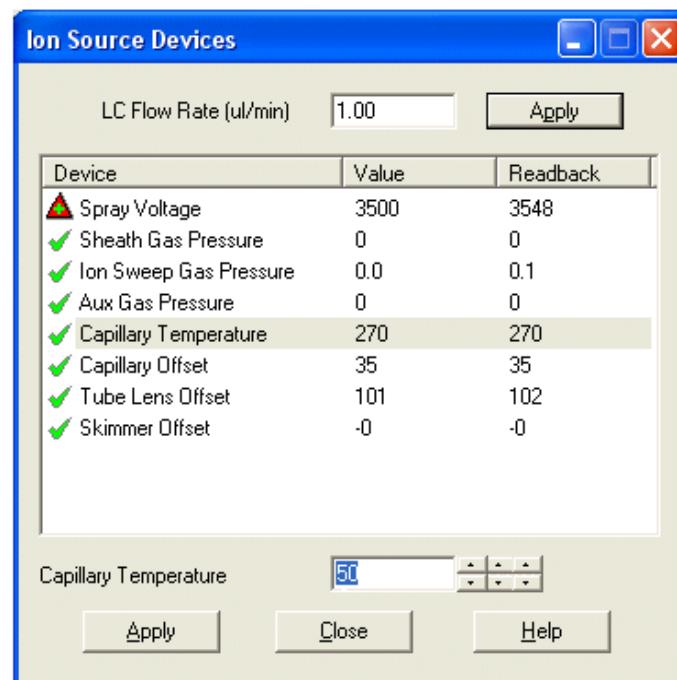


- a. In the EZ Tune window, click to open the Ion Source Devices dialog box. See [Figure 40](#).

6 Maintenance

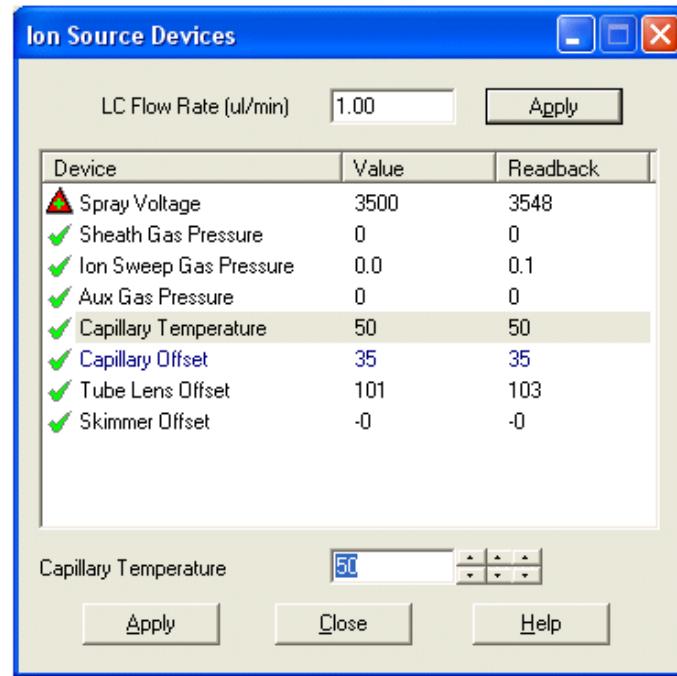
Maintaining the Ion Sweep Cone and Ion Transfer Tube

Figure 40. Ion Source Devices dialog box showing the ion transfer tube (capillary) at 270 °C



- b. Click **Capillary Temperature** in the Device list.
- c. Set the ion transfer tube (capillary) temperature to 50 °C or lower in the Capillary Temperature box and click **Apply**.
- d. Allow the ion transfer tube (capillary) to cool to 50 °C or lower. See [Figure 41](#).

Figure 41. Ion Source Devices dialog box showing the ion transfer tube (capillary) at 50 °C



4. Remove the Ion Max or Ion Max-S ion source housing from the front of the mass spectrometer. See “[Removing the Ion Max or Ion Max-S Ion Source Housing](#)” on [page 67](#).
5. Remove the ion sweep cone by pulling it off the ion source interface.
6. With the custom removal tool from the accessory kit (P/N 70111-20258), remove the ion transfer tube by turning it counterclockwise until you can pull it free from the ion source interface. See [Figure 42](#).

Figure 42. Removal tool attached to the ion transfer tube

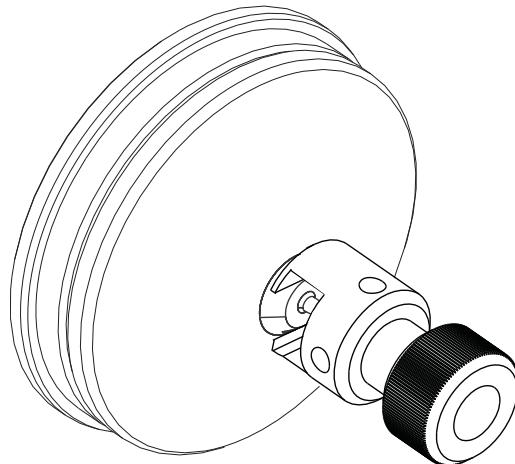
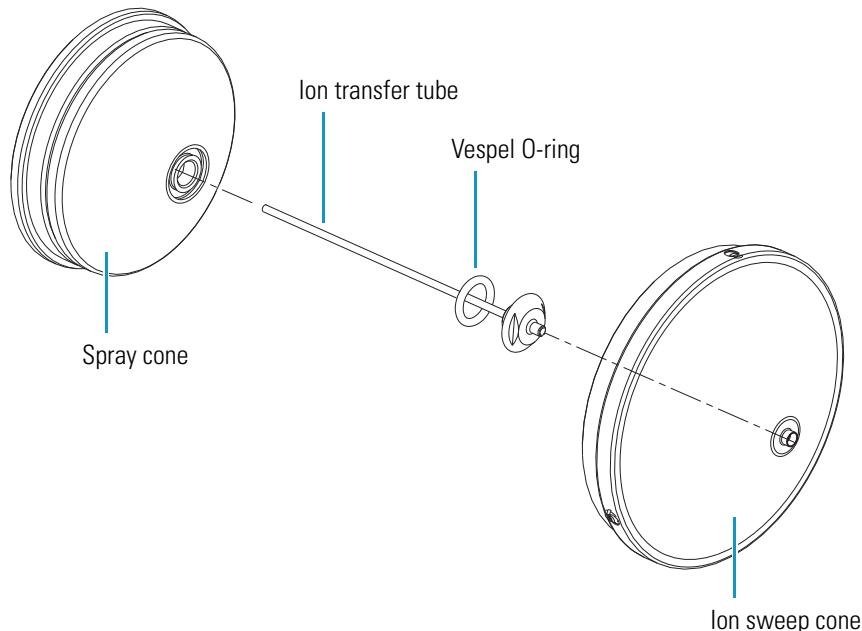


Figure 43. Spray cone, ion transfer tube, O-ring, and ion sweep cone of the ion source interface



7. Soak the ion transfer tube in a dilute solution of nitric acid to remove contaminants.

6 Maintenance

Maintaining the Ion Sweep Cone and Ion Transfer Tube

8. Sonicate the ion transfer tube in distilled water.
9. Clean the ion sweep cone by wiping the inside and outside with methanol and a Kimwipe.
10. Remove, clean with methanol, and inspect the Vespel™ O-ring (P/N 97055-20442) that is seated in the spray cone under the entrance end of the ion transfer tube. Replace it if necessary.
11. Reseat the O-ring in the spray cone.



CAUTION When you reinstall the ion transfer tube, take these precautions:

- Ensure that everything is properly aligned to prevent stripping the threads on the ion transfer tube.
- For mass spectrometers other than the TSQ Vantage, be careful not to bend the ion transfer tube. Rotate the tube as you insert it. (The ion transfer tube of the TSQ Vantage will bend slightly when you insert it.)

12. Insert the ion transfer tube into the heater block. Rotate the tube as you insert it. After you insert it, turn the tube clockwise until it is fingertight.
13. Align the gas inlet on the ion sweep cone with the sweep gas supply port on the ion source mount. Firmly press the ion sweep cone into the ion source mount. See [Figure 44](#) and [Figure 45](#).
14. Reinstall the Ion Max or Ion Max-S source housing on the mass spectrometer as described in the topic [“Installing the Ion Max or Ion Max-S Ion Source Housing”](#) on page 69.

Figure 44. Ion source interface, showing the sweep gas supply port in the API cone seal

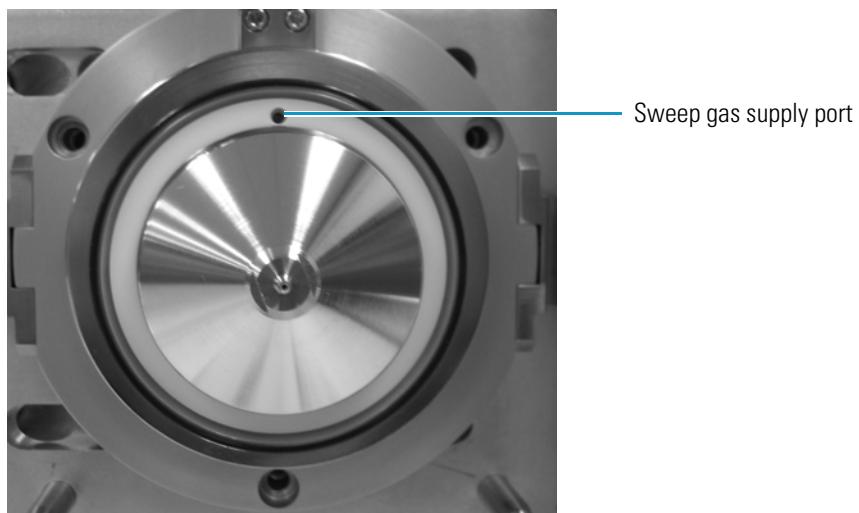
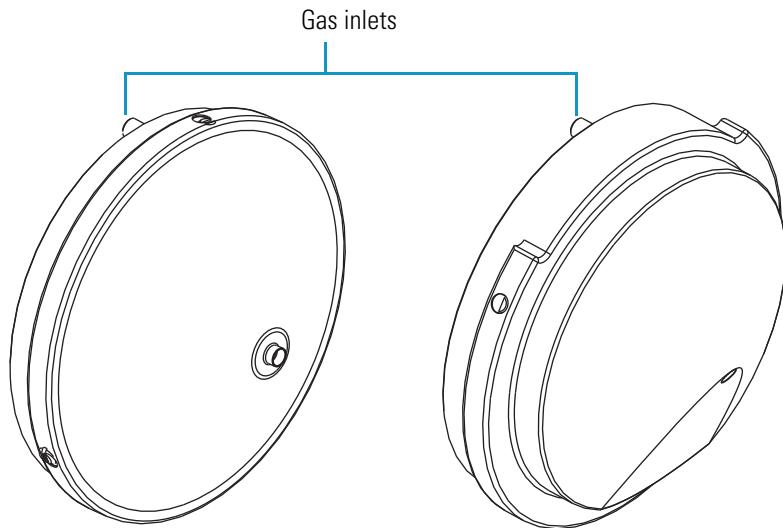


Figure 45. Ion sweep cones for FAIMS and APPI (left) and H-ESI, ESI, and APCI (right), showing the gas inlets



Note Unblocking the ion transfer tube should increase the Convectron gauge pressure to a normal value (approximately 1.5 Torr). If this method fails to clear the ion transfer tube, replace it. See [Table 6](#) for the correct ion transfer tube part number for your instrument.

