



TSQ Series II

TSQ Endura and TSQ Quantiva

Hardware Manual

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47 CFR 15, Subpart B, Class A: 2012	EN 61000-3-2: 2006 + A1 + A2	EN 61000-4-5: 2006
CISPR 11: 2009 + A1	EN 61000-3-3: 2008	EN 61000-4-6: 2009
ICES-003: 2012	EN 61000-4-2: 2009	EN 61000-4-8: 2010
EN 55011: 2009 + A1	EN 61000-4-3: 2006 + A1 + A2	EN 61000-4-11: 2004
EN 61326-1: 2013	EN 61000-4-4: 2004 + A1	

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- Appropriate pick-up time
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Preface

The *TSQ Endura and TSQ Quantiva Hardware Manual* describes the modes of operation and hardware components for the Thermo Scientific™ TSQ Endura™ and TSQ Quantiva™ triple-stage quadrupole mass spectrometry systems. It also provides the instruments' cleaning and maintenance procedures.

This guide is intended for the following Thermo Scientific mass spectrometers (MSs):

- TSQ Endura (requires one forepump)
- TSQ Quantiva (requires two forepumps)

Contents

- [Accessing Documentation](#)
- [Special Notices, Symbols, and Cautions](#)
- [Contacting Us](#)

❖ To suggest changes to the documentation or to the Help

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



Accessing Documentation


The TSQ Endura and TSQ Quantiva MSs include complete documentation. For system requirements, refer to the release notes on the software DVD.

❖ To view the product manuals

From the Microsoft™ Windows™ taskbar, choose **Start > All Programs > Thermo Instruments > model x.x**, and then open the applicable PDF file.

❖ To view the Help

Do the following as applicable:

- Thermo Tune application: Click the **Options** icon, , and choose **Tune Help**.
- Thermo Xcalibur™ Method Editor: Choose an option from the **Help** menu (or press the F1 key).

❖ To view user documentation from the Thermo Fisher Scientific website

1. Go to thermofisher.com.
2. Point to **Services & Support** and click **Manuals** on the left.
3. In the Refine Your Search box, search by the product name.
4. From the results list, click the title to open the document in your web browser, save it, or print it.

To return to the document list, click the browser **Back** button.










Special Notices, Symbols, and Cautions

Make sure you understand the special notices, symbols, and caution labels in this guide. Most of the special notices and cautions appear in boxes; those pertaining to safety also have corresponding symbols. Some symbols are also marked on the instrument itself and can appear in color or in black and white. For complete definitions, see [Table 1](#).

Table 1. Notices, symbols, labels, and their meanings (Sheet 1 of 2)

Notice, symbol, or label	Meaning
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 product.
Note	Highlights information of general interest.
Tip	Highlights helpful information that can make a task easier.

Table 1. Notices, symbols, labels, and their meanings (Sheet 2 of 2)

Notice, symbol, or label	Meaning
	Caution: Read the cautionary information associated with this task.
	Chemical hazard: Observe safe laboratory practices and procedures when handling chemicals. Only work with volatile chemicals under a fume or exhaust hood. Wear gloves and other protective equipment, as appropriate, when handling toxic, carcinogenic, mutagenic, corrosive, or irritant chemicals. Use approved containers and proper procedures to dispose of waste oil and when handling wetted parts of the instrument.
	Heavy object: Never lift or move the instrument by yourself; you can suffer personal injury or damage the instrument
	Hot surface: Before touching the API source assembly, allow heated components to cool.
	Pinch point: Keep hands away from the specified areas.
	Risk of electric shock: This instrument uses voltages that can cause electric shock and personal injury. Before servicing the instrument, shut it down and disconnect it from line power. While operating the instrument, keep covers on.
	Risk of eye injury: Eye injury can occur from splattered chemicals, airborne particles, or sharp objects. Wear safety glasses when handling chemicals or servicing the instrument.
	Sharp object: Avoid handling the tip of the syringe needle.
	Trip obstacle: Be aware of cords, hoses, or other objects located on the floor.

Read and understand the following cautions that are specific to the shutdown of the mass spectrometry system or to the removal of parts for cleaning.



CAUTION If you must turn off the MS in an emergency, turn off the main power switch located on the right-side power panel. This switch turns off all power to the MS, including the forepump, without harming components within the system. However, do not use this method as part of the standard shutdown procedure. Instead, see [Shutting Down the Mass Spectrometer Completely](#).

To turn off the LC, autosampler, and data system computer in an emergency, use their respective on/off switch or button.



CAUTION To avoid an electrical shock, be sure to follow the instructions in [Shutting Down the Mass Spectrometer Completely](#).



CAUTION Do not turn the instrument on if you suspect that it has incurred any kind of electrical damage. Instead, disconnect the power supply cord and contact Thermo Fisher Scientific technical support for a product evaluation. Do not attempt to use the instrument until it has been evaluated. (Electrical damage might have occurred if the system shows visible signs of damage or has been transported under severe stress.)



CAUTION Do not disconnect the power supply cord from the MS while the other end is still plugged into the electrical outlet.



CAUTION Do not place any objects (for example, the syringe pump or other containers with liquids) on top of the instrument, unless instructed to in the documentation. Leaking liquids might contact the electronic components and cause an electrical short circuit.



CAUTION Hot surface. Allow heated components to cool to room temperature (approximately 20 minutes) before servicing them.



CAUTION Place the MS in Standby (or Off) mode before you open the atmospheric pressure ionization (API) source. The presence of atmospheric oxygen in the API source when the MS is on could be unsafe. (The MS automatically turns off when you open the API source; however, it is best to take this added precaution.)






CAUTION Follow the instrument maintenance instructions. To avoid personal injury or damage to the instrument, do not perform any servicing other than that contained in the *TSQ Endura and TSQ Quantiva Hardware Manual* or related manuals unless you are authorized to do so.



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 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, you must decontaminate the pump and certify it as free of contamination before a Thermo Fisher Scientific field service engineer repairs or makes adjustments or before it is sent back to the factory for service.

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^a You can use your smartphone to scan a QR Code, which opens your email application or browser.

Introduction

The TSQ Endura and TSQ Quantiva mass spectrometers are members of the Thermo Scientific family of MSs. The TSQ Endura and TSQ Quantiva systems consist of the MS, a syringe pump, a divert/inject valve, and the Thermo Xcalibur data system.

Note The [Glossary](#) defines some of the terms used in this manual.

Contents

- [Mass Spectrometer Models](#)
- [Overview of an LC/MS Analysis](#)
- [LC/MS Functional Block Diagram](#)
- [Electronic Assemblies](#)
- [Controls and Indicators](#)
- [Cooling Fans](#)

Mass Spectrometer Models

For descriptions of the various hardware components, see [Chapter 3, “Vacuum System,”](#) [Chapter 4, “Ion Transmission and Mass Analysis,”](#) and [Chapter 5, “Syringe Pump and Divert/Inject Valve.”](#)

TSQ Endura MS

The TSQ Endura is a mass spectrometer that contains a triple-quadrupole [mass analyzer](#) and includes an external syringe pump, a divert/inject valve, and the Thermo Scientific EASY-Max NG™ API source. The instrument requires one forepump.



TSQ Quantiva MS

The TSQ Quantiva is a mass spectrometer that contains a triple-quadrupole mass analyzer and includes an external syringe pump, a divert/inject valve, and the Thermo Scientific Ion Max NG™ API source. The instrument requires two forepumps.



Overview of an LC/MS Analysis

Typical LC/MS analysis begins with the liquid chromatograph (LC) separating a mixture into its chemical components. The LC pump produces a solvent stream (the mobile phase) that passes through an HPLC column (containing the stationary phase) under high pressure. An autosampler introduces an aliquot of sample into this solvent stream. As the solvent stream passes through the LC column, the sample separates into its chemical components. The rate at which the components of the sample elute from the column depends on their relative affinities to the mobile phase and the stationary phase.

As the separated chemical components exit the LC column, they pass through a sample transfer line and enter the [mass spectrometer](#) for ionization and analysis. As the MS analyzes the ionized components and determines each [mass-to-charge ratio \(m/z\)](#) and relative intensity, it sends a data stream to the data system computer.

When the system setup includes a [syringe pump](#) and [divert/inject valve](#), there are three additional ways to introduce a sample into the MS, as described in [Table 2](#).

Table 2. Methods of sample introduction into the MS

Method	Description
Direct infusion	Connect the syringe pump directly to the atmospheric pressure ionization (API) source of the MS.
High-flow infusion	Use a union Tee to combine the flow from the syringe pump with the flow from an LC pump.
Manual loop injection	Connect a sample loop, a needle port fitting, and an LC pump to the divert/inject valve. After you fill the sample loop with sample, switch the position of the divert/inject valve, which places the contents of the sample loop in the path of the solvent flow produced by the LC pump.

Note Analysis by direct infusion or flow injection provides no chromatographic separation of components in the sample before they pass into the MS.

The MS consists of an API source, ion optics, a triple-stage mass analyzer, and an ion detection system. All are enclosed in a vacuum manifold, except for part of the API source.

Ionization of the sample takes place in the API source. The specific method used to ionize the sample is referred to as the ionization technique. The ion optics transmit the ions produced in the API source into the mass analyzer to determine the *m/z* values (of the ions produced in the API source). The polarity of the electric potentials applied to the API source and ion optics determines whether positively charged ions or negatively charged ions are transmitted to the mass analyzer. You can set up data acquisition methods for the MS to analyze positively or negatively charged ions or to switch between these polarity modes during a single run.

The data system serves as the user interface to the MS, autosampler, LC pump, and syringe pump. Refer to the Xcalibur Help for more information about the MS data processing and instrument control application.

Each sequence of loading a mass analyzer with ions followed by [mass analysis](#) of the ions is called a [scan](#). The ability to vary not only the ionization and [ion polarity modes](#), but the scan mode and scan type, provides greater flexibility in the instrumentation for solving complex analytical problems.

For information about the [heated-electrospray \(H-ESI\)](#), [atmospheric pressure chemical ionization \(APCI\)](#), and [atmospheric pressure photoionization \(APPI\)](#) techniques, refer to the *Ion Max NG and EASY-Max NG Ion Sources User Guide*. For information about the [nanoelectrospray ionization \(nanoESI or NSI\)](#) technique, refer to the nano source manual.

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

- The TSQ Endura and TSQ Quantiva operate as conventional MS systems with one stage of mass analysis. The ion source ionizes the sample, and mass filtering of the ion products occurs in the first rod assembly. The second and third rod assemblies transmit the resulting mass-selected ions to the ion detection system.¹

—or—

- The TSQ Endura and TSQ Quantiva operate as tandem MS systems with two stages of mass analysis. The ion source ionizes the sample, and mass filtering of the ion products occurs in 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 filtering 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.

During a scan, the first stage of mass analysis elucidates the structures of pure organic compounds and the structures of the components within mixtures. Furthermore, in a scan sequence that involves a second stage of mass analysis, the MS 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. Therefore, the MS makes it possible to investigate all pathways to form and fragment each ion in the [mass spectrum](#).

The two stages of mass analysis are ideal for very selective and sensitive analysis by reducing chemical noise in the final mass spectrum.

¹ You can also use the instrument as a single-stage MS by transmitting the ions through the first and second rod assemblies followed by mass analysis in the third rod assembly.

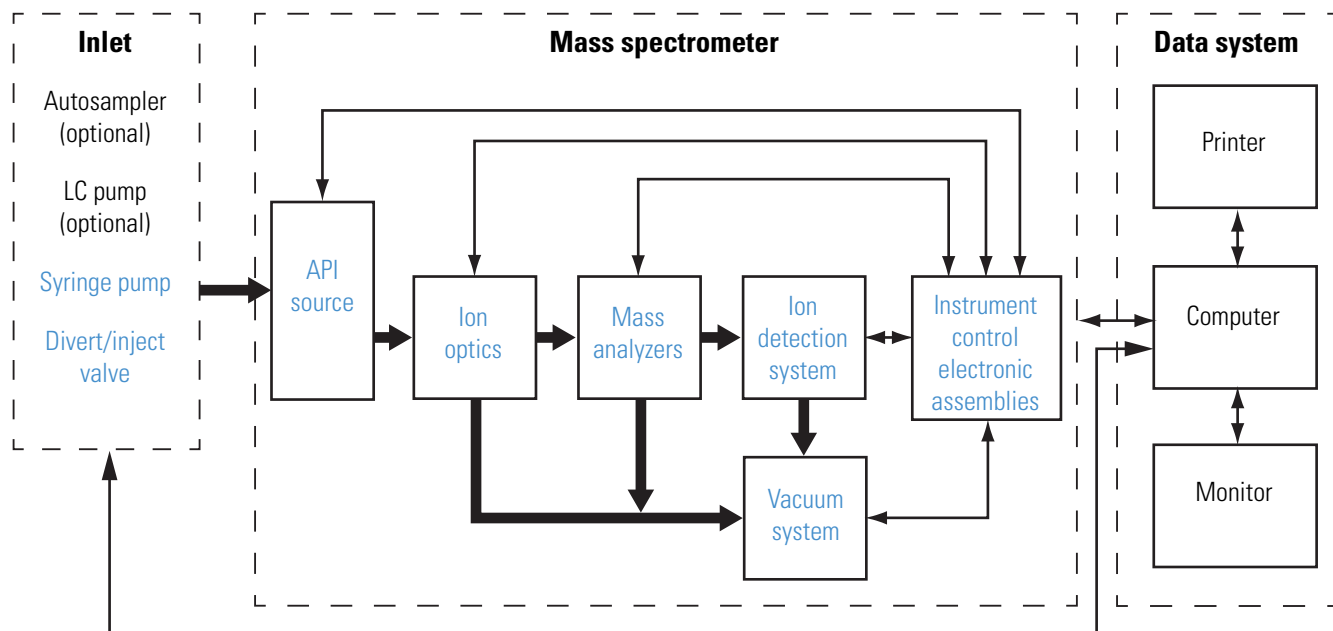
The MS uses several different scan modes and scan types to filter, fragment, or transmit ions in the mass analyzer, including the ionization and ion polarity modes. This ability to vary the scan mode and scan type provides greater flexibility in the instrumentation for solving complex analytical problems.

LC/MS Functional Block Diagram

Figure 1 shows a functional block diagram of the MS systems with links to additional information. The LC device is usually installed on the left side of the MS. A dedicated holder that sits on top of the MS contains the syringe pump and divert/inject valve.

In a typical 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 MS for analysis.

Figure 1. Functional block diagram of the TSQ Endura and TSQ Quantiva systems



Electronic Assemblies

The electronic assemblies that control the operation of the MS are distributed among various printed circuit boards (PCBs) and other modules, in the embedded computer, and on or around the vacuum manifold of the MS. You cannot service the electronic assemblies.

Note If you need assistance, contact your local Thermo Fisher Scientific field service engineer.