Table 6. Ion transfer tube part numbers

Instrument	Ion transfer tube part number
TSQ Vantage series	70005-20423
TSQ Quantum Access series	70111-20972
TSQ Quantum Ultra series	97055-20199
TSQ Quantum Discovery Max	70111-20396
TSQ Quantum Discovery	70111-20100
TSQ Quantum AM	70111-20100
TSQ Quantum	70111-20100

6 Maintenance

Maintaining the Ion Source Interface Assembly

The ion source interface assembly includes the ion sweep cone, ion transfer tube, capillary heater assembly, S-lens or tube lens, and exit lens or skimmer. The ion transfer tube has a finite lifetime. You must replace the ion transfer tube if the ion transfer tube bore becomes corroded.

You can easily remove the ion sweep cone and ion transfer tube to clean or replace them without venting the system. See “[Maintaining the Ion Sweep Cone and Ion Transfer Tube](#)” on [page 77](#).

To clean the ion source interface assembly components, other than the ion sweep cone and ion transfer tube, follow these procedures:

1. [Shutting Down and Venting the System](#)
2. [Removing the Ion Max or Ion Max-S Ion Source Housing](#)
3. [Removing the Ion Source Interface](#)
4. [Removing the S-Lens and Exit Lens \(TSQ Vantage\)](#)
5. [Cleaning the S-Lens and Exit Lens \(TSQ Vantage\)](#)
6. [Removing the Tube Lens and Skimmer \(TSQ Quantum Access, TSQ Quantum Access MAX, or TSQ Quantum Ultra\)](#)
7. [Cleaning the Tube Lens and Skimmer \(TSQ Quantum Access, TSQ Quantum Access MAX, or TSQ Quantum Ultra\)](#)
8. [Reinstalling the S-Lens and Exit Lens \(TSQ Vantage\)](#)
9. [Reinstalling the Tube Lens and Skimmer \(TSQ Quantum Access, TSQ Quantum Access MAX, or TSQ Quantum Ultra\)](#)
10. [Reinstalling the Ion Source Interface Assembly](#)
11. [Reinstalling the Ion Max or Ion Max-S Ion Source Housing](#)
12. [Starting Up the System](#)

Shutting Down and Venting the System

Shut down and vent the system. See “[Shutting Down the System Completely](#)” on [page 50](#).

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

You must remove the Ion Max or Ion Max-S ion source housing to access the ion source interface assembly. See “[Removing the Ion Max or Ion Max-S Ion Source Housing](#)” on [page 67](#).

Removing the Ion Source Interface

You must remove the ion source interface to access the exit lens or skimmer, the S-lens or tube lens, and the capillary heater assembly.

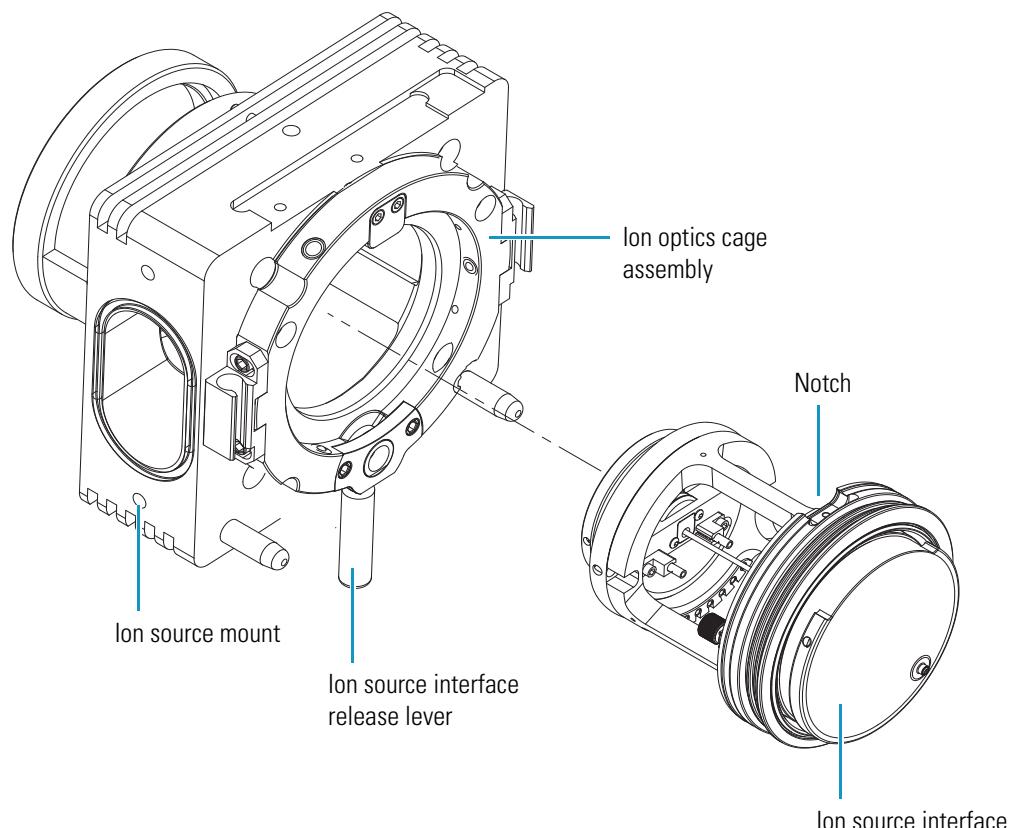


CAUTION Wait for the ion source interface to cool to ambient temperature before you remove it.

❖ To remove the ion source interface

1. Wear clean, talc-free gloves.
2. Using a right-to-left motion, move the ion source interface release lever several times to loosen the ion source interface from the ion optics cage assembly. See [Figure 46](#).
3. Grab the exposed outer grooves of the ion source interface and firmly pull the assembly straight out.
4. Place the assembly on a clean, lint-free surface.

Figure 46. Removing the ion source interface



6 Maintenance

Maintaining the Ion Source Interface Assembly

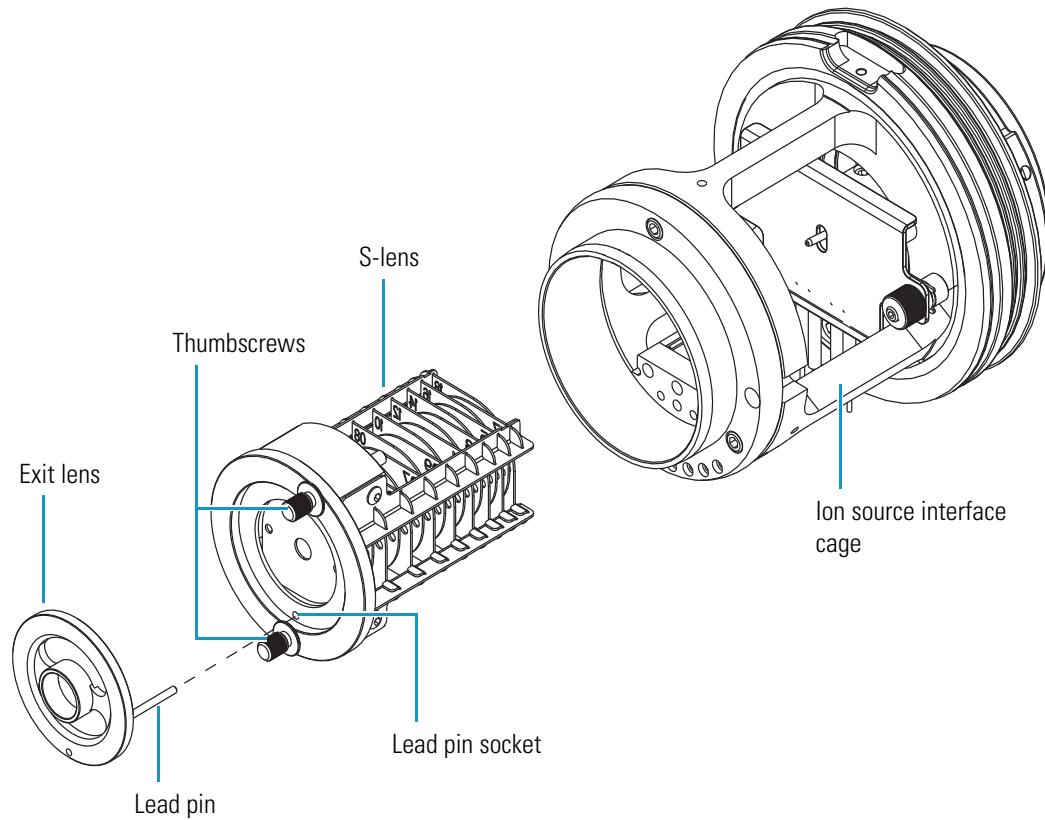
Removing the S-Lens and Exit Lens (TSQ Vantage)

You must remove the S-lens and exit lens from the ion source interface cage before they can be cleaned.

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

1. Wearing clean, lint- and powder- free gloves, 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. See [Figure 47](#).
2. Grasp the two thumbscrews and carefully pull the S-lens straight out of the ion source interface cage. Place it on a clean, lint-free surface.
3. Remove the exit lens from the S-lens and place it on a clean, lint-free surface.