Controls and Indicators

The TSQ Endura and TSQ Quantiva MSs have the following controls and indicators:

- [LEDs](#)
- [Power Entry Module](#)
- [Communications Panel](#)

LEDs

Figure 2 shows the LED indicators on the instrument front panel. See their descriptions in Table 3.

Figure 2. TSQ Endura and TSQ Quantiva front panel LEDs



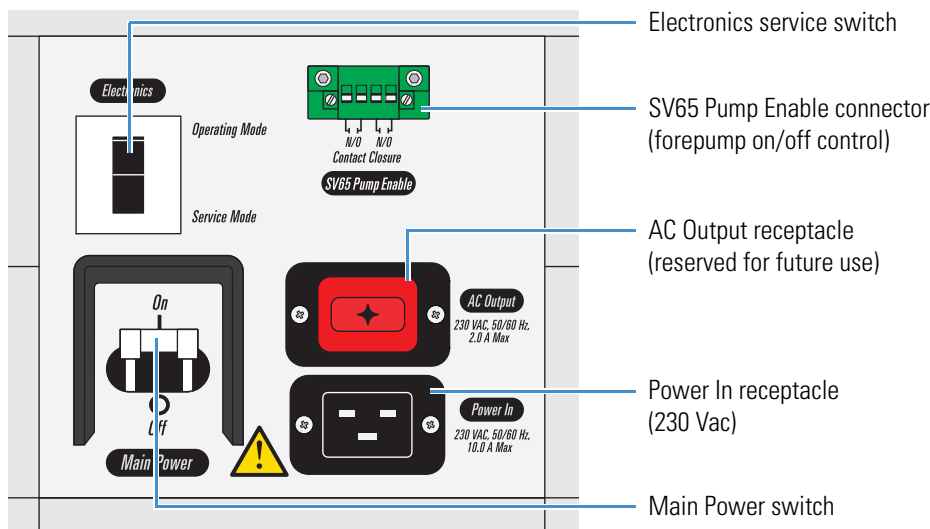
Table 3. LEDs for the TSQ Endura and TSQ Quantiva MSs

LED	State	Description
Power	Green	The MS is receiving power. (The electronics service switch is in the Operating Mode position.)
	Off	The MS is not receiving power. (The electronics service switch is in the Service Mode position.)
Vacuum	Green	The vacuum is within the allowable operating range.
	Yellow	The vacuum is outside the allowable operating range.
	Off	The MS is either off or in the process of starting up.
Communication	Green	The MS and data system are communicating.
	Yellow	The MS and data system are trying to establish a communication link.
	Off	The MS is off.
System	Green	The MS is on.
	Yellow	The MS is in standby mode.
	Off	The MS is off.
Scan	Flashing blue	The MS is on and scanning.
	Off	The MS is not scanning.

Power Entry Module

The MS receives line power at 230 Vac \pm 10%, 5 A, 50/60 Hz through the right-side power entry module (Figure 3).

Figure 3. Power entry module



Main Power Switch

In the Off position, the Main Power (circuit breaker) switch removes all power to the MS, including the external forepump or forepumps. In the On position, the MS receives power. In the standard operational mode, the switch stays in the On position.



CAUTION In an emergency do not use the electronics service switch to shut off power to the MS. Instead, place the main power circuit breaker switch (labeled *Main Power*) in the Off (down) position and disconnect the power cord from the electrical outlet.

Electronics Service Switch

The electronics service switch is a circuit breaker. In the Service Mode (down) position, the switch removes power to all components of the MS except for the fans and vacuum system. This setting allows you to service nonvacuum system components with the vacuum system still operating. In the Operating Mode (up) position, all components of the MS have power.

SV65 Pump Enable Connector

The MS turns the forepump or forepumps on and off by using the relay control cable that connects to the SV65 Pump Enable connector.

Communications Panel

The communications panel, which is located on the right side of the MS, provides a system Reset button, a contact closure interface (Peripheral Control), an analog input connector, USB ports for the external syringe pump and divert/inject valve, and a Gigabit Ethernet connection port for the data system computer.

When you briefly press the reset button, the embedded processing system and digital circuitry reset and the system software reloads from the data system. For more information about resetting the MS, see [Resetting the Mass Spectrometer](#).

Figure 4 shows the communication connectors, and Table 4 describes the pin-outs for these connectors.

Figure 4. Communication connectors (right side of the MS)

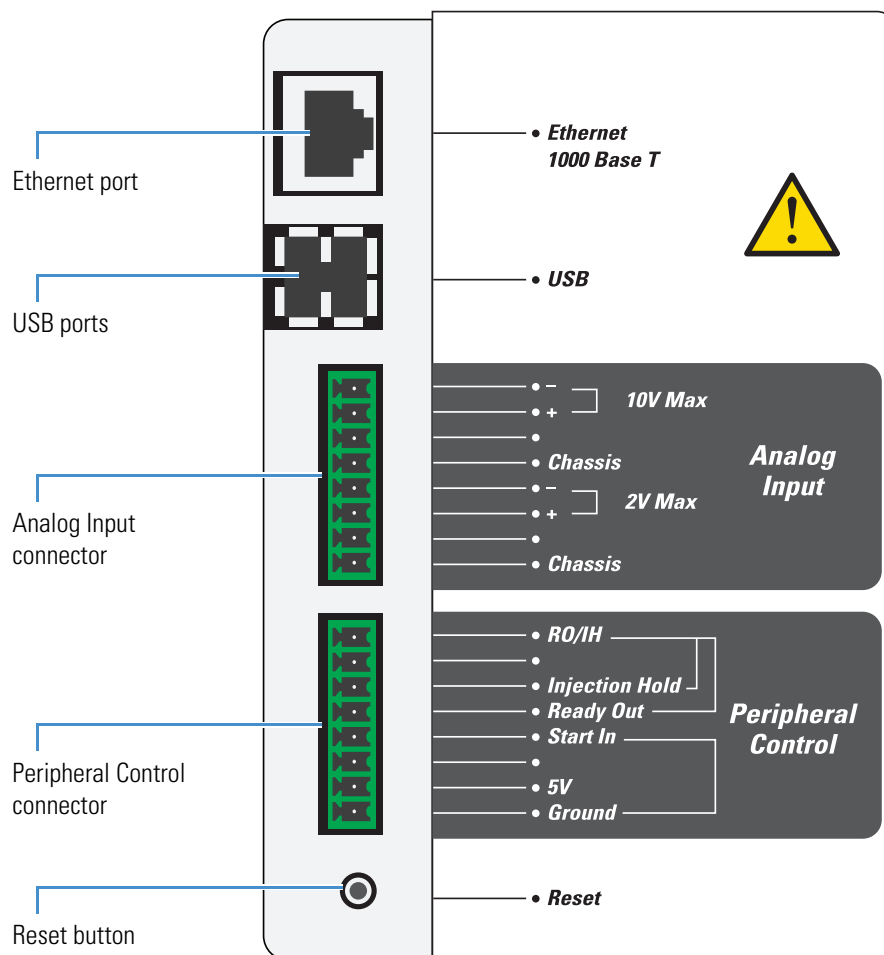


Table 4. Pin-out descriptions for the communication connectors (Sheet 1 of 2)

Pin	Name	Description
–	Reset	Resets the instrument to a power-up state. Note Use this button only if the instrument does not respond to the control program on the data system computer or if you need to restart the instrument without turning off the electronics service switch.
Peripheral Control		
1	Ground	Earth ground
2	5V	Provides a 5 Vdc, 500 mA output (with pin 1).
4	Start In	Receives the start signal from the contact closure connection of a connected external device. To activate this signal, the external device must pull the signal either low (below 0.75 Vdc) or high (above 2.4 Vdc), depending on the polarity, for at least 100 ms by using a relay, an open-collector driver, or a similar device that connects between pins 4 and 1. Note In the Instrument Configuration window, set the contact closure signal to “High-to-low edge” or “Low-to-high edge,” whichever matches the setting for the connected external device.
5	Ready Out	Provides a relay-driven programmable output signal to the connected external device. The relay opens when a method starts and closes when the method finishes. Output: Maximum 24 Vdc, 3 A
6	Injection Hold	Provides a relay-driven programmable output signal to the connected external device, such as a fraction collector. Output: Maximum 24 Vdc, 3 A
8	RO/IH	Common (return) connection for the Ready Out and Injection Hold pins

Table 4. Pin-out descriptions for the communication connectors (Sheet 2 of 2)

Pin	Name	Description
Analog Input		
The two analog channels connect to two separate 12-bit analog-to-digital converters (ADC) for on-demand conversion of the input voltage. The conversion rate depends on the MS rate.		
1	Chassis	Earth ground (for pins 3 and 4)
3, 4	2V Max: + (positive, pin 3) and – (negative, pin 4)	Provides a connection for an external device, such as an LC instrument. Input: 0–2 Vdc (voltage clamps at 5 Vdc)
5	Chassis	Earth ground (for pins 7 and 8)
7, 8	10V Max: + (positive, pin 7) and – (negative, pin 8)	Provides a connection for an external device, such as an LC instrument. Input: 0–10 Vdc (voltage clamps at 15 Vdc)
Other connectors		
–	USB (2 ports)	Provides a connection for the syringe pump and divert/inject valve.
–	Ethernet 1000 Base T	Provides a connection for the Ethernet switch.

Cooling Fans

Several fans, including those in the power supply subassemblies, provide internal cooling for the MS. Cooling air enters through the three main air intake fans on the right side of the MS. Exhaust air exits the instrument from the back ventilation slots.

The only user-serviceable part is the air filter in front of the air intake fans. For the recommended maintenance schedule, see [Chapter 8, “Maintenance.”](#)



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

Scan Parameters

This chapter describes some of the scan parameter settings that you set in the TSQ Endura or TSQ Quantiva Tune application.

Contents

- [Scan Types](#)
- [Scan Mass-To-Charge Ratio Ranges](#)
- [Data Types](#)
- [Ion Polarity Modes](#)

Scan Types

The TSQ Endura and TSQ Quantiva MSs operate in a variety of scan types. The most common can be divided into two categories: single mass spectrometry (MS) scan types and MS/MS scan types. The scan types in each category are as follows:

- MS scan types: full scan (Q1), full scan (Q3), selected ion monitoring (SIM) scan (Q1), and SIM scan (Q3)
- MS/MS scan types: product ion scan, precursor ion scan, neutral loss scan, and [selected reaction monitoring \(SRM\) scan type](#)

The available modes depend on the number and type of rod assemblies and the voltages applied to the rod assemblies.

The mass analyzers have three rod assemblies.¹ 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

¹ A rod assembly is a regular array of metal rods. See [Mass Analyzers](#).

If you apply only RF voltage, a rod assembly serves as an ion transmission device that passes all ions within a large range of m/z values (that is, virtually all ions that are present).

When you apply both RF and DC voltages to a rod assembly, ions of different m/z values have different stability profiles. This difference in stability allows the rod assembly to act as a mass filter.

On the MS, the quadrupole rod assemblies can operate with both RF and DC voltages or with only RF voltage. That is, Q1 and Q3 can act as either mass analyzers or ion transmission devices. The Q2 rod assembly operates exclusively with RF voltage. Therefore, Q2 is always an ion transmission device. For a summary of how the rod assemblies function in several of the major scan types, see [Table 5](#).

Table 5. Summary of scan types

Scan type	Quadrupole Q1	Q2 collision cell	Quadrupole Q3
Full scan (Q1)	Scan ^a	Pass all ions. ^b	Pass all ions.
Full scan (Q3)	Pass all ions.	Pass all ions.	Scan
SIM scan (Q1)	Set ^c	Pass all ions.	Pass all ions.
SIM scan (Q3)	Pass all ions.	Pass all ions.	Set
Product ion scan	Set	Fragment ions ^d ; then pass all fragments.	Scan
Precursor ion scan	Scan	Fragment ions; then pass all fragments.	Set
Neutral loss scan	Scan	Fragment ions; then pass all fragments.	Scan
SRM scan	Set	Fragment ions; then pass all fragments.	Set

^a Full scan or transmission of selected ions.

^b Pass ions or fragments within a wide range of m/z values.

^c Set to pass ions of a single m/z or a set of m/z values.

^d Collisions with argon gas cause ions to fragment.

Full Scan Q1 and Q3 Scan Types

The full scan Q1 and Q3 scan types 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, the ion source forms ions that 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. The full scan Q1 scan type uses Q1 as the mass analyzer; the full scan Q3 scan type uses Q3 as the mass analyzer.

Use [full-scan type](#) experiments to determine or confirm the m/z (identity) of unknown compounds or the m/z of each component in a mixture of unknown compounds. (Generally, you need a full mass spectrum to determine the m/z of an unknown compound.)

The full scan gives you more information about an analyte than does the [selected ion monitoring \(SIM\) scan type](#), but a full scan does not yield the sensitivity that the other two scan types can achieve. This scan type requires less time monitoring the signal for each ion than in the [selected reaction monitoring \(SRM\) scan type](#) or SIM. Full scan provides greater information but lower sensitivity than the other two scan types.

Before you perform a SIM or an SRM experiment, you must know what ions or reactions you are looking for. Therefore, 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 precursor ions of interest. Then, you might use SIM or SRM to do routine quantitative analysis of the compound.

Selected Ion Monitoring Scan Type

Selected ion monitoring (SIM) monitors a particular ion or set of ions. You can use SIM experiments to detect small quantities of a target compound in a complex mixture when you know the m/z of the target compound. Therefore, 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; it 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, which can result in a false positive.

Product Scan Type

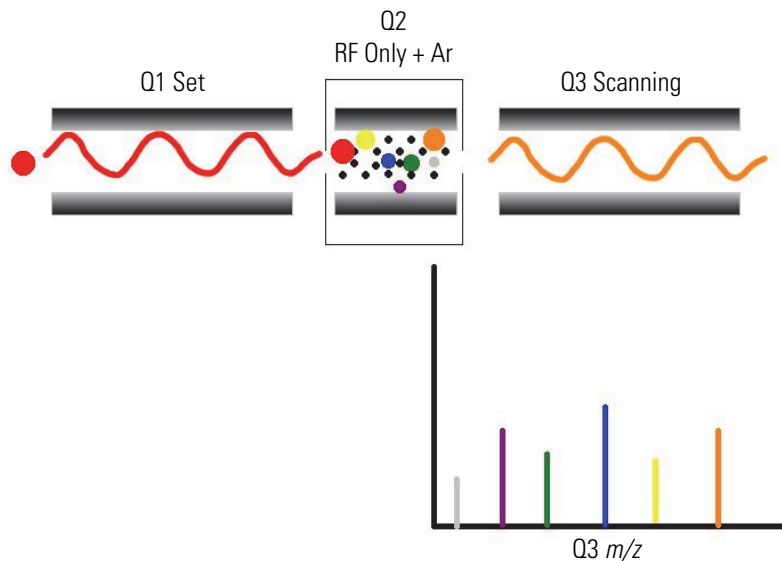
Product scan type performs two stages of analysis ([Figure 5](#)). In the first stage, the ion source forms ions that enter Q1, which is set to transmit ions of one m/z . Ions selected by this first stage of mass analysis are called precursor ions. (As a result, Q1 is referred to as the precursor mass analyzer, and the m/z of ions transmitted by the precursor mass analyzer is referred to as the precursor set mass.) After Q1 selects the precursor ions, they enter Q2, which is surrounded by the collision cell.

Note For ease of documenting the first, second, and third rod assemblies as separate pieces of hardware, this manual refers to them as Q1, Q2, and Q3, respectively. However, when discussing each rod assembly's function in MS/MS scan types, this manual uses the terms *precursor 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 the product mass analyzer (Q3) for the second stage of mass analysis. The product mass analyzer is scanned to obtain a mass spectrum that shows the product ions produced from the fragmentation of the selected precursor ion.

Experiments that use a product ion scan type can determine the m/z values of all the product ions from a specific precursor. These can be used to identify unknowns or as the basis for developing an SRM experiment.

Figure 5. Illustration of product scan type



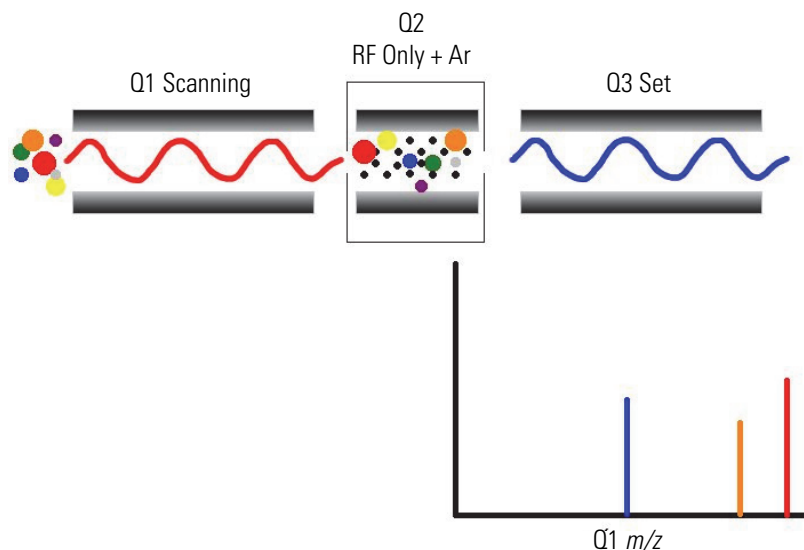
Precursor Scan Type

The precursor scan type also uses two stages of analysis (Figure 6). In the first stage, the ion source forms ions that are introduced into the precursor mass analyzer, which is scanned to transmit precursor ions sequentially into the collision cell.

In the second stage of analysis, in the collision cell, precursor ions can fragment to produce product ions by unimolecular decomposition of metastable ions or by CID. The collision cell forms ions that enter the product mass analyzer, which transmits a selected product ion. (The product set mass is the m/z of ions transmitted by the product mass analyzer.)

The resulting spectrum shows all the precursor ions that fragment to produce the selected product ion. For a mass spectrum obtained in the precursor scan type (precursor mass spectrum), note that data for the m/z axis is obtained from Q1 (the precursor ions), whereas data for the ion intensity axis is obtained from Q3 (from monitoring the product ion).

Figure 6. Illustration of the precursor scan type



You can use experiments that employ the precursor scan type (precursor experiments) in structure and fragmentation studies as well as in survey analyses of mixtures. In general, precursor experiments detect all compounds that decompose to a common fragment. You can use the experiments 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 Type

In the neutral loss scan type (Figure 7), the two mass analyzers (Q1 and Q3) link together so that they are scanned at the same rate over mass ranges of the same width. However, the respective mass ranges, are offset by a selected mass so that the product mass analyzer scans a selected number of mass units lower than the precursor mass analyzer.

As a result, the neutral loss scan type provides two stages of mass analysis. In the first stage, the precursor mass analyzer (Q1) separates ions that form in the ion source by their m/z values. These ions enter the collision cell.

In the second stage of analysis, ions in 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 m/z value.

To detect an ion, 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. Therefore, a neutral loss mass spectrum is a spectrum that shows all the precursor ions that lose a neutral species of a selected mass.

You can also perform a neutral gain (or association) experiment 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 precursor mass spectrum, Q1 (the precursor ion) provides data for the m/z axis, whereas Q3 (the product ion being monitored) provides data for the ion intensity axis.

You can use experiments that use the neutral loss scan type (neutral loss experiments) when surveying a large number of compounds for common functionality. However, you frequently lose neutral moieties from substituent functional groups (for example, CO_2 from carboxylic acids, CO from aldehydes, HX from halides, and H_2O from alcohols). Figure 8 shows a common fragment ion.

Figure 7. Illustration of the neutral loss scan type

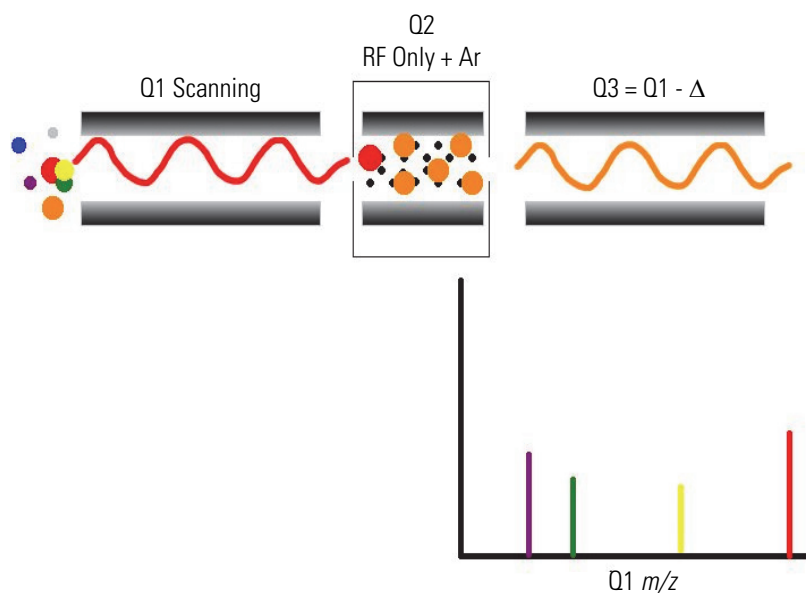
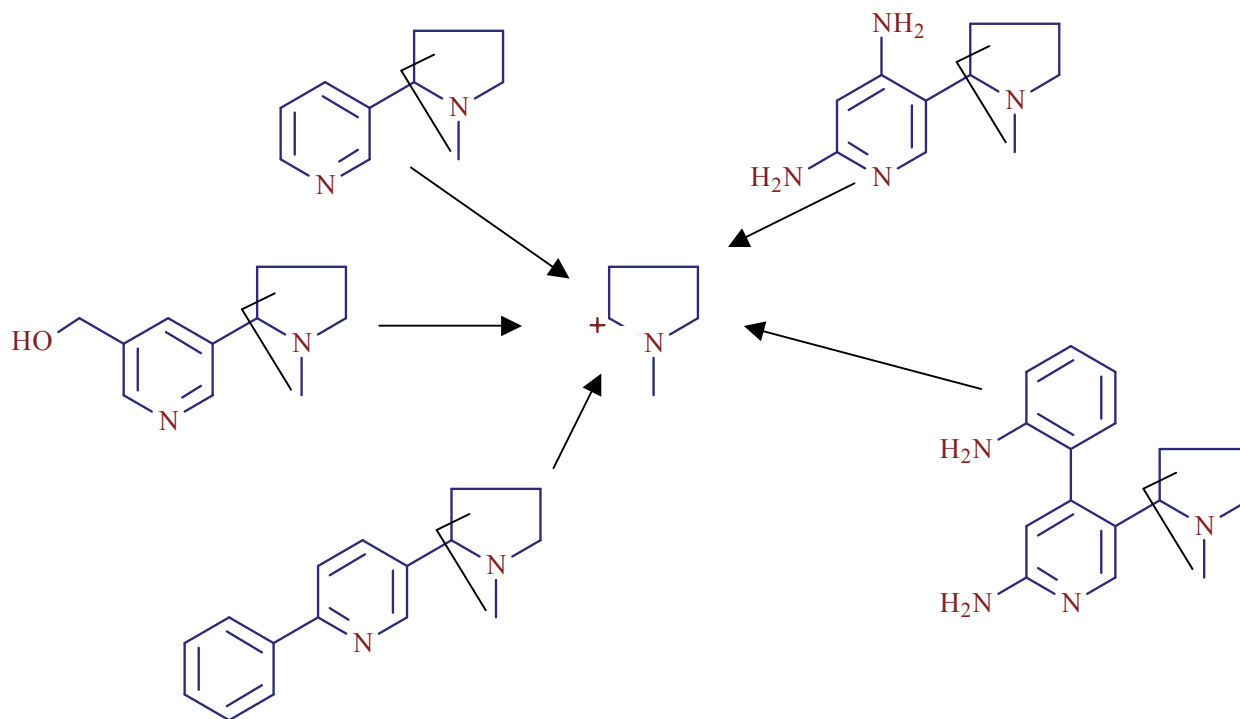


Figure 8. Examples of compounds with a common fragment



Selected Reaction Monitoring Scan Type

Selected reaction monitoring (SRM) monitors a particular transition or set of transitions, such as the fragmentation of an ion or the loss of a neutral moiety. SRM monitors a limited number of precursor/product ion pairs.

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 greater selectivity compared to SIM. Any interfering compound would have to form a precursor ion of the same m/z as the selected precursor ion from the target compound. Furthermore, that precursor ion would have to fragment to form a product ion of the same m/z as the selected product ion from the target compound.

Scan Mass-To-Charge Ratio Ranges

The TSQ Endura MS can operate in a range of m/z 10–3400. The TSQ Quantiva MS can operate in a range of m/z 10–1800.

Data Types

You can acquire and display mass spectral data (intensity versus m/z) in one of two data types:

- Profile data—With [profile data](#), you can see the inherent shape of the peaks in the mass spectrum. The mass spectrum divides each atomic mass unit into several sampling intervals. The intensity of the ion current is determined at each sampling interval. The intensity at each sampling interval is displayed with the intensities connected by a continuous line.
- Centroid data—With [centroid data](#), you can see the mass spectrum as a bar graph. This scan data type sums the intensities of each set of sampling intervals. This sum is displayed versus the integral center of mass of the many sampling intervals. Centroid data requires about one-tenth the computer disk space of what is required for profile data.

Ion Polarity Modes

The TSQ Endura and TSQ Quantiva MSs can operate in either positive or negative ion polarity mode. The MS controls whether positive ions or negative ions are transmitted to the mass analyzer for mass analysis by changing the polarity of the voltage potentials applied to the API source, ion optics, and ion detection system. The ion optics are located between the API source and the mass analyzer.

The information obtained from a positive ion mass spectrum is different from and complementary to the information from a negative ion spectrum. Therefore, 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.

Vacuum System

This chapter describes the principal components of the [vacuum system](#) for the TSQ Endura and TSQ Quantiva MSs.

Contents

- [Vacuum System Functional Block Diagram](#)
- [Schematic of the Internal Gas Supply Lines](#)
- [Inlet Gases Hardware](#)
- [Vacuum Manifold](#)
- [Vacuum Gauges](#)
- [Vacuum Pumps](#)
- [Atmospheric Pressure Ionization Source](#)
- [API Source Interface](#)

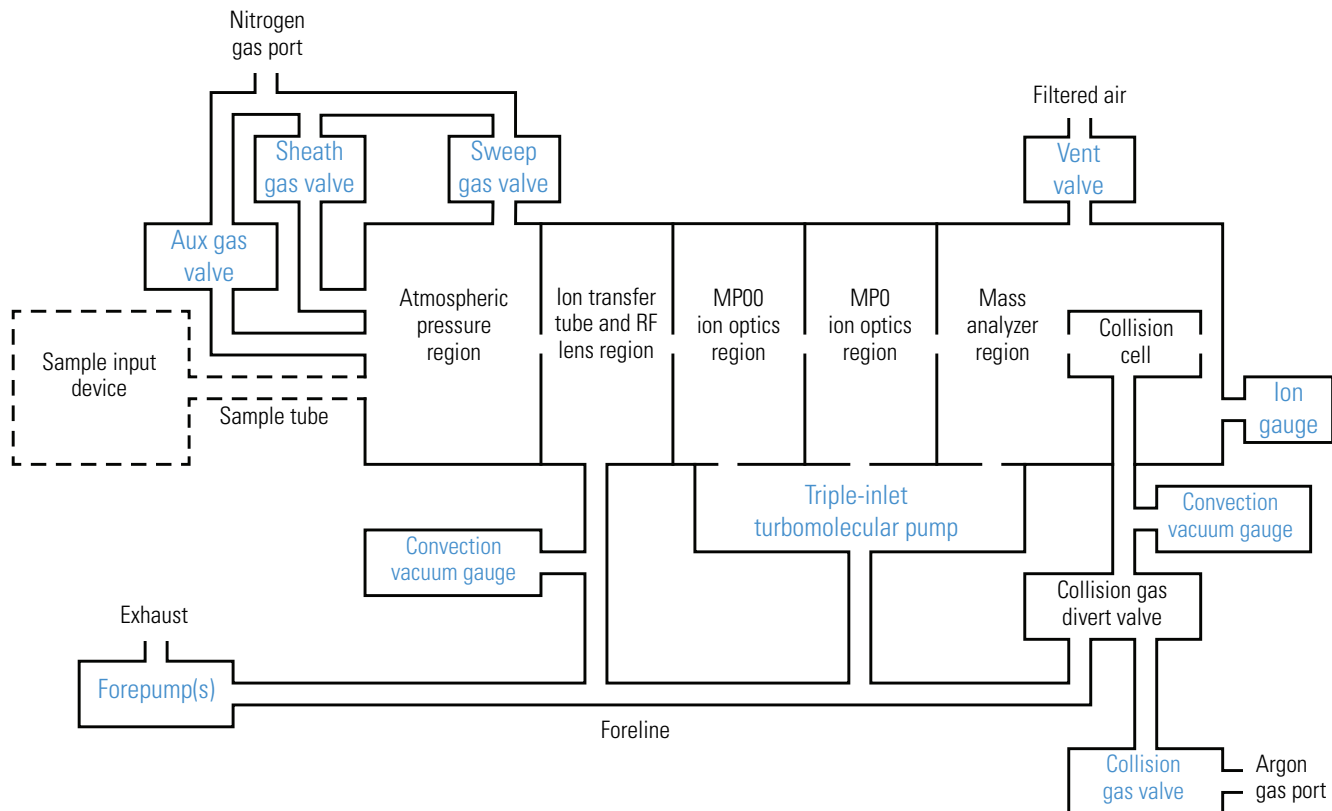
3 Vacuum System

Vacuum System Functional Block Diagram

Vacuum System Functional Block Diagram

The vacuum system evacuates the region around the API source interface, ion optics, mass analyzer, and ion detection system. [Figure 9](#) shows a functional block diagram of the vacuum system with links to additional information.