Figure 47. Removing the exit lens and S-lens from the ion source interface cage of the TSQ Vantage



Cleaning the S-Lens and Exit Lens (TSQ Vantage)

❖ To clean the S-lens and exit lens

Note Wear clean gloves when you handle 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. Sonicate the exit lens and S-lens separately for 15 minutes in 50:50 HPLC-grade methanol/water.
2. Rinse the exit lens and S-lens with fresh methanol.
3. 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.

Removing the Tube Lens and Skimmer (TSQ Quantum Access, TSQ Quantum Access MAX, or TSQ Quantum Ultra)

You must remove the tube lens and skimmer from the ion source interface assembly before they can be cleaned.

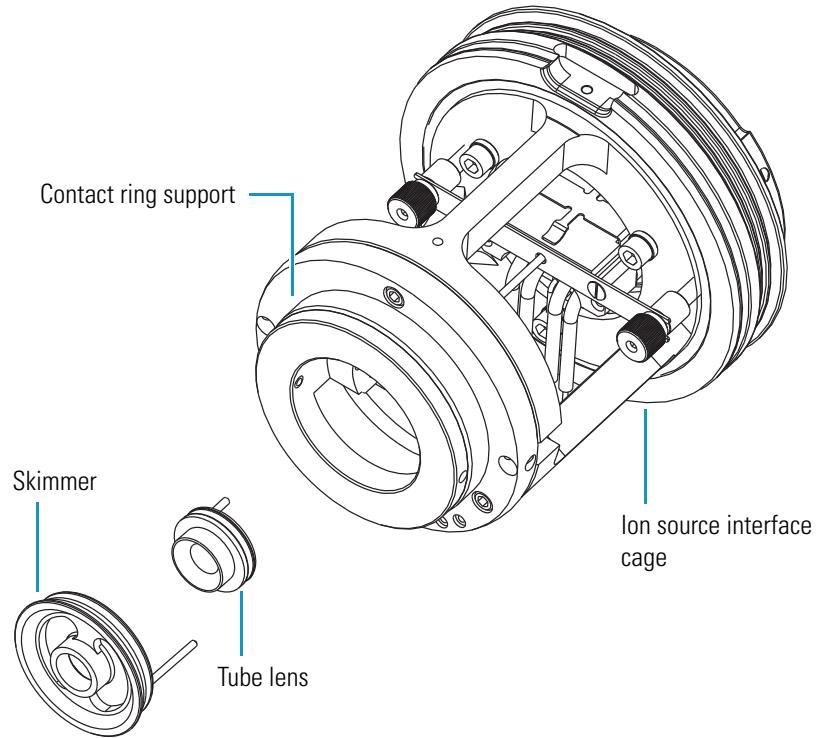
❖ To remove the tube lens and skimmer from the ion source interface assembly

1. Wearing clean, lint- and powder- free gloves, reach behind the skimmer with your fingers and gently press the skimmer out of the contact ring support. If necessary, loosen the set screws. See [Figure 48](#).
2. Place the skimmer on a clean, lint-free surface.
3. Push the tube lens, from the back, out of the contact ring support.
4. Place the tube lens on a clean, lint-free surface.

6 Maintenance

Maintaining the Ion Source Interface Assembly

Figure 48. Removing the skimmer and tube lens from the ion source interface cage of the TSQ Quantum Access, TSQ Quantum Access MAX, or TSQ Quantum Ultra



Cleaning the Tube Lens and Skimmer (TSQ Quantum Access, TSQ Quantum Access MAX, or TSQ Quantum Ultra)

❖ To clean the tube lens and skimmer

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

CAUTION Do not clean the tube lens or skimmer with detergents, acidic or caustic substances, or abrasives.



The sharp edge of the skimmer cone is fragile and any deformation might result in a loss of efficient ion transmission. Use care not to drop the skimmer when cleaning it. Sonicate the skimmer alone with the cone side up.

Sonicate the tube lens and skimmer alone in organic or aqueous solution. For most cleaning applications, HPLC-grade methanol is the solvent of choice. However, use of buffers or salt solutions might require that you use an aqueous solution. If you need to use a solvent other than methanol, after cleaning the component, flush the component with distilled water and then flush it with methanol as a final wash. You can air dry the skimmer and tube lens or blow dry them with nitrogen gas. In all cases, ensure that all solvent has evaporated from the components before reassembly.

Reinstalling the S-Lens and Exit Lens (TSQ Vantage)

❖ To reinstall the S-lens and exit lens

1. Reinstall the exit lens onto the S-lens:
 - a. Wearing clean, lint- and powder- free gloves, extend the thumbscrews on the S-lens. See [Figure 47 on page 84](#).
 - b. Insert the exit lens lead pin into the lead pin socket and seat the exit lens onto the S-lens.
2. Reinstall the exit lens and S-lens into the ion source interface cage:
 - a. Hold the S-lens by the thumbscrews and orient the thumbscrews toward the thumbscrew holes on the ion source interface. Only one orientation will work.
 - b. Carefully insert the S-lens into the ion source interface cage.
 - c. Tighten the thumbscrews until fingertight.

Reinstalling the Tube Lens and Skimmer (TSQ Quantum Access, TSQ Quantum Access MAX, or TSQ Quantum Ultra)

❖ To reinstall the tube lens and skimmer

1. Reinstall the tube lens into the ion source interface cage (see [Figure 49](#)):
 - 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.
 - b. Insert the lead pin into the socket and firmly press the tube lens into the contact ring support.



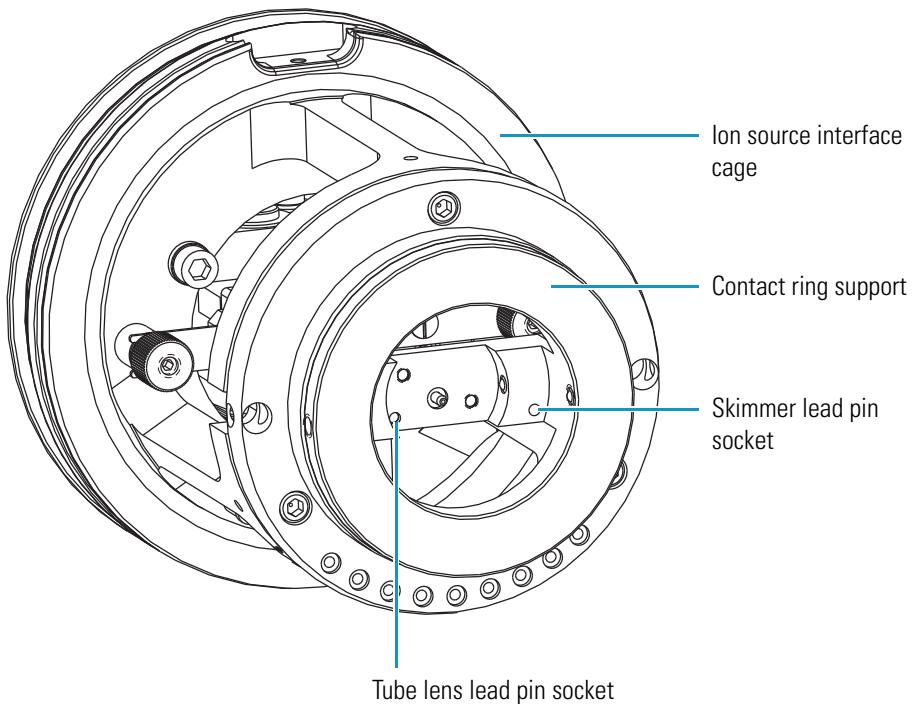
CAUTION Ensure that you do not scratch or nick the skimmer cone.

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.

6 Maintenance

Maintaining the Ion Source Interface Assembly

Figure 49. Ion source interface cage of the TSQ Quantum Access, TSQ Quantum Access MAX, or TSQ Quantum Ultra, showing the skimmer and tube lens lead pin sockets



Reinstalling the Ion Source Interface Assembly

❖ To reinstall the ion source interface assembly

1. Orient the ion source interface assembly so that the sweep gas inlet notch on the ion source interface is aligned with the sweep gas supply block on the ion source mount.
2. Carefully slide the ion source interface assembly into the ion optics cage assembly.

Reinstalling the Ion Max or Ion Max-S Ion Source Housing

Reinstall the Ion Max or Ion Max-S ion source housing as described in the topic [“Installing the Ion Max or Ion Max-S Ion Source Housing” on page 69](#).

You might also need to reinstall an ion source probe and LC liquid lines, as appropriate, as described in the corresponding topics in the *TSQ Series Getting Connected Guide*.

Starting Up the System

Start up the system as described in the topic [“Starting Up the System after a Complete Shutdown” on page 52](#).

Cleaning the Q00 Ion Optics

Because an accumulation of chemicals on the surfaces of the tube lens, skimmer, and Q00 rf lens forms an insulating layer that can modify the electrical fields that control ion transmission, clean ion optics components are essential for the proper operation of the instrument. The tube lens and skimmer require cleaning less often than the API source. The Q00 rf lens requires 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.

Clean or replace the Q00 ion optics components by doing the following:

1. [Shutting Down and Venting the System](#)
2. [Removing the Ion Max or Ion Max-S Ion Source Housing](#)
3. [Removing the Ion Source Interface](#)
4. [Removing the Ion Optics Cage Assembly](#)
5. [Disassembling the Ion Optics Cage Assembly](#)
6. [Cleaning Q00 and L0](#)
7. [Reassembling the Ion Optics Cage Assembly](#)
8. [Reinstalling the Ion Optics Cage Assembly](#)
9. [Reinstalling the Ion Source Interface Assembly](#)
10. [Reinstalling the Ion Max or Ion Max-S Ion Source Housing](#)
11. [Starting Up the System](#)

Shutting Down and Venting the System

Shut down and vent the system as described in the topic “[Shutting Down the System Completely](#)” on [page 50](#).

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

Remove the Ion Max or Ion Max-S ion source housing to access the ion source interface assembly. Remove the Ion Max or Ion Max-S ion source housing as described in the topic “[Removing the Ion Max or Ion Max-S Ion Source Housing](#)” on [page 67](#).

Removing the Ion Source Interface Assembly

Remove the ion source interface assembly to access the Q00 ion optics assembly. Remove the ion source interface assembly as described in the topic “[Removing the Ion Source Interface](#)” on [page 83](#).