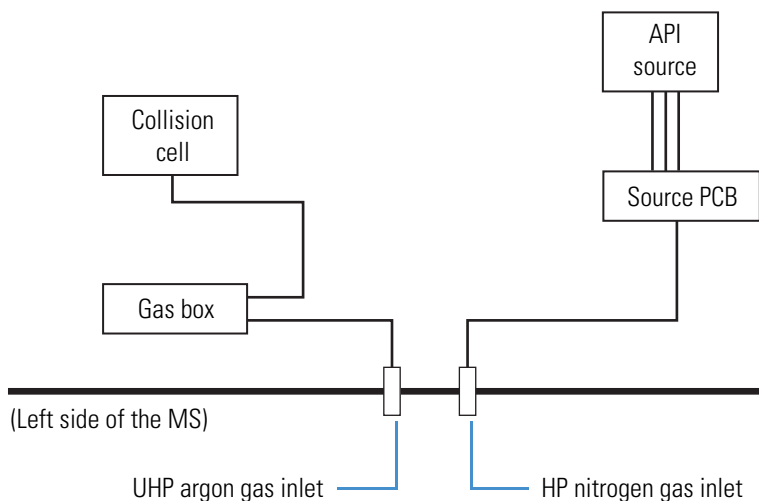
Figure 9. Functional block diagram of the vacuum system



Schematic of the Internal Gas Supply Lines

Figure 10 shows a schematic drawing of the gas lines in the MS.

Figure 10. Schematic of the internal gas supplies



Inlet Gases Hardware

The inlet gas hardware controls the flow of gases into the MS: the argon collision gas; the nitrogen sheath gas, auxiliary gas, and sweep gas; and the nitrogen venting gas. Figure 11 shows the gas inlets on the left side of the MS.

Note For a list of guidelines for the operating parameters of the API source, refer to Chapter 1 in the *TSQ Endura and TSQ Quantiva Getting Started Guide*.

- Argon Gas Valves—The data system controls the valves that regulate the argon gas pressure (see [Checking the Gas Supplies](#)). You can set the collision gas pressure (CID gas) in the Tune application.

Argon gas (135 ± 70 kPa [20 ± 10 psi], 99.995% minimum purity) enters the left side of the MS through a 1/8 in. port. The valves for the collision gas control the flow of argon gas into and out of the Q2 collision cell. When activated, a solenoid valve shuts off the argon gas flow to the cell.

- Nitrogen Gas Valves—The data system controls the valves that regulate the nitrogen pressure (see [Checking the Gas Supplies](#)). You can set the gas flow rates in the Ion Source pane of the Tune application.

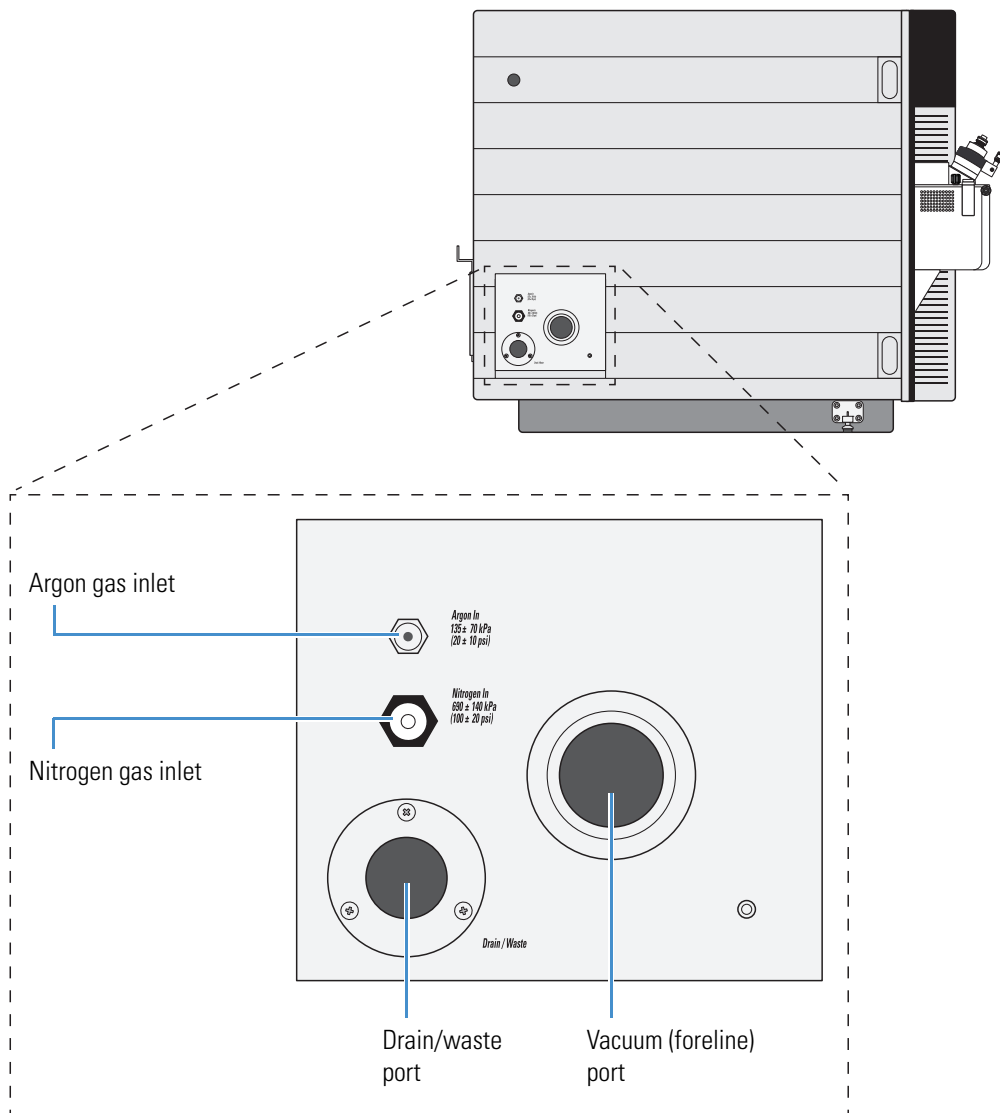
Dry nitrogen gas (690 ± 140 kPa [100 ± 20 psi], 99% purity) enters the left side of the MS through a 1/4 in. port. The valves for the sheath, auxiliary, and sweep gases control the flow of dry nitrogen gas into the API source (Figure 9). Sheath gas is the inner-coaxial nitrogen gas that helps nebulize the sample solution into a fine mist as the solution exits the API spray insert nozzle. Auxiliary gas is the outer-coaxial nitrogen gas that helps the

sheath gas in the nebulization and evaporation of the sample solution by focusing the vapor plume and lowering the humidity in the API source. Sweep gas is the off-axis nitrogen gas that flows out from behind the optional ion sweep cone to aid in solvent declustering and adduct reduction. The optional ion sweep cone has an inlet for the sweep gas.

- Vent Valve—The solenoid-operated vent valve allows the [vacuum manifold](#) to be vented with filtered air. The vent valve on the vacuum manifold is closed when the solenoid is energized.

The vacuum manifold vents when the MS no longer receives external power, as with a power failure or when you turn off the main power switch. Power is briefly provided to the vent valve after losing external power to protect against the accidental loss of power. When power to the vent valve solenoid shuts off for more than a very brief period of time, the vent valve opens and the manifold vents air.

Figure 11. Gas inlets and vacuum (foreline) port (left side of the MS)



Vacuum Manifold

The vacuum manifold (Figure 12), a thick-walled, aluminum chamber, encloses the API source interface, ion optics, mass analyzer, and ion detection system assemblies. It has multiple removable top cover plates, various electrical feedthroughs, and gas inlets.

Table 6 lists the five vacuum regions, the pumps that evacuate them, and the chamber pressures. The block diagram in Figure 9 shows the vacuum regions.

Table 6. Vacuum regions, evacuation devices, and typical pressures

Region	Components	Evacuated by	Pressure	
			TSQ Endura	TSQ Quantiva
1	API source	N/A	Atmosphere	
2	RF lens	Forepump or forepumps	Less than 2 Torr	Less than 4.5 Torr
3	MP00 ion optics	Triple-inlet turbomolecular pump (first inlet [molecular drag])	50 mTorr	
4	MP0 ion optics	Triple-inlet turbomolecular pump (second inlet [interstage])	1 mTorr	
5	Mass analyzer	Triple-inlet turbomolecular pump (third inlet [high vacuum])	Less than 10^{-5} Torr	

Vacuum Gauges

The MS contains three types of vacuum gauges that measure the pressure in specific regions of the vacuum manifold. In the Tune application, you can observe the readback values for the vacuum gauges on the By Function page in the Status pane (under Vacuum).

- Convection pressure gauge—Measures pressure down to a fraction of a milliTorr (mT). The instrument uses two convection gauges:
 - Source pressure gauge—Measures the pressure in the RF lens and [API ion transfer tube](#) region in the vacuum manifold and the foreline, which connects the triple-inlet turbomolecular pump and the forepump or forepumps.
 - Collision gas pressure gauge—Measures the pressure in the collision cell.
- Ionization gauge—Measures the pressure in the analyzer region of the vacuum manifold.

The ionization gauge produces energetic electrons that cause molecular ionization. A collector attracts positive ions formed in the ionization gauge, and the collector current is related to the pressure in the vacuum manifold. The ionization gauge is also involved in vacuum protection.

Vacuum Pumps

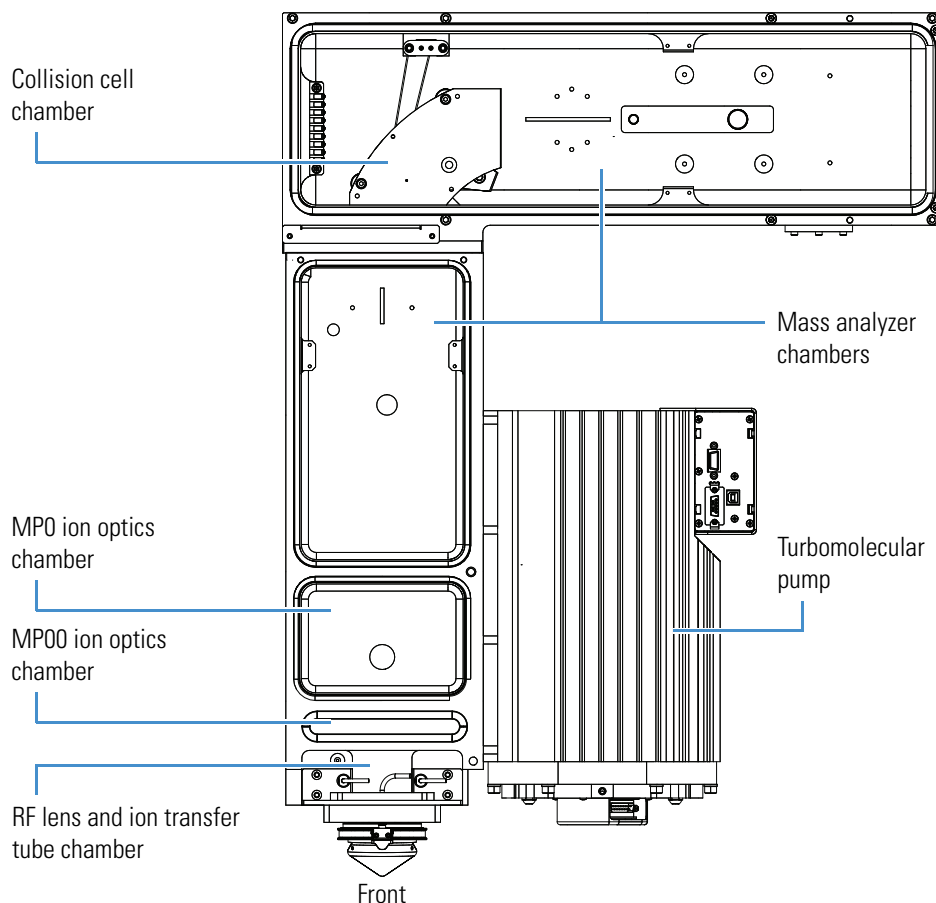
The MS requires either one (TSQ Endura MS) or two (TSQ Quantiva MS) external forepumps, and both instruments require an internal **turbomolecular pump** to provide the vacuum pressures for the five vacuum regions (Figure 9). The forepumps create the vacuum necessary to properly operate the turbomolecular pump. It also evacuates the ion transfer tube region of the vacuum manifold.

The forepumps' detachable power supply cords plug into separate, single-phase 230 Vac wall outlets. The relay control cable that connects between the MS's SV65 Pump Enable connector (Figure 3) and forepumps remotely turns the forepumps on and off. The Main Power switch controls the SV65 Pump Enable connector, not the electronics service switch.

As shown in Figure 12, one triple-inlet **turbomolecular pump** controls the vacuum for multiple vacuum regions. The turbomolecular pump also sends status information, such as its temperature or rotational speed, to the data system computer.

The Main Power switch turns off the turbomolecular pump. The electronics service switch has no effect on these pumps. Power to the turbomolecular pumps automatically shuts off if the temperature of the turbomolecular pumps becomes too high.

Figure 12. Placement of the turbomolecular pump next to the vacuum manifold



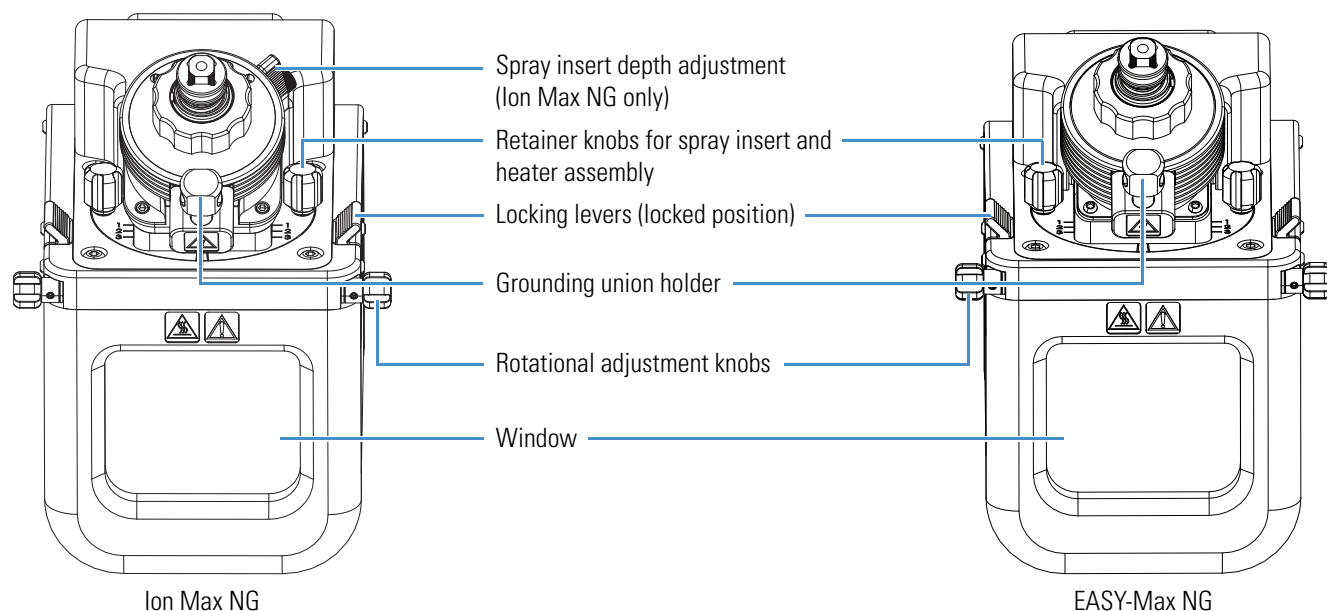
Atmospheric Pressure Ionization Source

The atmospheric pressure ionization (API) source forms gas phase sample ions from sample molecules that are contained in solution. The API source also serves as the interface between the LC and the MS. You can configure the EASY-Max NG API source (provided with the TSQ Endura MS) or the Ion Max NG API source (provided with the TSQ Quantiva MS) for the following ionization techniques: [heated-electrospray \(H-ESI\)](#), [atmospheric pressure chemical ionization \(APCI\)](#), and [atmospheric pressure photoionization \(APPI\)](#). Figure 13 shows both API sources.

The MS has a front, built-in drain that routes the solvent waste from the API source to the solvent waste container connected to the left-side drain/waste port. For information about the solvent waste connection, refer to the *TSQ Endura and TSQ Quantiva Getting Connected Guide*.

For information about the API source, refer to Chapter 2 in the *TSQ Endura and TSQ Quantiva Getting Started Guide*. For instructions on how to install the spray insert, refer to the *Ion Max NG and EASY-Max NG Ion Sources User Guide*.

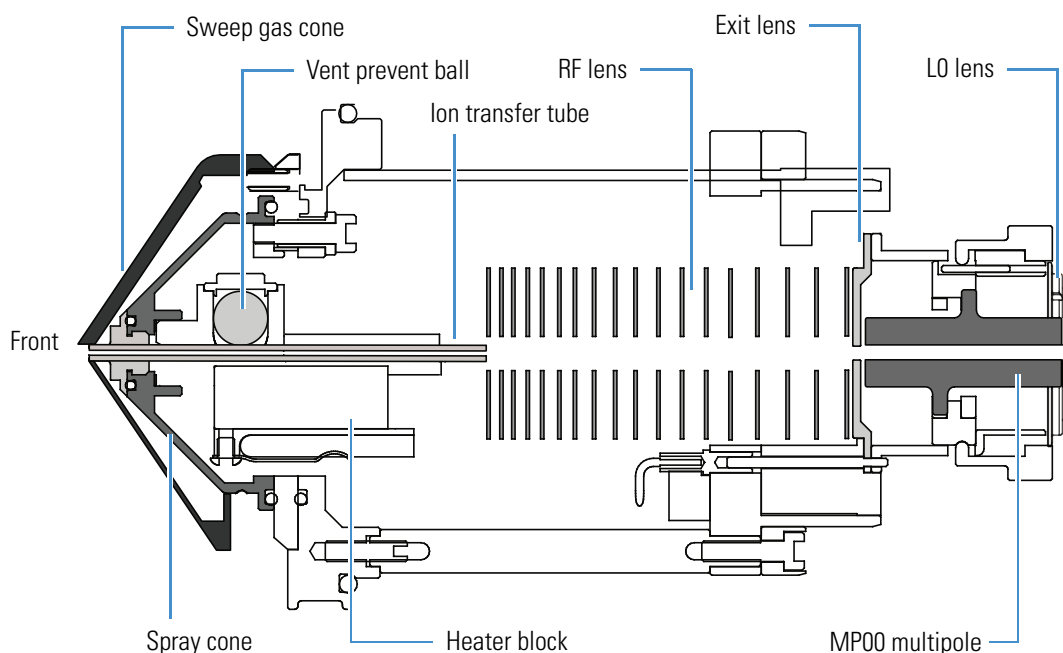
Figure 13. Ion Max NG and EASY-Max NG ion sources



API Source Interface

The API source interface includes an ion sweep cone, an ion transfer tube, two cartridge heaters, a heater block, a sensor, a vent prevent ball, the RF lens, the exit lens, and lens L0 (Figure 14). Except for the atmospheric pressure side of the ion sweep cone that is within the API source, the API source interface components are located in a vacuum chamber compartment that the forepump evacuates to a pressure of approximately 1.5 Torr (for the TSQ Endura MS) or 4.0 Torr (for the TSQ Quantiva MS).

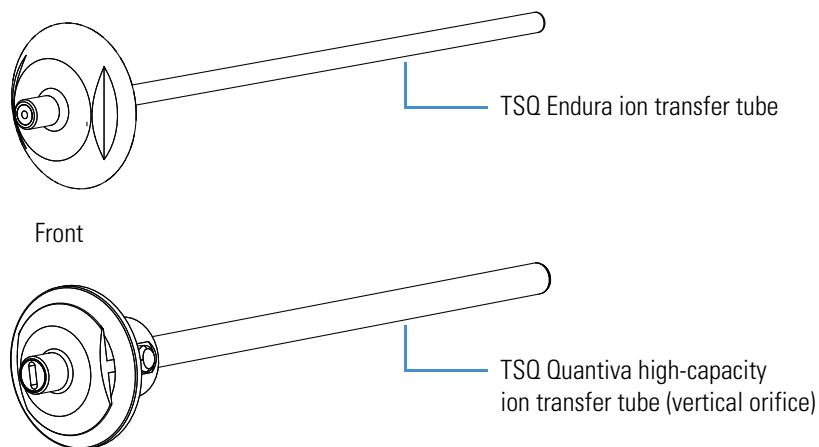
Figure 14. API source interface (TSQ Endura MS cross section)



The ion sweep cone is a metal cone over the ion transfer tube. The ion sweep cone channels the sweep gas toward the entrance of the ion transfer tube, acts as a physical barrier that protects the entrance of the ion transfer tube, and increases source robustness. The net result is a significant increase in the number of samples to analyze without a loss of signal intensity. In addition, keeping the ion transfer tube entrance as clean as possible reduces the need for frequent maintenance. The ion sweep cone improves ruggedness when analyzing complex matrices, such as plasma or nonvolatile salt buffers. Remove the ion sweep cone before performing NSI experiments.

The ion transfer tube (Figure 15) is a metal, cylindrical tube that assists in desolvating ions produced by the API spray insert while transferring them into the vacuum system. The high-capacity ion transfer tube (in the TSQ Quantiva MS) has a vertical 2×0.6 mm (0.08×0.02 in.) rectangular orifice, and the regular ion transfer tube (in the TSQ Endura MS) has a 0.58 mm (0.02 in.) diameter orifice.

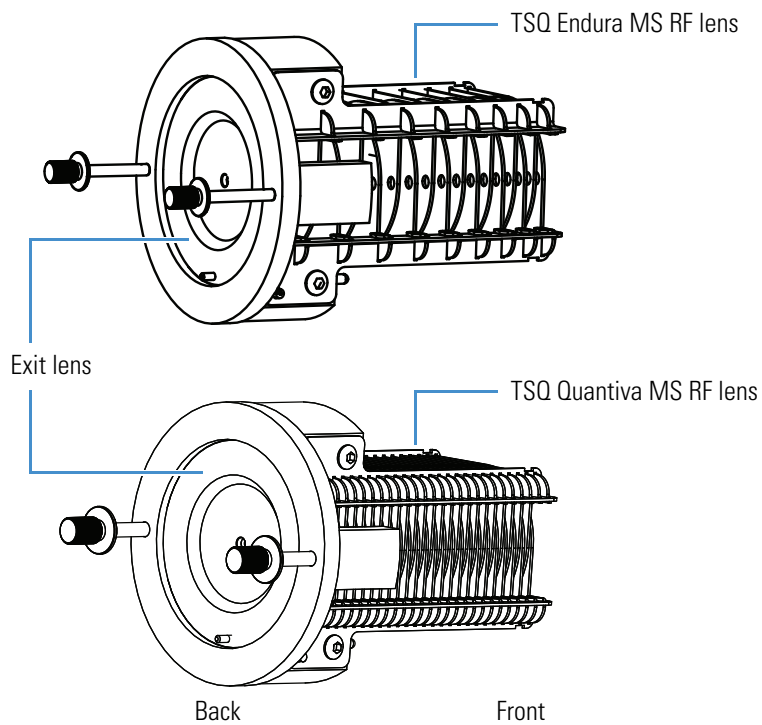
Figure 15. Ion transfer tubes



The heater block contains two heater cartridges that surround the ion transfer tube and heat the tube to temperatures up to 400 °C (752 °F). A thermocouple measures the temperature of the heater block. Typical temperatures of the ion transfer tube are 270 °C (518 °F) for H-ESI and 250 °C (482 °F) for APCI, but these temperatures vary with the flow rate and the mobile phase composition. A decreasing pressure gradient draws ions into the ion transfer tube in the atmospheric pressure region and transports them to the API source interface region of the vacuum manifold. When you remove the ion transfer tube (after it has cooled to room temperature), the vent prevent ball drops into place to stop air from entering the vacuum manifold. Therefore, you can remove the ion transfer tube for cleaning or replacement without venting the system.

Ions from the ion transfer tube pass through the RF lens and then the exit lens (Figure 16). The RF lens is an ion transmission device consisting of progressively spaced, stainless-steel electrodes. The RF lens differs slightly between the TSQ Endura MS and the TSQ Quantiva MS. The MS applies an RF voltage to the electrodes, and adjacent electrodes have voltages of opposite phase. As the RF amplitude increases, ions of progressively higher m/z values pass through to the exit lens and move toward the MP00 RF lens. The exit lens acts as a vacuum baffle between the higher pressure API source interface region and the lower pressure MP00 RF lens region of the vacuum manifold. The RF lens and exit lens mount to the API source interface cage.

Figure 16. RF and exit lenses



3 Vacuum System

API Source Interface

Ion Transmission and Mass Analysis

This chapter provides descriptions of the ion optics elements, mass analyzer, and ion detection system in the TSQ Endura and TSQ Quantiva MSs.

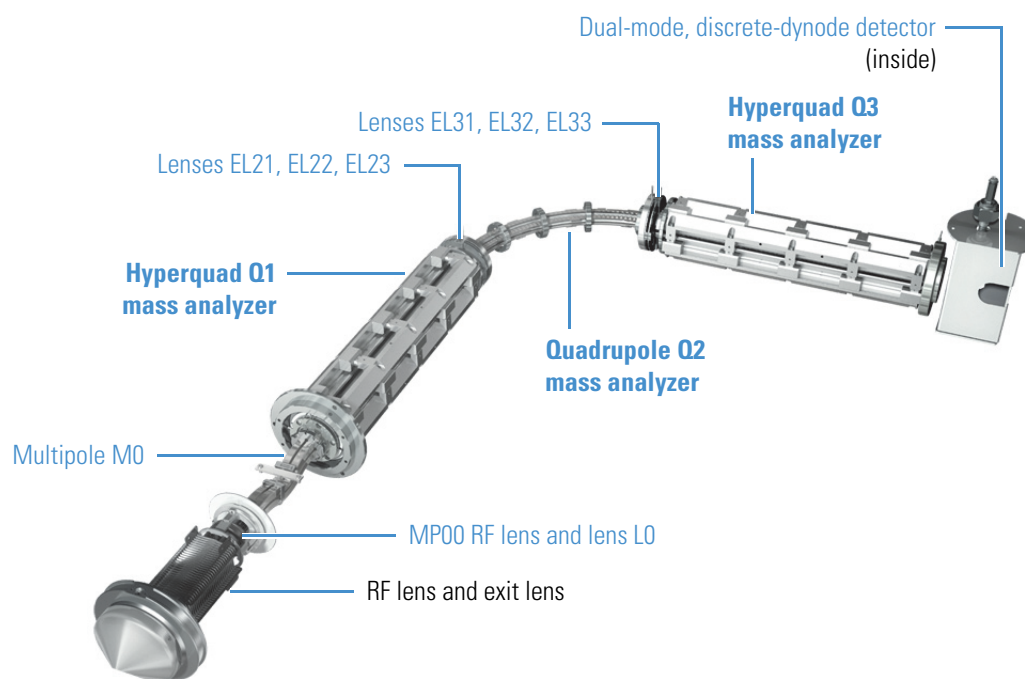
Contents

- Ion Optics
- Mass Analyzers
- Dual-Mode, Discrete-Dynode Ion Detection System

Ion Optics

Figure 17 shows a schematic of the ion transmission path through the MS and provides links to additional information.

Figure 17. Schematic of the MS ion transmission path



The ion optics focus the gas-phase sample ions into the mass analyzer. See the following topics:

- [MP00 Ion Optics](#)
- [MP0 Ion Optics](#)

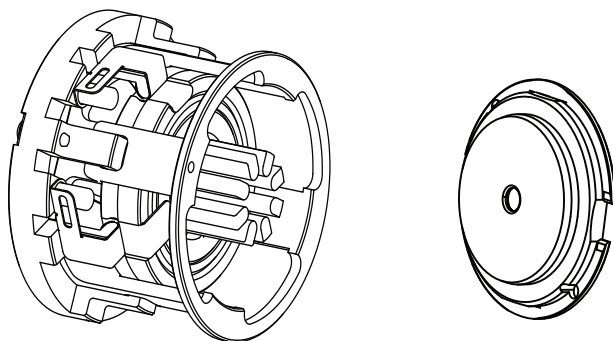
MP00 Ion Optics

Ions pass through the exit lens and move toward the MP00 ion optics, which are located between the API source interface and the MP0 ion optics. The MP00 ion optics include the MP00 RF lens and the L0 lens. For the location of these components, see [Figure 17](#).

The MP00 RF lens is an array of eight metal elements ([Figure 18](#)). The MS applies an RF voltage to the elements, generating an electric field that guides the ions along the axis of the lens.

The lens L0 is a metal disk with a small hole in the center through which the ion beam passes ([Figure 18](#)). The MS applies an electrical potential (positive for positive ions and negative for negative ions) to lens L0 to aid in ion transmission. Lens L0, which mounts to the MP00 RF lens, also acts as a vacuum baffle between the MP00 and MP0 ion optics chambers.