6 Maintenance

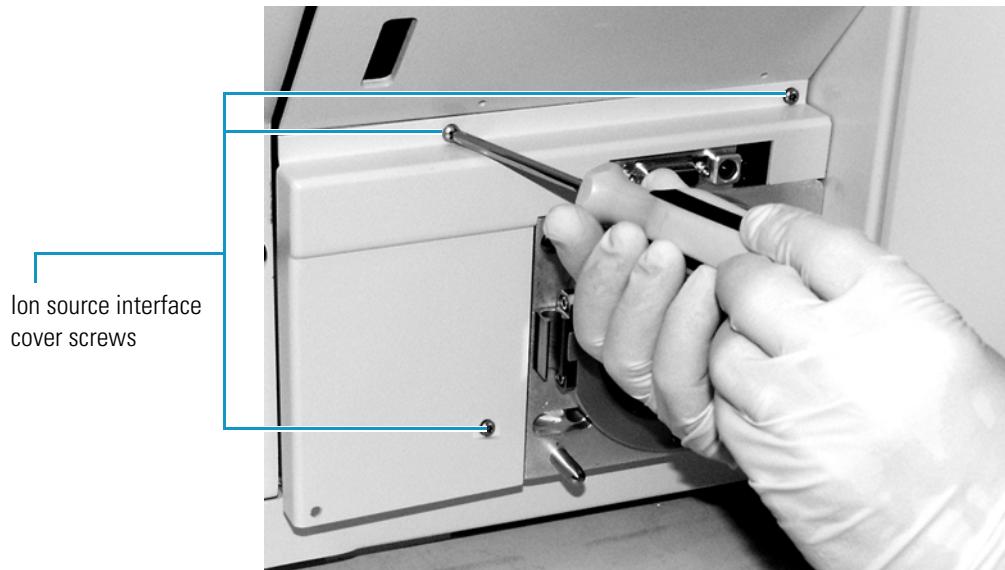
Cleaning the Q00 Ion Optics

Removing the Ion Optics Cage Assembly

❖ To remove the ion optics cage assembly

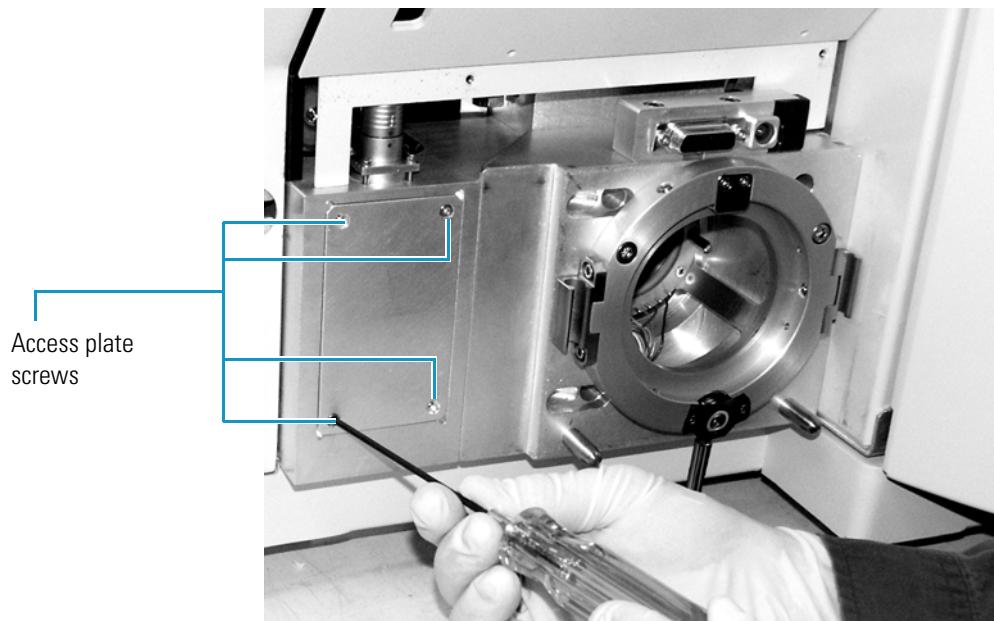
1. Using a Phillips screwdriver, remove the three screws fastening the ion source interface cover to the mass spectrometer, and place the cover in a safe place. See [Figure 50](#).

Figure 50. Removing the ion source interface cover screws



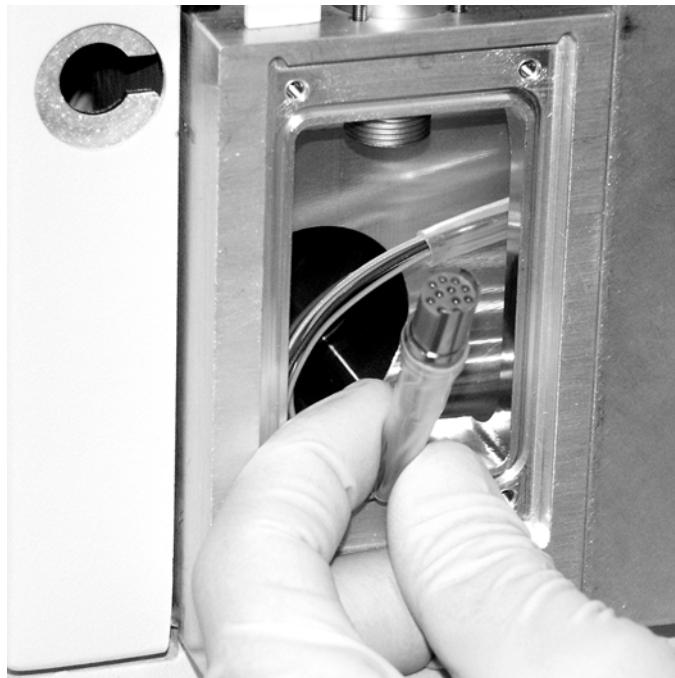
2. Using a hex ball driver, remove the roughing pump adapter access plate. See [Figure 51](#).

Figure 51. Removing the roughing pump adapter access plate screws



3. Unplug the ion source cable harness from the connector. See [Figure 52](#).

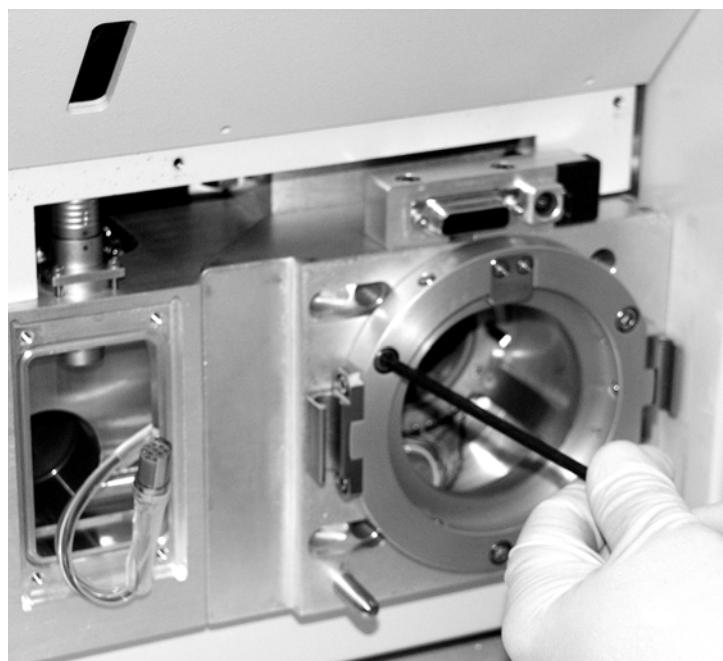
Figure 52. Unplugging the ion source cable harness connector



4. Remove the ion optics cage assembly:

- a. Using a hex ball driver, remove the three screws fastening the ion optics cage assembly to the ion source mount assembly. See [Figure 53](#).

Figure 53. Removing the ion optics cage assembly retaining screws



6 Maintenance

Cleaning the Q00 Ion Optics

- b. Carefully feed the cable harness back through the roughing pump adapter and out of the front of the cage assembly to ensure that it does not get trapped between the cage and the ion source mount assembly while you are removing the cage assembly. See [Figure 54](#).

Figure 54. Pulling the ion source cable harness out of the ion optics cage assembly



- c. Carefully slide the ion optics cage assembly out of the ion source mount assembly. See [Figure 55](#).
- d. Place the ion optics cage assembly on a clean, lint-free surface.

Figure 55. Removing the ion optics cage assembly



6 Maintenance

Cleaning the Q00 Ion Optics

Disassembling the Ion Optics Cage Assembly

The Q00 rf lens and L0 lens must be removed from the ion optics cage assembly before they can be cleaned.

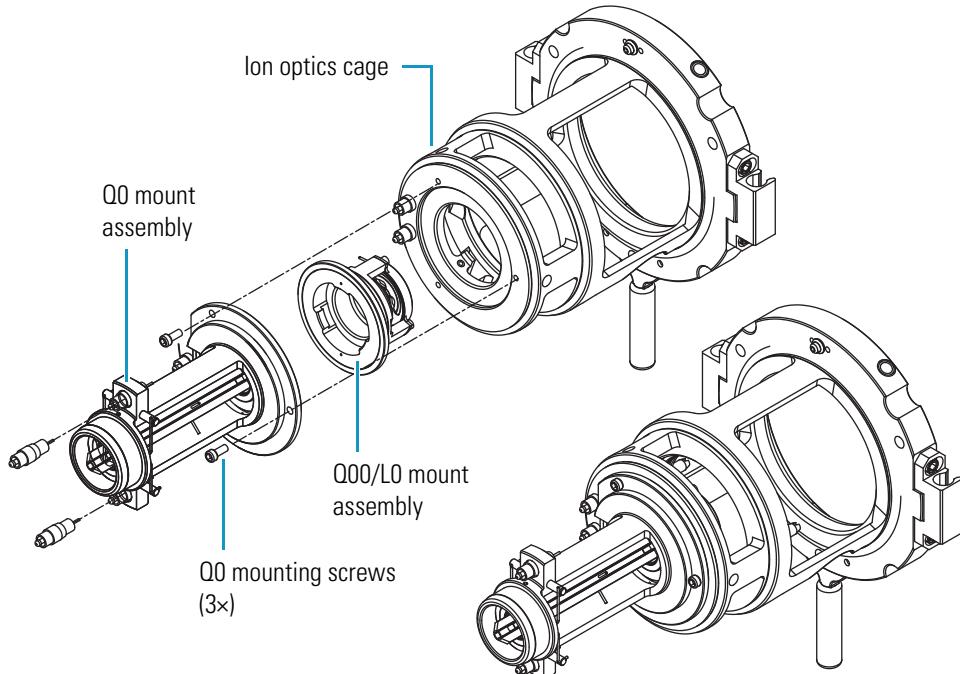
Note Make careful note of the proper orientation of all wiring before removing any electrical lead from its contact.