Figure 18. MP00 RF lens (left) and lens L0 (right)

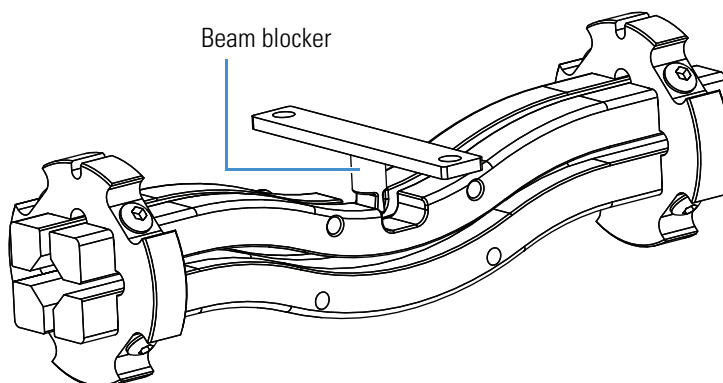


MP0 Ion Optics

The MP0 ion optics transmit ions from the MP00 ion optics to the mass analyzer. The MP0 ion optics include multipole MP0 and lenses TK1 and TK2. See [Figure 17](#) for the location of these components.

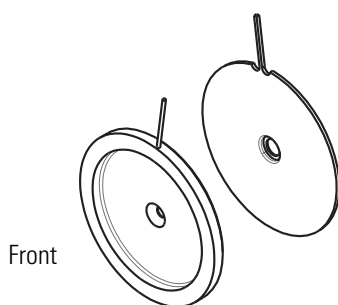
Multipole MP0 is an array of square-metal rods that act as an ion transmission device ([Figure 19](#)). The MS applies an RF voltage to the elements, generating an electric field that guides the ions along the axis of the multipole. The MP0 offset voltage increases the translational kinetic energy (TKE) of ions emerging from MP00. The rods are curved so that charged ions follow the curve of the rod. Because neutral species do not follow the curve, they strike the neutral beam blocker and are removed from the beam.

Figure 19. Multipole MP0 and beam blocker



The TK1 and TK2 lenses are metal discs with a circular hole in the center through which the ion beam passes (Figure 20). Together they act as a two-element cone lens. The MS applies an electrical potential to the lens to accelerate (or decelerate) ions as they approach each lens and to focus the ion beam as it passes through each lens. Lenses TK1 and TK2 act as a vacuum baffle between the multipole MP0 and quadrupole Q1.

Figure 20. TK1 (left) and TK2 (right) lenses



Mass Analyzers

This section describes the components of the mass analyzer, voltages applied to the mass analyzer electrodes, and mass analyzer operation during mass analysis. Ion manipulation and mass analysis occur in a mass analyzer, which consists of three quadrupole rod assemblies (Q1, Q2, and Q3) and two lens sets (EL21, EL22, EL23 and EL31, EL32, EL33). See Figure 17.

Note For ease of documenting the first, second, and third rod assemblies as separate pieces of hardware, this manual refers to them as Q1, Q2, and Q3, respectively. However, when discussing each rod assembly's function in MS/MS scan types (see Chapter 2), this manual uses the terms *precursor mass analyzer*, *collision cell* (ion transmission device surrounded by the collision cell), and *product mass analyzer*, respectively.

The following subtopics discuss the mass analyzer in detail:

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

Quadrupole Rod Assemblies

The three rod assemblies in the mass analyzers are numbered from the API source end of the manifold and are designated Q1, Q2, and Q3 (Figure 17). Quadrupoles Q1 and Q3 enable high-resolution scans without signal loss.

For the TSQ Endura MS, quadrupoles Q1 and Q3 (also known as a hyperquads) are square arrays of circular rods (Figure 21). For the TSQ Quantiva MS, quadrupoles Q1 and Q3 are square arrays of precision-machined and precision-aligned, true hyperbolic rods (Figure 22). Quartz spacers act as electrical insulators between adjacent rods.

Figure 21. Quadrupole Q1 or Q3 (TSQ Endura MS)

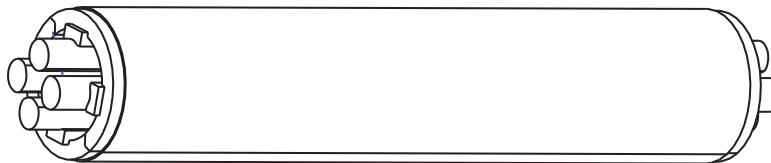
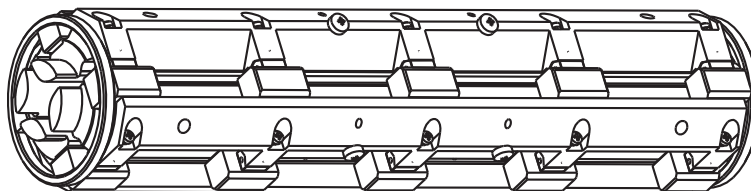


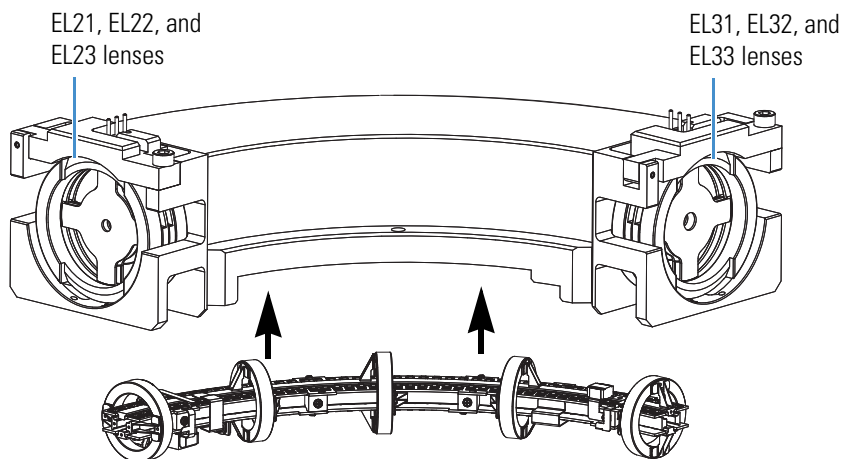
Figure 22. Hyperquad Q1 or Q3 (TSQ Quantiva MS)



Quadrupole Q2 is a square-profile quadrupole rod assembly that always acts as an ion transmission device. The rods bend into a 90-degree arc (Figure 23), which does the following: reduces the footprint of the instrument, prevents the transmission of unwanted neutral species to the detector that are generated during fragmentation, and dramatically lowers the noise level in the data.

Quadrupole Q2 has become synonymous with the term *active collision cell*. Technically, the collision cell is the chamber that encloses Q2 where CID can take place if the argon (or nitrogen) collision gas is present. The active collision cell has an axial field down its length to speed throughput. This allows up to 500 SRM transitions per second.

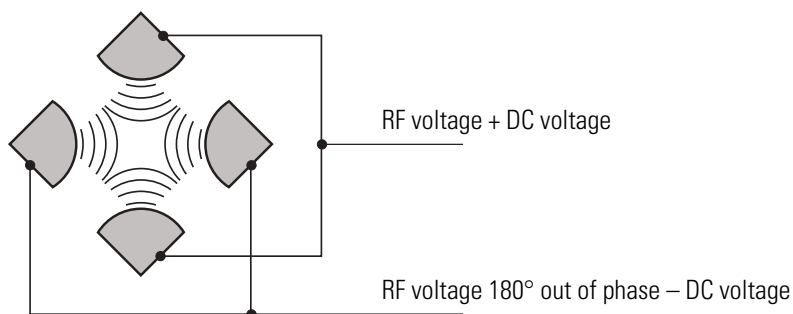
Figure 23. Quadrupole Q2 (bottom) separated from the active collision cell housing (top)



Applied RF and DC Fields

In a quadrupole rod assembly, because rods opposite each other in the array connect electrically, the four rods are considered two pairs of two rods each. The MS applies RF and DC voltages to the rods. As shown in [Figure 24](#), although the RF voltages applied to the four rods are the same, the two pairs are 180 degrees out of phase (that is, one pair has a positive voltage and the other a negative voltage).

Figure 24. Polarity of the RF and DC voltages applied to the Q1 and Q3 mass analyzers



The quadrupole coil module provides the voltages for operating the quadrupole. The RF voltage applied to the quadrupole rods is of constant frequency (approximately 1.095 MHz for the TSQ Endura MS and 1.005 MHz for the TSQ Quantiva MS).

Because the frequency of this AC voltage is in the radio frequency range, it is referred to as RF voltage. The ratio of RF voltage to DC voltage determines the ability of the MS to separate ions of different m/z values.

As mentioned, the first and third quadrupole rod assemblies (Q1 and Q3) can act as mass filters or as ion transmission devices. When the MS applies both RF and DC voltages, quadrupoles Q1 and Q3 act as mass filters, and when it applies only RF voltage, they act as ion transmission devices. In the ion transmission mode, the quadrupoles allow ions to pass in a wide window of m/z values.

The square quadrupole rod assembly (Q2) operates in the ion transmission mode only. Surrounding quadrupole Q2 is a collision cell where CID takes place if the argon (or nitrogen) collision gas is present in the cell.

Mass Analysis

The mass analyzers (quadrupoles Q1 and Q3) are square arrays that are charged with a variable ratio of RF voltage and DC voltage. The variable amplitude of RF and DC voltages applied to the quadrupole rods generates an electric field that gives stable oscillations to ions with a specific m/z and unstable oscillations to all others.

When the MS applies one particular set of RF and DC voltages to the mass analyzer rods, only ions of one m/z (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 a different m/z (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 of transmitting ions of one m/z after another continues as the RF and DC voltages change in value.

The MS can rapidly and precisely change the potentials on the quadrupole rods to obtain a fast scan rate.

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

Collision Cell and CID Efficiency

In the MS/MS scan modes, the MS 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 electric field that gives stable oscillations to ions in a wide window of m/z values. An axial field down the length of Q2 speeds throughput.

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 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.

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 MS 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 MS automatically computes the necessary Q3 quadrupole offset voltage and then varies the voltage, as appropriate, as each scan proceeds.

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 precursor ions are formed) and Q2 (where they collide with collision gas). As the offset voltage on Q2 increases, so does the TKE of the precursor ions. As a result, the energy of ion/Ar (or ion/N) collisions also increases. You can set the collision energy from 0 to ± 65 V.

Before obtaining any mass spectra, the MS 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 MS determines the optimum quadrupole offset voltage for Q1 and for Q3.

Mass Analyzer Lenses

The mass analyzer has three lens sets. See [Figure 23](#). Those between quadrupoles Q1 and Q2 are designated as EL21, EL22, and EL23; those between quadrupoles Q2 and Q3 are designated as EL31, EL32, and EL33; and the lens between Q3 and the ion detection system is designated as L4 (or the exit lens). Circular holes in the center of the lenses allow the ion beam to pass through.

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 quadrupoles Q1 and Q2) and the L3x lens set (between quadrupoles Q2 and Q3) serve the following 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, be sure to maintain a low pressure in the mass analyzers.

4 Ion Transmission and Mass Analysis

Dual-Mode, Discrete-Dynode Ion Detection System

- To retain the collision gas: Lenses EL23 and EL31 form two of the walls of the collision cell, so they tend to hold the collision gas in the collision cell. However, the collision gas escapes through the same lens holes through which the ion beam passes.
- 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.

However, 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.

Dual-Mode, Discrete-Dynode Ion Detection System

The ion detection system (Figure 17) includes a high-voltage conversion dynode and an electron multiplier. Typically, the electron multiplier is set to a gain of about 5×10^5 (that is, for each ion or electron that enters, 5×10^5 electrons exit) in MS mode and 2×10^6 in MS/MS mode. The electrometer circuit converts the current that leaves the electron multiplier through the anode to a voltage, and the data system records the voltage.

Syringe Pump and Divert/Inject Valve

This chapter describes the external syringe pump and divert/inject valve that ship with the TSQ Endura or TSQ Quantiva MS. For information about installing these components, refer to the *TSQ Endura and TSQ Quantiva Getting Connected Guide*.

Contents

- [Syringe Pump](#)
- [Divert/Inject Valve](#)

Syringe Pump

The external Chemyx™ Fusion 100T syringe pump delivers sample solution from an installed syringe, through the sample transfer line (red PEEK), and into the API source. The motorized pusher block ([Figure 25](#)) depresses the syringe plunger at the flow rate specified in the data system. (The default flow rate for calibration is 5 µL/min.)

You can start and stop the syringe pump from the data system; refer to the data system Help for instructions. You can also start and stop the syringe pump by pressing the syringe pump buttons.

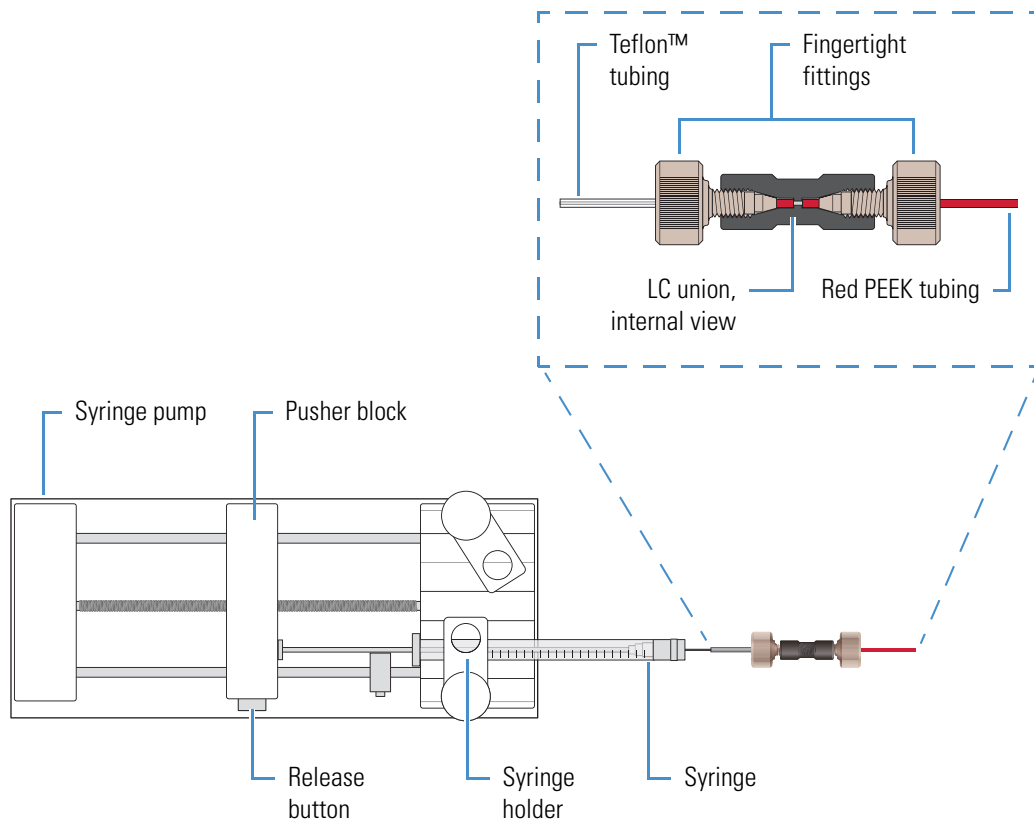
Note If you choose to provide a syringe pump other than the Fusion 100T, ensure that it can provide a steady, continuous flow of 1–5 µL/min.