❖ To disassemble the ion optics cage assembly

Note Wear clean gloves when you handle the ion optics components.

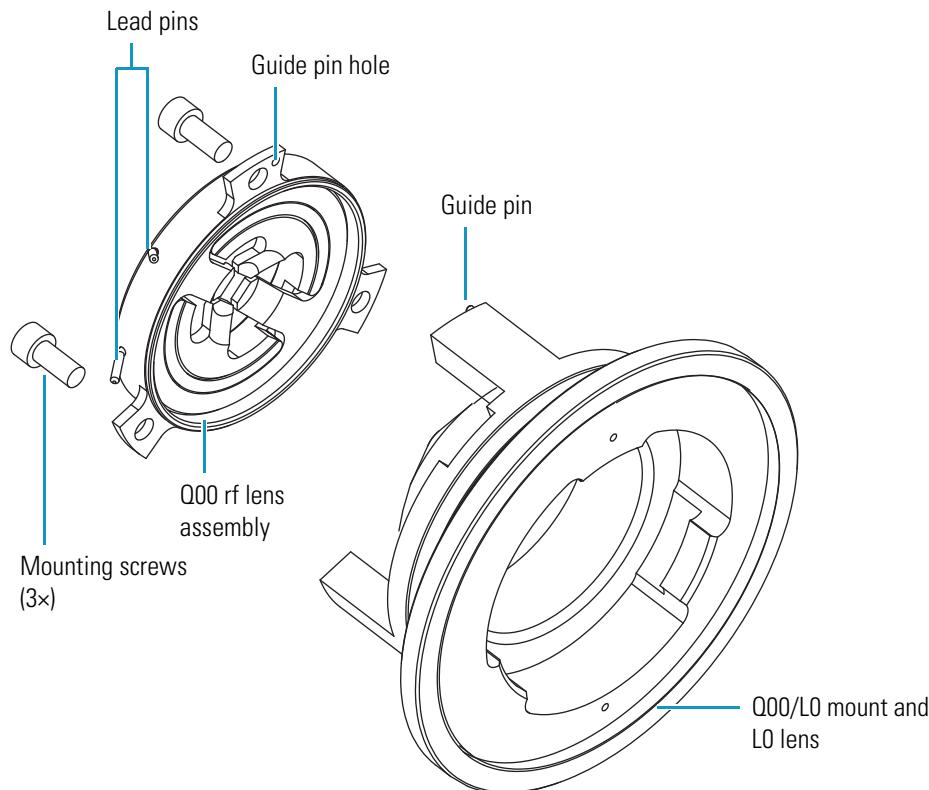
1. Using a hex ball driver, remove the three screws that fasten the Q0 mount assembly to the ion optics cage. See [Figure 56](#).

Figure 56. Ion optics cage assembly with Q0 mount assembly and Q00/L0 mount assembly removed



2. Remove the Q0 mount assembly. Place it on a clean, lint-free surface.
3. Using needle nose pliers, disconnect the two rf lead wires from the Q00 lead pins.
4. Carefully push the Q00/L0 mount assembly out of the ion optics cage by pressing on the mount assembly with your fingers.
5. Using a hex ball driver, remove the three Q00 mounting screws that fasten the Q00 rf lens assembly to the Q00/L0 mount. Leave the lens L0 mounted in the PEEK Q00/L0 mount.

Figure 57. Exploded diagram of the Q00/L0 mount assembly



6. Place all components onto a clean, lint-free surface.



CAUTION Do not disassemble the Q00 rf lens assembly any further.

Cleaning Q00 and L0

❖ To clean the Q00 rf lens and L0 lens

1. Clean the Q00 rf lens and L0 lens with a Kimwipe™ soaked in methanol.



CAUTION Do not use abrasives to clean the Q00 rf lens. Do not soak the Q00 rf lens and L0 lens in solvent.

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

2. Dry the parts with a rapid stream of nitrogen gas.
3. Inspect each part for contamination and dust. If necessary, repeat the cleaning procedure.

6 Maintenance

Cleaning the Q00 Ion Optics

Reassembling the Ion Optics Cage Assembly

❖ To reassemble and mount the Q00/L0 assembly

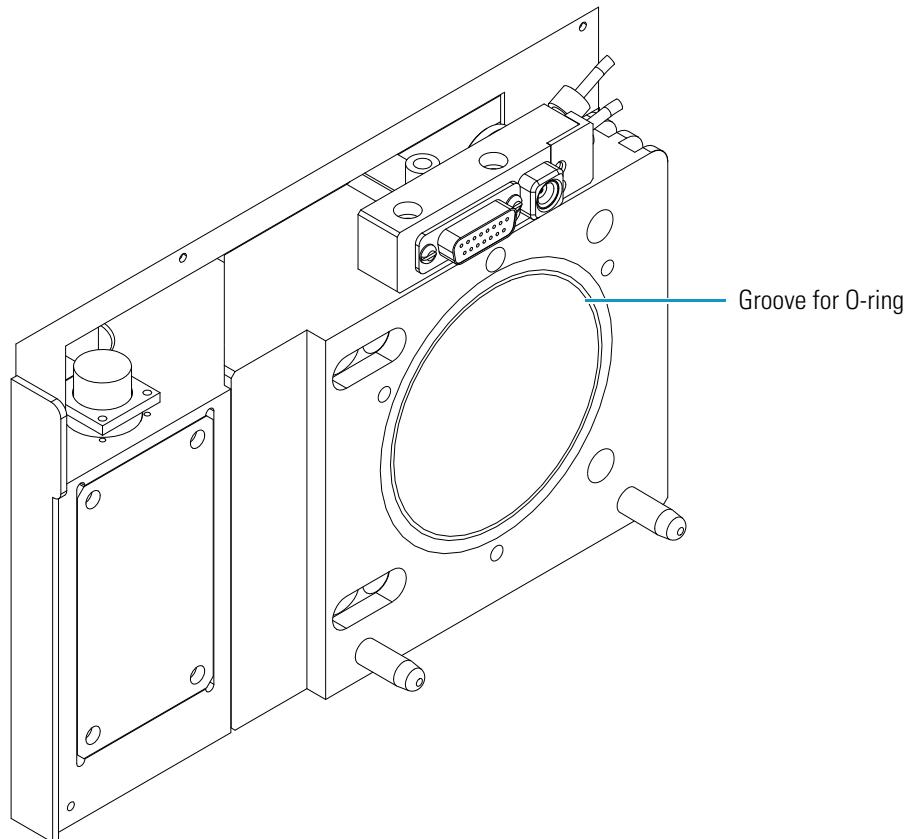
1. Reinstall the Q00 assembly on the Q00/L0 mount:
 - a. Orient the Q00 assembly so that the guide pin on the Q00/L0 mount inserts into the guide pin hole in the Q00 assembly.
 - b. Secure the Q00 assembly with the 3 Q00 mounting screws.
2. Reinstall the Q00/L0 mount assembly in the ion optics cage:
 - a. Orient the Q00/L0 mount assembly so that the lead pins are closest to the lead wires in the ion optics cage.
 - b. Press the Q00/L0 assembly into the ion optics cage. See [Figure 56](#).
3. Use needle nose pliers to carefully reconnect the top rf lead wire to the top Q00 lead pin and the bottom rf lead wire to the bottom Q00 lead pin.
4. Reinstall the Q0 mount assembly onto the ion optics cage:
 - a. Orient the Q0 mount assembly so that the flat side is on the same side as the two contacts.
 - b. Secure the Q0 mount assembly on the ion optics cage with the 3 Q0 mounting screws. See [Figure 56](#).

Reinstalling the Ion Optics Cage Assembly

❖ To reinstall the ion optics cage assembly

1. Reinstall the 3.25 in. ID Viton™ O-ring into the groove on the ion source mount assembly. See [Figure 58](#).

Figure 58. Ion source mount assembly, showing groove for O-ring

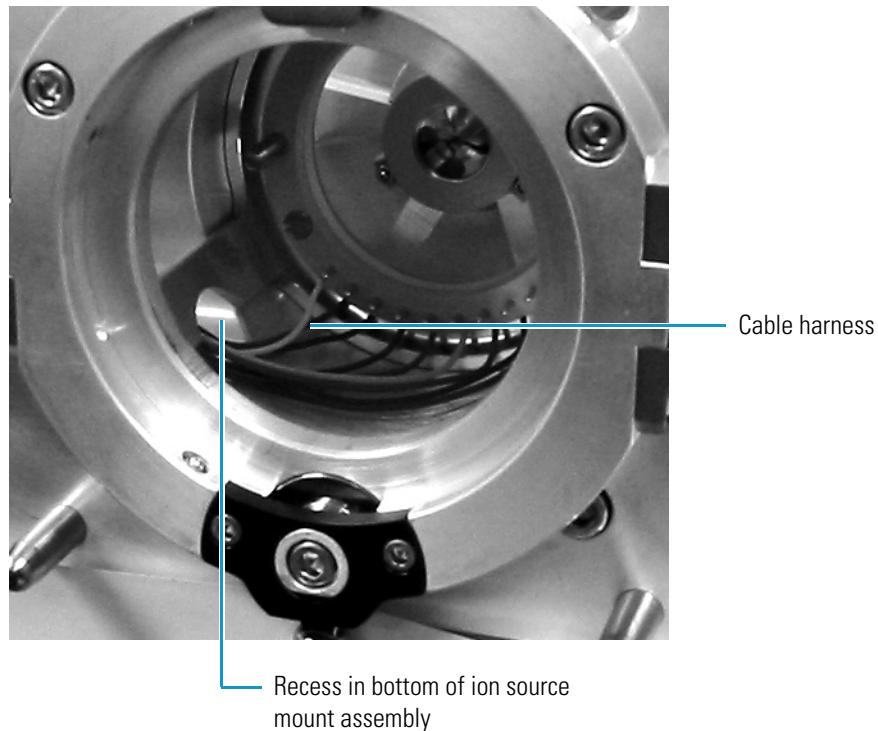


2. Orient the ion optics cage assembly with the contact pins down, and then partially insert it into the ion source mount assembly.
3. Feed the cable harness into the roughing pump adapter and reconnect the cable. Rotate the ion optics cage assembly if necessary.
4. Insert the ion optics cage assembly completely so that the two interstage contact pins are inserted into the sockets in the ion source mount assembly.
5. Ensure that the 3.25 in. ID Viton O-ring is properly seated between the ion optics cage assembly and the ion source mount assembly.
6. Carefully press the wiring harness down into the recess in the bottom of the ion source mount assembly so that the wires are out of the path of the ion source interface assembly that you will install in the next procedure. See [Figure 59](#).

6 Maintenance

Cleaning the Q00 Ion Optics

Figure 59. Ion optics cage assembly, installed



7. Reinstall the three ion optics cage assembly screws that fasten the cage assembly to the ion source mount assembly. See [Figure 53](#).
8. Plug in the ion source cable harness connector. Secure the connector. See [Figure 52](#).
9. Reinstall the roughing pump adapter access plate and screws. See [Figure 51](#).
10. Reinstall the ion source interface cover and screws. See [Figure 50](#).

Reinstalling the Ion Source Interface Assembly

Reinstall the ion source interface assembly as described in the topic [“Reinstalling the Ion Source Interface Assembly”](#) on page 88.

Reinstalling the Ion Max or Ion Max-S Ion Source Housing

Reinstall the Ion Max or Ion Max-S ion source housing as described in the topic [“Installing the Ion Max or Ion Max-S Ion Source Housing”](#) on page 69.

Starting Up the System

Start up the system as described in the topic [“Starting Up the System after a Complete Shutdown”](#) on page 52.

Maintaining the Forepump

The forepump is located under the TSQ work table. Inspecting, adding, purging, and changing the oil are all that is required to maintain the forepump.

Forepump oil is a translucent, light amber color, which you must check often. 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. Plan to change the pump oil after every 3000 hours (about four months) of operation. Refer to the manufacturer's documentation for procedures for purging, adding, and changing the forepump oil.

Cleaning the Fan Filters

You must clean the two fan filters every four months. The fan filters are located on the rear of the front cover and on the right side cover of the TSQ Series mass spectrometer.

❖ To clean the fan filters

1. Remove the fan filter from the right side cover:
 - a. On the TSQ Vantage, using a Phillips screwdriver, remove the six screws that hold the blue appliqué to the right-side cover.
 - b. Remove the appliqué.
 - c. Loosen and remove the four screws that hold the filter bracket to the right-side cover. Note that from the outside of the mass spectrometer the filter bracket appears to be a grille.
 - d. Remove the filter and filter bracket.
2. Remove the fan filter from the front cover:
 - a. Remove the front cover of the TSQ mass spectrometer:
 - i. Disconnect all tubing to the divert/inject valve and syringe pump.
 - ii. Depress the two (blue) spring catches that are located on either side of front cover.
 - iii. Pull the front cover straight off by about 6 in. (15 cm) to access the Front Panel PCB cable and the two grounding wires.
 - iv. Disconnect the Front Panel PCB cable from the TSQ mass spectrometer by pushing the connector retainer up and then pulling the cable free.
 - v. Pull the two grounding wires free from their respective spade connectors.
 - vi. Remove the front cover.

6 Maintenance

Cleaning the Fan Filters

- b. Loosen and remove the four screws that hold the filter bracket to the front cover.
- c. Remove the filter and filter bracket.
3. Wash the fan filters in a solution of soap and water.
4. Rinse the fan filters with tap water.
5. Squeeze the water from the fan filters and allow them to air dry.
6. Reinstall the fan filter on the right-side cover:
 - a. Place the filter in the filter bracket and position the filter bracket and filter on the right-side cover.
 - b. Install and tighten the four screws that hold the filter bracket to the right-side cover.
 - c. On the TSQ Vantage, position the blue appliqué on the right-side cover.
 - d. Install and tighten the six screws that hold the appliqué to the right-side cover.
7. Reinstall the fan filter on the front cover:
 - a. Place the filter in the filter bracket and position the filter bracket and filter on the rear of the front cover.
 - b. Install and tighten the four screws that hold the filter bracket to the front cover.
 - c. Reinstall the front cover of the TSQ mass spectrometer:
 - i. Position the front cover about 6 in. (15 cm) from the TSQ mass spectrometer.
 - ii. Reconnect the grounding wire to the space connector.
 - iii. Reconnect the Front Panel PCB cable to the TSQ mass spectrometer by inserting the cable into the connector. Push the connector retainer down to secure the cable.
 - iv. Align the front cover with the two guide pins on the TSQ mass spectrometer.
 - v. Push the front cover against the TSQ mass spectrometer until the two spring catches lock.
 - vi. Reconnect all tubing to the divert/inject valve and the syringe pump.

Diagnostics and PCB and Assembly Replacement

The TSQ system diagnostics can test many components of the TSQ mass spectrometer. If there is a problem with the instrument electronics, the diagnostics can often locate the problem. Replacing a faulty PCB or assembly can usually correct the problem. After the PCB or assembly is replaced, the diagnostic tests are rerun to verify that the instrument is functioning properly.

Note Three levels of protection are possible:

- No protection—All operators can access all workspaces.
- Automatic protection—Tune Master uses the default password, lctsq, to protect the secure workspaces.
- Custom password protection—The Key Operator (or Laboratory Administrator or Manager) can select a password to protect the secure workspaces.

If your TSQ system has been password protected, you must obtain the password before you can access the secure workspaces (including the System Tune and Calibration workspace). If the instrument password is lost, you must reinstall the TSQ software to reset the default password (lctsq).

Contents

- [Running the TSQ System Diagnostics](#)
- [Replacing a Fuse](#)
- [Replacing PCBs and Power Supplies](#)

Running the TSQ System Diagnostics

The TSQ system diagnostics are used to test the major electronic circuits within the instrument and indicate whether the circuits pass or fail the tests. If there is a problem with the instrument electronics, the TSQ system diagnostics can often locate the problem.

CAUTION Non-expert users should run only the following diagnostics:



- Ion Source Board
- System Control
- Analyzer Control Board

The TSQ system diagnostics do not diagnose problems that are not electrical in nature. For example, they do not diagnose poor sensitivity due to misaligned or dirty components or to improper tuning. Therefore, it is important that the person running the diagnostics be familiar with system operation and basic hardware theory as well as the details of the diagnostics.

Typically, only a Thermo Fisher Scientific field service engineer runs diagnostic tests because certain tests can overwrite system parameters. However, before calling a Thermo Fisher Scientific field service engineer to run diagnostics, consider the following:

- Did the system fail when you were running samples?
- Did problems occur after you performed maintenance on the instrument, data system, or peripherals?
- Did you change the configuration of the system, 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 either of the last two questions above, the problem is probably mechanical, not electrical. Verify again that alignment, configurations, and cable connections are correct before you call the Thermo Fisher Scientific field service engineer. Keep careful notes documenting the nature of the problem and the corrective steps you have taken. If you are not successful in correcting the problem, you can e-mail this information to your field service engineer. The Field Service department can then do a preliminary evaluation of the problem before an engineer arrives at your site.

❖ **To run diagnostics**



CAUTION Non-expert users should run only the following diagnostics:

- Ion Source Board
- System Control
- Analyzer Control Board

1. Open TSQ Tune Master:
 - a. Right-click the **Start** button and select **Explore**.
 - b. Browse to the **C:\Thermo\Instruments\TSQ\system\programs** folder.
 - c. Double-click **TSQTune**.
2. Choose **Workspace > Full Instrument Control** to display the Full Instrument Control Workspace.
3. Choose **Workspace > Diagnostics** to display the Diagnostics Workspace.
4. Select Test Name: **Ion Source Board**, **System Control**, or **Analyzer Control Board**.
5. Select how many times you want to run the tests.
6. Click on the **Start** button to start the diagnostics.

Replacing a Fuse

Fuses protect the various circuits by opening the circuits whenever overcurrent occurs. On the TSQ mass spectrometer, a failed fuse indicates a failed board or electronic module that must be replaced by a Thermo Fisher Scientific field service engineer.



CAUTION Due to the complexity of accessing the TSQ mass spectrometer electronic assemblies, only a Thermo Fisher Scientific field service engineer can replace fuses.

Replacing PCBs and Power Supplies

The electronic assemblies that control the operation of the mass spectrometer are distributed among various PCBs and other modules located in the tower, in the embedded computer, and on or around the vacuum manifold of the mass spectrometer.



CAUTION The TSQ mass spectrometer electronic assemblies are close-packed to minimize the size of the system. Due to the complexity of removing and reinstalling the TSQ mass spectrometer electronic assemblies, only a Thermo Fisher Scientific field service engineer can replace electronic assemblies.