In the Tune application version 3.0 and later, you can prime the syringe while it is in the provided syringe pump.

5 Syringe Pump and Divert/Inject Valve

Divert/Inject Valve

Figure 25. Syringe pump setup (top view)

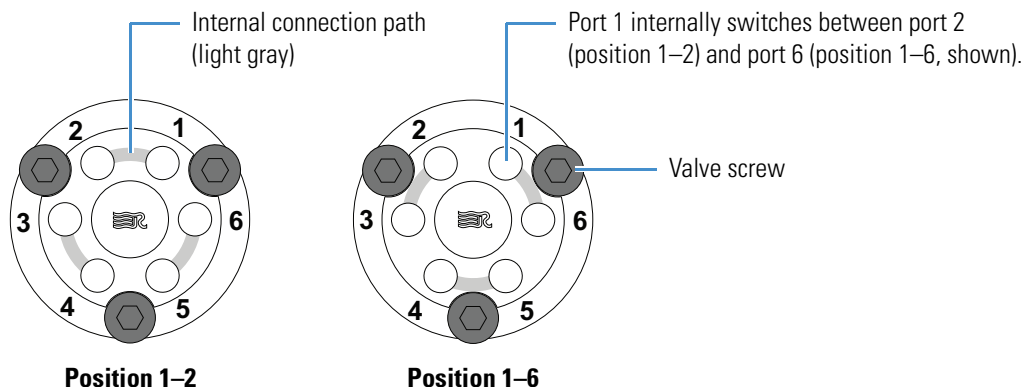


Divert/Inject Valve

The external Rheodyne™ MX Series II™ divert/inject valve is a 6-port motorized valve that switches between two positions. In the first position, port 1 connects internally to port 2, port 3 connects to port 4, and port 5 connects to port 6. In the second position, the valve rotates one position so that port 1 connects internally to port 6, port 2 connects to port 3, and port 4 connects to port 5. [Figure 26](#) shows the valve's internal flow paths for both positions.

The Method Editor in the Xcalibur application identifies the valve's two positions as "1–2" (port 1 to 2) and "1–6" (port 1 to 6).

Figure 26. Divert/inject valve positions



Configurations

You can configure (plumb) the divert/inject valve as a loop injector (for flow injection analysis) or as a divert valve. The divert valve can switch the solvent front, gradient endpoint, or any portion of the LC run to waste. [Figure 27](#) shows both of these configurations.

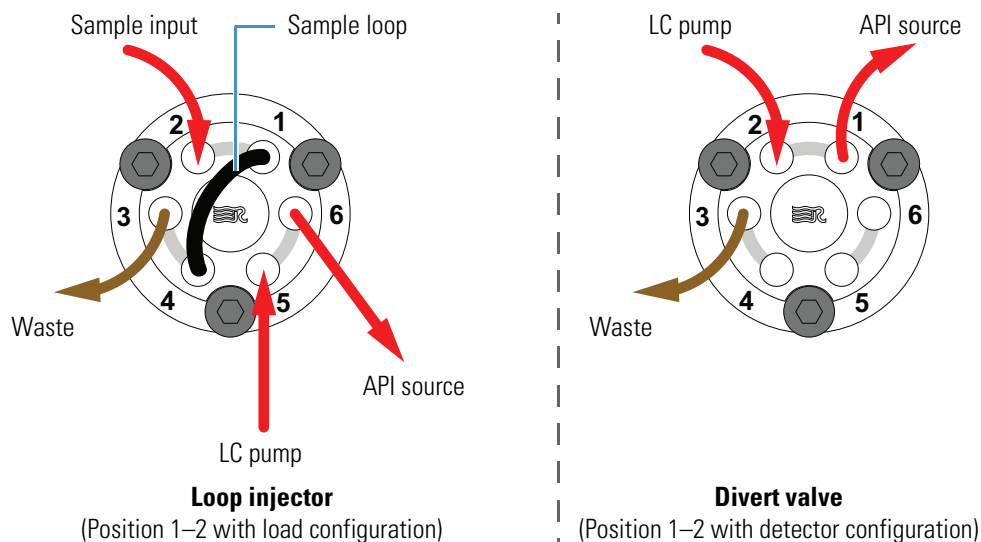
In the loop injector valve configuration, the valve switches between these two positions:

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

In the divert valve configuration, the valve switches between these two positions:

- Detector (position 1-2)—Solvent flow from the LC pump enters the valve through port 5 and exits through port 6 into the API source.
- Waste (position 1-6)—Solvent flow from the LC pump enters the valve through port 5 and exits through port 4 to waste.

Figure 27. Divert/inject valve plumbed as a loop injector and as a divert valve

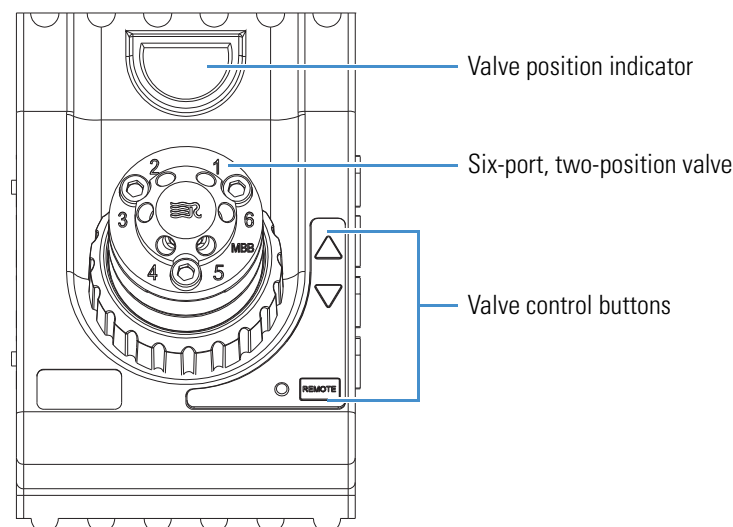


Controlling the Divert/Inject Valve

You can control the divert/inject valve as follows:

- Use the MS’s data system to specify the parameters in the Divert Valve Properties pane of the Method Editor. For instructions, refer to the Xcalibur Method Editor Help.
- Use the valve’s control buttons (Figure 28) to divert the LC flow between the MS 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. For instructions, refer to the manufacturer’s manual.

Figure 28. Divert/inject valve (front view)



System Shutdown, Startup, and Reset

When you are not using the TSQ Endura or TSQ Quantiva system for short periods of time, place the MS in standby mode. For longer periods, for example, two or more months, you can shut it down completely. In addition, many maintenance procedures for the system require shutting down the MS completely.

Contents

- [Shutting Down the System in an Emergency](#)
- [Placing the Mass Spectrometer in Standby Mode](#)
- [Turning On the Mass Spectrometer](#)
- [Shutting Down the Mass Spectrometer Completely](#)
- [Starting the System After a Complete Shutdown](#)
- [Resetting the Mass Spectrometer](#)
- [Resetting Calibration Parameters](#)
- [Restarting the Data System](#)
- [On/Off Status for MS Components Under Varying Power Conditions](#)

Shutting Down the System in an Emergency




CAUTION To turn off the MS in an emergency, **turn off the main power switch** located on the right-side power panel ([Figure 3](#)). This switch turns off all power to the MS, including the forepump, without harming components within the instrument. However, do not use this method as part of the standard shutdown procedure. Instead, see [Shutting Down the Mass Spectrometer Completely](#).

To turn off the LC, autosampler, and data system computer in an emergency, use their respective on/off switch or button.

Placing the Mass Spectrometer in Standby Mode

If you are temporarily not using the TSQ Endura or TSQ Quantiva MS, you do not need to shut it down completely. Instead, place the MS in standby mode.

❖ To place the mass spectrometer in Standby mode

1. Complete all data acquisition, if any.
2. In the Windows taskbar, choose **Start > All Programs > Thermo Instruments > model x.x > model Tune** to open the Tune window.
3. If your LC/MS system includes an LC pump, turn off the liquid flow to the API source.
For instructions, refer to the LC pump's manual.
4. In the Tune window, place the MS in **Standby** mode, .


The center of the selected power mode icon changes from white to green. The System LED on the front panel turns yellow. To keep the API source clean, the MS reduces the auxiliary and sheath gas flows to their standby default settings (2 arbitrary). The MS turns off the electron multiplier, conversion dynodes, 8 kV power to the API source, main RF voltage, and ion optic RF voltages. For a more complete list, see [On/Off Status for MS Components Under Varying Power Conditions](#).



CAUTION Hot surface. Allow heated components to cool to room temperature (approximately 20 minutes) before you touch or service them.

Turning On the Mass Spectrometer

❖ To turn on the mass spectrometer

In the Tune window, place the MS in **On** mode, .

The System LED on the front panel turns green.

Shutting Down the Mass Spectrometer Completely

Shut down the TSQ Endura or TSQ Quantiva system completely only when you are not using it for an extended period of time or when you must shut it down for maintenance or service. Instead, place the system in standby mode (see [Placing the Mass Spectrometer in Standby Mode](#)).



CAUTION Hot surface. Allow heated components to cool to room temperature (approximately 20 minutes) before you touch or service them.

❖ **To shut down the mass spectrometer completely**

1. Follow the procedure, [Placing the Mass Spectrometer in Standby Mode](#).
2. Place the electronics service switch in the Service Mode (down) position.

This turns off all LEDs on the front panel and the power to the nonvacuum system electronics.

3. Turn off the Main Power switch.

The following occurs:

- All power to the MS, including the turbomolecular pumps and the one or two forepumps, turns off.
 - After approximately 5 seconds, power to the vent valve solenoid shuts off, the vent valve opens, and the vacuum manifold vents with dry nitrogen. You can hear a hissing sound.
 - After about 2 minutes, the vacuum manifold is at atmospheric pressure.
4. Unplug the MS's power cord from the electrical outlet.



CAUTION Do not disconnect the power supply cord from the MS while the other end is still plugged into the electrical outlet.

5. (Optional) Follow the next procedure, [To turn off the LC, gases, data system, and autosampler](#).

Tip When performing routine or preventive system maintenance on the MS, you do not need to turn off the LC, gases, data system, and autosampler. In this case, the shutdown procedure is complete.

If you plan to have the system off for an extended period of time, Thermo Fisher Scientific recommends that you also turn off the LC, gases, data system, and autosampler.

❖ **To turn off the LC, gases, data system, and autosampler**

1. If the LC system is included, turn it off as described in the LC manual.
2. Turn off the argon and nitrogen gas supplies at their tanks.
3. Shut down the data system computer and turn off the monitor.
4. If an autosampler and printer are included, use their On/Off switches to turn them off.

Starting the System After a Complete Shutdown

To start the TSQ Endura or TSQ Quantiva system after it has been shut down completely, follow these procedures:

- [Starting the LC](#)
- [Starting the Data System](#)
- [Starting the Mass Spectrometer](#)
- [Starting the Autosampler](#) (if applicable)

Starting the LC

To start the LC system, follow the startup procedure described in the manufacturer's manual.

Note Do not turn on the liquid flow to the MS until you start the data system.

Starting the Data System

❖ **To start the data system**

Turn on the computer, monitor, and optional printer.

Starting the Mass Spectrometer

Make sure that the data system is running before starting the MS. The MS does not operate until it receives instructions from the data system.

❖ **To start the mass spectrometer**

1. Turn on the flows for the argon and nitrogen gases at their tanks if they are off.
2. Ensure that the Main Power switch is off and that the electronics service switch is in the Service Mode position.
3. Plug in the power cord for the MS.
4. Turn on the Main Power switch.

This turns on the forepump or forepumps and the turbomolecular pumps. All LEDs on the front panel are off.

5. If the MS was turned off for an extended period of time, follow the procedures in "Pumping Down the Mass Spectrometer," in Chapter 5 of the *TSQ Endura and TSQ Quantiva Getting Started Guide*. Otherwise, wait at least 1 hour to allow the MS to pump down.

IMPORTANT (TSQ Quantiva MS only) Before you pump down the MS, remove the ion transfer tube, which has a vertical orifice (Figure 15), reinserting it after the pump down process is complete.

6. Place the electronics service switch in the Operating Mode (up) position.

The following occurs:

- The Power LED on the front panel turns green to indicate that the electronics have power. However, the electron multiplier, conversion dynodes, 8 kV power to the API source, main RF voltage, and ion optic RF voltage remain off.
- After several more seconds, the Communication LED turns yellow and then green to indicate that the MS and the data system are communicating. Make sure that the instrument console window is active. The data system transfers operational software to the MS.
- After a few minutes, the System LED turns yellow to indicate the software transfer from the data system to the MS is complete and that the MS is in standby mode. When you change the mode from standby to on, the System LED turns green to indicate that the MS is functional.

IMPORTANT On the front panel, the Vacuum LED illuminates green only when the pressure in the mass analyzer region, as measured by the ionization gauge, is below the maximum allowable pressure of 1×10^{-4} Torr.

To ensure that the calibrations are correct, wait until the vacuum system is optimized completely, which takes approximately 15–24 hours of continuous pumping.

Starting the Autosampler

Turn on the autosampler by using its on/off power switch. If necessary, configure the autosampler. For procedures for placing sample vials, preparing solvent and waste containers, installing syringes, and so on, refer to the autosampler manual. The *TSQ Endura and TSQ Quantiva Getting Connected Guide* provides procedures for connecting the MS to the autosampler by using a contact closure cable.

Resetting the Mass Spectrometer

In the unlikely event that communication is lost between the MS and data system computer, you can reset the MS by using the reset button located on the right-side communications panel.

The following procedure assumes that power to the MS and data system computer are on and that both are operational. If the MS, data system computer, or both are off, see [Starting the System After a Complete Shutdown](#).

❖ To reset the mass spectrometer

Hold down the reset button for 3 seconds.

The following occurs:

- The embedded computer restarts. All LEDs on the front panel turn off except the Power LED.
- After several more seconds, the Communication LED turns yellow and then green to indicate that the MS and the data system are communicating. The data system transfers operational software to the MS.
- After a few minutes, the System LED turns yellow to indicate that the software transfer from the data system to the MS is complete and that the MS is in standby mode. Or, the System LED turns green to indicate that the MS is functional.