Replaceable Parts

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

Contents

- [MS Accessory Kit](#)
- [TSQ Vantage Instrument Specific Accessory Kit](#)
- [TSQ Quantum Ultra, Ultra AM, and Ultra EMR Instrument Specific Accessory Kit](#)
- [HESI-II Probe Kit](#)
- [TSQ Quantum Access Instrument Specific Accessory Kit](#)
- [TSQ Accurate Mass Calibration Compounds Kit](#)
- [Fittings, Ferrules, and Sample Loops](#)

MS Accessory Kit

Accessory Kit	70111-62034
Fuse, 0.25 A, 250 V, 5x20	00006-01700
Fuse, 0.25 A, 250 V, 5x20	00006-05080
Fuse, 0.50 A, 250 V, 5x20	00006-07608
Fuse, 1.0 A, 250 V, 5x20	00006-07610
Fuse, 2.0 A, 250 V	00006-09102
Fuse, 1.0 A, 250 V, 5x20	00006-10510
Fuse, 4.0 A, 250 V	00006-10705
Fuse, 0.16 A, 250 V, 5x20	00006-11204
Fuse, 4 A, 250 V	00006-11420
Fuse, 1.0 A, 250 V	00006-14015
Fuse, 6.3 A, 250 V, 5x20	00006-11450
Fitting, ferrule, Swagelok, Back, 1/8 in.	00101-02500
Fitting, ferrule, Swagelok, Back, 1/4 in.	00101-04000
Fitting, ferrule, Swagelok, Front, 1/8 in.	00101-08500
Fitting, ferrule, Swagelok, Front, 1/4 in.	00101-10000
Fitting, Swagelok, Nut, 1/4 in., brass	00101-12500

8 Replaceable Parts

TSQ Vantage Instrument Specific Accessory Kit

Fitting, Swagelok, Nut, 1/8 in., brass	00101-15500
Fitting, HPLC adaptor, 10-32 x 1/4-28	00101-18080
Ferrule, 0.008 in. ID, KEL-F™, HPLC	00101-18114
Fitting, Fingertight 2, Upchurch™	00101-18195
Ferrule, Fingertight 2, Upchurch	00101-18196
Fitting, HPLC, Tee, 0.020 orifice, PEEK	00101-18204
Tubing, fused silica, 0.150 mm x 0.390 mm	00106-10498
Tubing, fused silica, 0.10 mm ID x 0.19 mm OD	00106-10499
Tubing, fused silica, 0.05 mm ID x 0.19 mm OD, deactivated	00106-10502
Tube, hypodermic 28-gauge x 10 in.	00106-20000
Fitting, HPLC, 10-32, long, one piece	00109-99-00016
Septa	00301-16999
Syringe, 500 µL, Gastight™, Removable needle	00301-19016
Tubing, PEEK, 0.005 ID x 1/16 in. OD, Red, 5 ft. (1.5 m long)	00301-22912
Tubing, Teflon™, 0.030 in. ID x 1/16 in. OD	00301-22915
Syringe Adapter Kit	70005-62011
Needle, Corona, APCI	70005-98033
Tool, ion transfer tube removal	70111-20258
O-ring, graphite Vespel (for ion transfer tube)	97055-20442

TSQ Vantage Instrument Specific Accessory Kit

Accessory Kit	70111-62081
5/32 Ball driver	00025-10020
Reserpine	00301-12901
Ultramark 1621 (EMR only)	00301-12200
Ion transfer tube	70005-20423
Polytyrosine, liquid	00301-22924
Polytyrosine, solid	00301-22925
Cable, LC/MS	60053-63035

TSQ Quantum Ultra, Ultra AM, and Ultra EMR Instrument Specific Accessory Kit

Accessory Kit	70111-62057
5/32 Ball driver	00025-10020
Ultramark 1621 (EMR only)	00301-12200
Reserpine	00301-12901
Needle seal	07055-20271
ESI needle	07055-20273
Kit, metal needle, H-ESI	97055-62026
Ion transfer tube	97055-20199
Polytyrosine, liquid	00301-22924
Polytyrosine, solid	00301-22925
Cable, LC/MS	60053-63035

HESI-II Probe Kit

HESI-II Probe Kit	OPTON 20037
High-flow needle insert assembly	OPTON-53010
Low-flow needle insert assembly.....	OPTON-53011

The HESI-II Probe Kit contains the HESI-II probe with a factory-installed high-flow needle insert. The high-flow metal needle insert is suitable for flow rates equal to or greater than 5 μ L/min. For low-flow rate applications, order the low-flow needle insert assembly.

TSQ Quantum Access Instrument Specific Accessory Kit

Accessory Kit	70111-62059
Reserpine	00301-12901
Ultramark 1621	00301-12200
Needle seal	00950-00952
ESI needle	00950-00990
Ion transfer tube	70111-20972
Polytyrosine, liquid.....	00301-22924
Polytyrosine, solid.....	00301-22925
Kit, metal needle, high flow	70005-62013
Kit, metal needle, low flow	97144-62080
Cable, LC/MS	60053-63035
CsI	HAZMAT-01-00004

TSQ Accurate Mass Calibration Compounds Kit

Calibration Compounds Kit	70111-62029
Polyethelene glycol, 1000 molecular weight, 5 g	00301-07710
Polyethelene glycol, 200 molecular weight, 5 g	00301-07712
Polyethelene glycol, 400 molecular weight, 5 g	00301-07714
Polyethelene glycol, 600 molecular weight, 5 g	00301-07716

Fittings, Ferrules, and Sample Loops

Ferrule, Fingertight 2, Upchurch. (for: PEEK tubing and Teflon tube)	00101-18196
Ferrule, 0.016 in. ID, PEEK, Upchurch (for: Fused-silica capillary infusion line)	00101-18120
Ferrule, 0.012 in. ID, Kel-F, Upchurch (for: High flow metal needle and low flow metal needle)	00101-18114
Ferrule, 0.008 in. ID, Kel-F, Upchurch (for: Fused-silica capillary sample line).....	00101-18116
Ferrule, LC, 1/16 in., stainless steel, Rheodyne	2522-3830
Fitting, Fingertight, Upchurch.....	00101-18195
Fitting, Fingertight, Upchurch.....	00101-18081

8 Replaceable Parts

Fittings, Ferrules, and Sample Loops

Fitting, adapter, Kel-F, 10-32 x 1/4-28, Upchurch (connects directly to ESI probe inlet).....	00101-18080
Nut, LC, 1/16 in., stainless steel, Rheodyne.....	2522-0066
Fitting, LC union, 0.010 in. orifice, PEEK.....	00101-18202
Fitting, LC TEE union, 0.020 in. orifice, PEEK.....	00101-18204
Fitting, adapter union, PEEK, Upchurch.....	00101-18206
5 μ L sample loop, stainless steel.....	00110-22010

Index

A

accessory kit 105
 air leaks, checking for 62
 analyzer assembly, lenses, voltages applied to 35
 analyzer chamber, location (figure) 38
 Analyzer Control PCB, discussion 44
 analyzer region, vacuum manifold, description 38
 anode, electron multiplier, description 35
 API probe, flushing 64
 argon inlet, location (figure) 42
 argon supply
 checking 62
 pressure 62
 atmospheric pressure ionization (API) source
 description 69
 ion source interface 22
 autosampler
 about 14
 configuring 14
 startup 53
 auxiliary gas pressure 42
 auxiliary gas valve, description 42
 auxiliary gas, on/off status 58

C

calibration
 and H-SRM (note) 61
 discussed 61
 frequency (note) 54, 61
 capillary, heated. See ion transfer tube
 cathode, electron multiplier, description 35
 Cautions
 capillary heater cage assembly temperature 83
 emergency shutdown 47
 forepump and line power 40
 lower ion transfer tube temperature before removing 77
 nitrogen supply and API source operation 62

replacing fuses 103
 replacing PCBs and power supplies 103
 scratching the skimmer cone 87
 solvent waste backing into ion source housing 70
 centroid scan, defined 12
 CID. See collision-induced dissociation
 circuit breaker 20
 cleaning procedures
 API probe, flushing 64
 ESI probe, flushing 64
 exit lens 85
 frequency 75
 ion sweep cone 76
 ion transfer tube 66, 76
 Q00 ion optics 89
 Q00 rf lens 89, 95
 sample transfer line 64
 sample tube 64
 skimmer 85–86
 S-lens 85
 sweep cone 66
 tube lens 85–86
 collision cell
 figure 30
 location (figure) 38
 collision energy (Q2 offset voltage) 34
 collision gas valve, description 41
 collision gas, description 32
 collision-induced dissociation (CID), discussion 32
 Communication LED
 description 19
 mass spectrometer reset 55
 mass spectrometer startup 53
 compliance
 EMC iii
 FCC v
 regulatory compliance iii
 WEEE vii
 computer, features 44

Convection gauge
description 40
location (figure) 38
pressure readings (table) 63, 81
conversion dynode
description 35
figure 36
on/off status 58

D

daily maintenance
API probe, flushing 64
emptying solvent waste bottle 66
ion sweep cone, flushing 66, 76
ion transfer tube, flushing 66, 76
sample tube, flushing 64
transfer line, flushing 64

daily system checks
air leaks 62
argon supply 62
check list 64
list 61
nitrogen supply 62
overview 61

data system
description 44
instrument interface 45
interconnect diagram 46
LAN interface 45
LC interface 45
personal computer 44
primary Ethernet adapter 45
resetting 55
shutdown 51

data types, discussed 11

data-dependent scan mode, discussed 9

diagnostics

Caution 102

running 102

divert/inject valve

description 16

location (figure) 17

loop injection 16

plumbing (figure) 17

dynode 35

E

electron multiplier
anode, description 35
description 35
on/off status 58

electronic assemblies
description 42, 103
ion detection system 43
Power Entry Module, description 42
rf voltage generation, description 43
electronics service switch
and complete shutdown 50
location 48
mass spectrometer components on/off status 58
embedded computer
description 43
resetting 55
EMC compliance iii
emergency shutdown procedure 47
ESI probe, flushing 64
Ethernet Link OK LED 22
exit lens
cleaning 85
reinstalling 87
removing 84

F

FCC compliance v
filters 42
fittings, replaceable parts 107
forepump
description 40
maintenance 99
on/off status 58
power cord (Caution) 40
front panel LEDs
Communication 19
description 19
figure 19
Power 19
Scan 19
System 19
Vacuum 19
full scan type 10
functional description
data system 44
divert/inject valve 16
liquid chromatograph 15
mass analyzer 28
mass spectrometer 18
syringe pump 15
TSQ 13
fuses, mass spectrometer, replacing 103

I

- inlet gasses hardware
 - auxiliary gas valve 42
 - collision gas valve 41
 - description 37
 - sheath gas valve 41
- Instrument Configuration window, opening 14
- interconnect diagram 46
- ion detection system
 - conversion dynode 35
 - electron multiplier 35
 - electron multiplier gain 36
 - electronic assemblies 43
- ion gauge
 - description 40
 - pressure readings (table) 63, 81
- Ion Max API source
 - housing (figure) 68
 - housing, rear (figure) 69
 - installing 69
 - maintenance 73
- Ion Max-S API source
 - housing (figure) 68
 - installing 69
- ion optics
 - cage assembly location (figure) 83–84, 86
 - description 24
 - Q0 quadrupole, discussion 27
 - Q00, description 24
- ion optics cage assembly
 - disassembling 94
 - exploded view (figure) 94
 - reinstalling 97
- ion polarity modes, discussed 3
- ion source interface
 - cross-sectional view 23
 - description 22
 - figure 83–84, 86
 - ion transfer tube 23
 - location (figure) 80
 - maintenance 82
 - reinstalling 88
 - release lever (location) 70
 - removing 83
- ion source mount
 - figure 70
 - guide pins 70
 - location (figure) 83–84, 86
- ion source, description 3
- ion sweep cone
 - cleaning 79
 - description 24
- figure 79
- flushing 66, 76
- location (figure) 23
- ion transfer tube
 - description 23
 - figure 24
 - flushing 66, 76
 - location (figure) 23
 - lower temperature before removing (Caution) 77
 - part numbers 81
 - removing and cleaning 76
 - setting temperature 77
- ion transmission device
 - defined 4
 - rod assembly 4

L

- leaks, checking for 62
- LEDs
 - Communication LED 19
 - Communication LED, mass spectrometer reset 55
 - Communication LED, mass spectrometer startup 53
 - divert/inject valve LEDs 20
 - Ethernet Link OK 22
 - Power LED 19
 - Power LED, mass spectrometer reset 55
 - Power LED, mass spectrometer startup 53
 - Pump On, location (figure) 22
 - Scan LED 19
 - syringe pump LED 16, 19
 - System LED 19
 - System LED, mass spectrometer reset 55
 - System LED, mass spectrometer startup 53
 - Vacuum LED 19
 - Vent Valve Closed 21
- lens L0, description 27
- lenses
 - analyzer assembly, voltages applied to 35
 - L21, L22, L23, figure 30
 - L31, L32, L33, figure 30
- liquid chromatograph (LC)
 - about 15
 - configuring 15
 - functional description 15
 - interconnect diagram 46
 - startup 52
 - supported 15
- loop injection, divert/inject valve 16

M

- main power circuit breaker, description 20

maintenance
API probe, flushing 64
exit lens, cleaning 85
forepump 99
frequency (table) 74
Ion Max API source 73
Ion Max-S API source 73
ion source interface 82
ion sweep cone, cleaning 76
ion transfer tube, cleaning 66, 76
ion transfer tube, removing and cleaning 76
Q00 ion optics, cleaning 89
Q00 rf lens, cleaning 89, 95
sample transfer line, flushing 64
sample tube, flushing 64
skimmer, cleaning 85–86
S-lens, cleaning 85
sweep cone, cleaning 66
tube lens, cleaning 85–86
mass analysis
collision-induced dissociation (CID) 32
discussion 32
rf and dc fields (figure) 30
mass analyzer
defined 4
description 28
on/off status 58
mass ranges 12
mass spectrometer
collision gas valve 41
diagnostics 102
electronic assemblies 42, 103
emergency shutdown 47
frequency of cleaning 75
front panel LEDs 19
functional description 18
fuses, replacing 103
inlet gasses hardware 37
interconnect diagram 46
ion detection system electronic assemblies 43
ion gauge 40
LEDs and system startup 55
maintenance procedures (table) 74
mass analyzer 28
Off condition 58
Power Entry Module, description 42
pressure readings (table) 63, 81
resetting 55
RF voltage generation electronic assemblies 43
shutdown 50
Standby condition 49
starting up 52
turbomolecular pump 39

vacuum manifold 38
vacuum system 36
vent valve 41
mechanical pump 40
MS main power circuit breaker
mass spectrometer components on/off status 58

MS/MS scan modes
neutral loss 7
parent 6
product 5

N

neutral Loss scan mode
illustration (figure) 8
neutral loss scan mode
discussed 7
example (figure) 9
nitrogen
pressure 42
rate of consumption 62
nitrogen inlet, location (figure) 42
nitrogen supply
Caution 62
checking 62
pressure 62

O

Off condition, on/off status of components 58
offset voltage, quadrupole 33

P

parent scan mode
discussed 6
illustration (figure) 6
part numbers 105
password 101
personal computer, features 44
power cord, forepump (Caution) 40
Power Entry Module, description 42
Power LED
description 19
mass spectrometer reset 55
mass spectrometer startup 53
power panel, figure 20–21
pressure levels, checking 62
printer, setting up 45
procedures
cleaning the exit lens 85
cleaning the skimmer 86
cleaning the S-lens 85

cleaning the tube lens 86
 complete system shutdown 50
 configuring the LC 15
 disassembling the ion optics cage assembly 94
 installing the Ion Max API source 69
 installing the Ion Max-S API source 69
 maintaining the forepump 99
 placing system in standby 49
 reinstalling the exit lens 87
 reinstalling the ion optics cage assembly 97
 reinstalling the ion source interface 88
 reinstalling the skimmer 87
 reinstalling the S-lens 87
 reinstalling the tube lens 87
 removing skimmer 85
 removing the exit lens 84
 removing the S-lens 84
 removing tube lens 85
 resetting mass spectrometer 55
 product scan mode
 discussed 5
 illustration (figure) 6
 profile scan, defined 11
 pumps
 forepump 40
 turbomolecular pump 39

Q

Q0 ion optics chamber, location (figure) 38
 Q0 ion optics, discussion 27
 Q0 mount assembly, location (figure) 94
 Q0 quadrupole
 description 27
 figure 27
 Q00 ion optics
 cleaning 89
 cleaning components 95
 cross-sectional view 23
 reassembling 96
 skimmer 25
 Q00 RF lens
 description 26
 figure 26
 on/off status 58
 Q00 rf lens
 cleaning 89, 95
 location (figure) 23
 Q00/L0 mount assembly
 exploded view (figure) 95
 location (figure) 94
 Q1 quadrupole, figure 29
 Q1MS and Q3MS scan modes 5

Q2 rod assembly, figure 30
 Q3 quadrupole, figure 29
 quadrupole mass analyzer
 functional description 29, 32
 quadrupole offset voltage 33
 quadrupoles
 mass analysis 29, 32
 Q0, description 27
 Q1 and Q3 29
 RF and dc fields (figure) 31
 rf and dc fields (figure) 30

R

regulatory compliance iii
 replaceable parts
 accessory kit 105
 fittings 107
 part numbers 105
 sample loops 107
 RF voltage generation, discussion 43
 right side power panel
 discussion 21
 figure 21
 rod assemblies
 description 30
 ion transmission 4
 mass analysis 4
 mass analyzer(s), quadrupole 29, 32
 Q1, Q2, and Q3 (note) 5
 roughing pump 40

S

safety precautions xvi
 sample loop, replaceable parts 107
 sample transfer line, flushing 64
 sample tube, flushing 64
 scan data types
 centroid scan 12
 profile scan 11
 Scan LED, description 19
 scan modes
 data-dependent 9
 discussed 3
 mass spectrometer 3
 neutral loss 7
 neutral loss, example (figure) 9
 neutral loss, illustrated (figure) 8
 parent 6
 parent, illustrated (figure) 7
 product 5
 Product, illustrated (figure) 6

Q1MS and Q3MS 5
summary (table) 4

scan types
discussed 10
full-scan 10
selected ion monitoring (SIM) 10
selected reaction monitoring (SRM) 11

selected ion monitoring (SIM) scan type 10

selected reaction monitoring (SRM) scan type 11

sheath gas pressure 41

sheath gas valve, description 41

sheath gas, on/off status 58

shutdown
data system 51
emergency procedure 47
mass spectrometer 50
nonemergency procedure 50

side cover plate (vacuum manifold), description 39

skimmer
cleaning 86
description 25
figure 26
location (figure) 23
reinstalling 87
removing 85

S-lens
cleaning 85
on/off status 58
reinstalling 87
removing 84

solvent waste bottle, emptying 66

solvents
cleaning 86
purity requirements xvii

Standby condition
on/off status of components 58
placing system in 49

startup
autosampler 53
liquid chromatograph 52
mass spectrometer 52
operating conditions, setting 54

sweep gas supply port, location (figure) 80

switches 21

syringe pump
description 15
figure 16

system checks
argon and nitrogen supplies 62
sample tube polyimide elongation 62
vacuum levels 62

System Control PCB, description 43

System LED
mass spectrometer reset 55
mass spectrometer startup 53

system reset button
description 21
location (figure) 21
mass spectrometer reset 55

system shutdown
emergency procedure 47
nonemergency procedure 50

T

tables
mass spectrometer components on/off status 58
mass spectrometer maintenance procedures 74
pressure readings 63, 81
summary of scan modes 4

troubleshooting 101

TSQ
autosampler 14
calibrating 61
calibration, frequency 54
complete shutdown 50
daily system checks 61
data system 44
data types 11
diagnostics 102
divert/inject valve 16
emergency shutdown 47
front panel LEDs 19
functional block diagram (figure) 13–14
functional description 13
interconnect diagram 46
ion polarity modes 3
LEDs and system startup 55
liquid chromatograph 15
mass ranges 12
mass spectrometer 18
operating conditions, setting 54
overview 1
regulatory compliance iii
replaceable parts 105
scan modes 3
scan types 10
shutdown, emergency procedure 47
shutdown, nonemergency procedure 50

Standby condition 49

starting up 52

syringe pump 15

tuning 61

tuning, frequency 54

tube lens
 cleaning 86
 description 24
 figure 24
 location (figure) 23
 on/off status 58
 reinstalling 87
 removing 85
 voltages 24

Tune Master window, opening 15

tuning
 discussed 61
 frequency (note) 54
 tube lens offset voltage 24

turbomolecular pump
 description 39
 on/off status 58

V

Vacuum LED

and analyzer region pressure 19
 description 19

vacuum levels, checking 62

vacuum manifold
 analyzer chamber, location (figure) 38
 collision cell chamber, location (figure) 38
 description 38
 feedthroughs 39
 interior (figure) 38
 pressure readings (table) 63, 81
 Q0 ion optics chamber, location (figure) 38
 side cover plate, description 39

vacuum pumps

forepump 40
 turbomolecular pump 39

vacuum service switch

and mass spectrometer shutdown 50
 location 48
 mass spectrometer components on/off status 58

vacuum system

auxiliary gas valve 42
 block diagram 37
 checking pressure levels 62
 collision gas valve 41
 description 36
 forepump 40
 ion gauge 40
 powering off 21
 pressure readings 63, 81
 sheath gas valve 41
 turbomolecular pump 39
 Vacuum LED 19

vacuum service switch 21
 vent valve 41

vent valve
 description 41
 LED 21

Vent Valve Closed LED 21

voltages
 conversion dynode 35
 ion transfer tube 23
 Q0 ion optics 27
 Q0 offset 27
 Q00 offset 26
 quadrupole rf and dc 30
 tube lens offset 24

W

WEEE compliance vii