Resetting Calibration Parameters

If you must reset the calibration parameters to their factory default values, contact your local Thermo Fisher Scientific service engineer for assistance.

IMPORTANT

- Before resetting the instrument parameters to their default values, make sure that the system problems you are experiencing are not due to improper API source settings (such as spray voltage, sheath and auxiliary gas flow, or ion transfer tube temperature).
- If you reset the instrument to the factory calibration settings, always repeat the calibration of the internal electronic devices as specified in the *TSQ Endura and TSQ Quantiva Getting Started Guide*. Otherwise, all instrument calibrations might produce incorrect results.

Restarting the Data System

If possible, use the Windows restart procedure to shut down and restart the data system so that Windows can properly close applications and save changes to any open Thermo Scientific application.

Note After you reset the data system, the communications link between the data system and the MS is automatically reestablished. When this occurs, the Communication LED turns yellow and then green. If the system is unable to reestablish the communications link, hold down the reset button for 3 seconds.

❖ **To restart the data system by using Windows**

1. On the Windows taskbar, choose **Start**, and then click the arrow next to Shut Down.
2. Choose **Restart**, and then click **OK**.



❖ **To restart the data system by using the power button**

1. Press the power button on the data system computer.
2. Wait at least 20 seconds after the computer shuts down.
3. Press the power button again.

On/Off Status for MS Components Under Varying Power Conditions

Table 7 summarizes the on/off status of MS components, voltages, and API gas flows.



Table 7. On/Off status of MS components, voltages, and API gas flows (Sheet 1 of 2)

Mass spectrometer component	Standby mode 	Off ^a mode 	Electronics service switch, Service Mode position	Main Power switch, Off (0) position
Vent valve	Closed	Closed	Closed	Open
APCI corona discharge needle	Off	Off	Off	Off
Conversion dynode				
Electron multiplier				
ESI needle				
Gas, argon (collision [CID gas]) ^b				
Power supply, electron multiplier and conversion dynode				
Vaporizer temperature ^a				

6 System Shutdown, Startup, and Reset

On/Off Status for MS Components Under Varying Power Conditions

Table 7. On/Off status of MS components, voltages, and API gas flows (Sheet 2 of 2)

Mass spectrometer component	Standby mode 	Off ^a mode 	Electronics service switch, Service Mode position	Main Power switch, Off (0) position
Ion transfer tube DC offset	On	Off	Off	Off
Ion transfer tube temperature				
Mass analyzer, DC offset voltage				
Mass analyzer, RF voltage				
MP00 and MP0 ion optics, DC offset voltage				
MP00 and MP0 ion optics, RF voltage				
RF lens voltage		On	On	
Embedded computer				
Gases, auxiliary, sheath, and sweep ^c				
Gauge, convection vacuum (collision cell)				
Gauge, ionization vacuum (mass analyzer)				
Fans				
Forepumps		On	On	
Gauge, convection vacuum (foreline)				
Turbomolecular pump and controller				
Vent Delay PCB				

^a The electronics service switch is in the Operating Mode (up) position.

^b You can control this setting in your method even when the instrument is in standby mode.

^c In standby mode, the Tune application sets the API gases to their standby default settings (2 arbitrary) to keep the API source clean.

Daily Operation

To ensure the proper operation of the TSQ Endura or TSQ Quantiva system, Thermo Fisher Scientific recommends that you perform daily preventive maintenance. This chapter specifies the items to check before operating the system and the cleaning procedures to perform after completing the analyses.

Clean the ion sweep cone, the spray cone, and the ion transfer tube on a regular basis to prevent corrosion and to maintain optimum performance of the API source; see [Cleaning the Ion Sweep Cone, Spray Cone, and Ion Transfer Tube](#). If you use a mobile phase that contains a nonvolatile buffer or inject high concentrations of sample, you might need to clean these parts more often. You do not need to clean the system to flush the ion sweep cone and ion transfer tube.

Note You do not need to calibrate and tune the MS as part of your daily routine. Generally, you must calibrate the MS every one to three months of operation for optimum performance over the entire mass range of the mass detector.

For information about calibration, refer to the *TSQ Endura and TSQ Quantiva Getting Started Guide*.

Contents

- [Before Operating the Mass Spectrometer](#)
- [After Operating the Mass Spectrometer](#)

Before Operating the Mass Spectrometer


Follow these preventive maintenance procedures every day before beginning the first analysis:

- [Checking the System Mode](#)
- [Checking the Vacuum Pressure Levels](#)
- [Checking the Gas Supplies](#)
- Checking the oil level of the forepumps (See [Maintaining the Forepumps](#).)

Checking the System Mode

Make sure that the system is turned on. See [Turning On the Mass Spectrometer](#).

Checking the Vacuum Pressure Levels

Before daily operation begins, check the vacuum pressure levels and check for major air leaks in the system. A major air leak can indicate insufficient pressure levels to turn on the system. In the Tune window, a green square, , indicates that the readback value is good.



CAUTION For proper performance, operate the system at the proper vacuum levels. Poor vacuum levels can cause reduced sensitivity and reduced electron multiplier life.

You can check the current values of the pressures in the ion transfer tube-RF lens and foreline (labeled *Source Pressure*) and in the analyzer region (labeled *Analyzer Pressure*) in the Status pane of the Tune window.

❖ To check the vacuum pressures


1. Open the Tune window.
2. Click the **Status** tab and click the **Expand** icon, , next to Vacuum.
3. Compare the current values of the pressures in the vacuum manifold with the values listed in [Table 8](#) for the TSQ Endura MS and [Table 9](#) for the TSQ Quantiva MS. If the current values are higher than normal, you might have an air leak.

Table 8. Typical pressure readings for the TSQ Endura MS

Conditions	Ion source pressure reading (foreline, ion transfer tube, S lens region)	Analyzer pressure reading (analyzer region)
Collision gas off, ion transfer tube orifice sealed	Less than 0.05 Torr	Less than 6×10^{-6} Torr (after pumping for at least 12 hours)
Collision gas off, ion transfer tube orifice open	1.5 Torr	Less than 9×10^{-6} Torr
Collision gas set to 1.5 mTorr, ion transfer tube orifice open	1.5 Torr	Approximately 3×10^{-5} Torr

Table 9. Typical pressure readings for the TSQ Quantiva MS

Conditions	Source pressure reading (foreline, ion transfer tube, RF lens region)	Analyzer pressure reading (analyzer region)
Collision gas off, ion transfer tube orifice sealed	Less than 0.05 Torr	Less than 6×10^{-6} Torr (after pumping for at least 12 hours)
Collision gas off, ion transfer tube orifice open	3.8–4.2 Torr	Less than 9×10^{-6} Torr
Collision gas set to 1.5 mTorr, ion transfer tube orifice open	3.8–4.2 Torr	Approximately 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 MS.

If the pressure remains high, your system might have an air leak. First inspect the vacuum lines and fittings external to the MS for leaks and take corrective action if necessary. If you suspect an air leak within the MS, contact Thermo Fisher Scientific.

❖ **To check the system for major air leaks**

Listen for a rush of air or a hissing sound coming from the MS.

Possible causes of a major leak might be a loose or disconnected fitting, an improperly positioned O-ring, or an open valve.

❖ **To fix an air leak**

1. Shut down the system (see [Shutting Down the Mass Spectrometer Completely](#)).
2. Visually inspect the vacuum system and vacuum lines for leaks.
3. Check each fitting and flange on the system for tightness and tighten any 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.

Checking the Gas Supplies

Check the argon supply on the regulator of the argon gas tank. Make sure that there is sufficient gas for the analysis. If necessary, replace the tank. Verify that the pressure of argon gas reaching the MS is 135 ± 70 kPa (20 ± 10 psi). If necessary, adjust the pressure with the tank pressure regulator.

Check the nitrogen gas supply on the regulator of the nitrogen gas tank or liquid nitrogen boil-off tank. Make sure that there is sufficient gas for the analysis. Based on 24-hour per day operation, typical nitrogen consumption is 2800 liters per day ($100 \text{ ft}^3/\text{day}$). If necessary, replace the tank. Verify that the pressure of nitrogen gas reaching the MS is 690 ± 140 kPa (100 ± 20 psi). If necessary, adjust the pressure with the tank pressure regulator.

For more information about gas requirements, refer to the *TSQ Endura and TSQ Quantiva Preinstallation Requirements Guide*.

After Operating the Mass Spectrometer

After operating the system, follow these preventive maintenance procedures every day, unless otherwise indicated:

- [Flushing the Inlet Components](#) (as needed)
- [Purging the Oil in the Forepump](#)
- [Emptying the Solvent Waste Container](#)
- [Placing the System in Standby Mode](#)

Flushing the Inlet Components

This section describes how to flush the syringe and the inlet components (sample transfer line, sample tube, and spray insert) at the end of each work day (or more often if you suspect they are contaminated). You can also use an LC pump to flush the 50:50 methanol/water solution through the inlet components to the API source at a flow rate of 200–400 $\mu\text{L}/\text{min}$ for approximately 15 minutes.

Tip You do not need to flush the inlet components daily. However, if a mass spectrum shows unwanted contamination peaks, follow this procedure.



CAUTION When the MS's ion transfer tube is installed, do not flush it with cleaning solution, which flushes the residue into the MS.

❖ **To flush the inlet components**

1. Turn off the liquid flow from the syringe pump.
2. Place the MS in **Standby** mode.
3. Remove the syringe from the syringe pump as follows:
 - a. Lift the syringe holder off of the syringe.
 - b. Press the pusher block's release button and slide the block to the left.
 - c. Remove the syringe from the holder.
 - d. Carefully remove the syringe needle from the Teflon tube on the syringe adapter assembly.
4. Rinse the syringe with a solution of 50:50 methanol/water.
5. Flush the sample transfer line, sample tube, and spray insert as follows:
 - a. Load the clean syringe with a solution of 0.1% formic acid in 50:50 methanol/water (or another appropriate solvent).
 - b. Carefully reinsert the syringe needle into the Teflon tube on the syringe adapter assembly.
 - c. Slowly depress the syringe plunger to flush the solution through the sample transfer line, sample tube, and spray insert.
 - d. Remove the syringe needle from the syringe adapter assembly.

This completes the procedure to flush the inlet components.

Purging the Oil in the Forepump

Purge (decontaminate) the oil in the forepump daily to remove water and other dissolved chemicals, which can cause corrosion and decrease the lifetime or the performance of the forepump. For instructions, refer to the forepump's documentation.

The best time to purge the oil is at the end of the working day after you flush the inlet components. Remember to close the purge valve before continuing normal operation.

Emptying the Solvent Waste Container

Check the solvent level in the solvent waste container daily. If necessary, empty the container and dispose of the solvent waste according to local and national regulations.

Placing the System in Standby Mode

After you complete the daily maintenance procedures, place the MS in standby mode as described in [Placing the Mass Spectrometer in Standby Mode](#).

7 Daily Operation

After Operating the Mass Spectrometer

Maintenance

You are responsible for performing routine maintenance procedures to ensure optimum performance of the TSQ Endura or TSQ Quantiva system. Optimum performance depends on maintaining all parts of the instrument.



CAUTION Heavy object. Never lift or move the instrument by yourself; you can suffer personal injury or damage the instrument.



CAUTION Before performing instrument maintenance, either shut down the MS completely or place it in Standby mode as specified in the applicable procedure. Then, allow heated components to cool to room temperature (approximately 20 minutes) before you touch or service them.

For a list of replaceable parts, see [Chapter 10, “Replaceable Parts.”](#)

Note The following components are slightly different between the TSQ Endura MS and the TSQ Quantiva MS: sweep cone, ion transfer tube, API source interface, RF lens, MP00 RF lens, and lens L0. Unless otherwise noted, use the TSQ Endura MS procedures.

Contents

- [Maintenance Schedule](#)
- [Guidelines](#)
- [Tools and Supplies](#)
- [Maintaining the API Source Housing](#)
- [Maintaining the API Source Interface](#)
- [Maintaining the Forepumps](#)
- [Maintaining the Air Filter](#)
- [Pumping Down the Mass Spectrometer](#)

Maintenance Schedule

Table 10 lists the maintenance procedures and their recommended frequency.

Table 10. Mass spectrometer maintenance procedures and frequency

MS component	Procedure	Recommended frequency	Reference
API source	Flush (clean) the sample transfer line, sample tube, and spray insert.	Daily	page 54
	Clean the API source housing.		page 61
	Clean the APPI fan filter.	As needed	
	Replace the APPI lamp.		<i>Ion Max NG and EASY-Max NG Ion Sources User Guide</i>
	Replace the H-ESI needle insert.	If the metal needle is obstructed	
	Replace the APCI fused-silica tubing.	If the tubing is obstructed	
API source interface	Clean the ion sweep cone and spray cone.	Daily, or more often depending on analytical conditions	page 62
	Remove and clean the ion transfer tube.	Weekly, or if the ion transfer tube bore is contaminated or obstructed	
	Replace the ion transfer tube.	If the bore becomes corroded or blocked	
	Clean the exit lens or RF lens.	As needed, depending on analytical conditions	
	Clean MP00 RF lens and lens L0.	As needed, depending on analytical conditions	
Forepump (each)	Purge (decontaminate) the oil and check for leaks.	Daily	
	Add oil.	As needed, based on oil level	Manufacturer's manual
	Change the oil.	Every 12 months of typical use, or if the oil is cloudy or discolored	
Cooling fans	Clean the air filter.	Every 4 months	page 72

For instructions about maintaining the LC modules, refer to that instrument's manual.

Guidelines

For optimal results, follow these guidelines when performing the procedures in this chapter:

- Always wear a new pair of lint- and powder-free gloves when handling internal components. Never reuse gloves after you remove them because the surface contaminants on them recontaminate clean parts.
- Always place the components on a clean, lint-free work surface.
- Have nearby the necessary tools, supplies, and replacement parts (when applicable).
- Never overtighten a screw or use excessive force.
- Proceed methodically.

IMPORTANT

- Put on a new pair of lint- and powder-free gloves before starting each removal, cleaning, and reinstallation procedure.
- Make sure that you do not introduce any scratches or surface abrasions while handling the API source interface components. Even small scratches can affect performance if they are close to the ion transmission path. Avoid using tools, such as metal pliers, that might scratch these components.

Tools and Supplies

The MS requires very few tools to perform routine maintenance procedures. You can remove and disassemble many of the components by hand. [Table 11](#) lists the necessary chemicals, tools, and equipment for maintaining the instrument. (One of the tools is in the TSQ Source Installation Kit.) In addition, you can use the contents of the PM Cleaning Kit (P/N 70111-62112).



CAUTION To prevent corrosion, do not use nitric acid to clean metal parts.



CAUTION Avoid exposure to potentially harmful materials.

By law, producers and suppliers of chemical compounds are required to provide their customers with the most current health and safety information in the form of Material Safety Data Sheets (MSDSs) or Safety Data Sheet (SDS). The MSDSs and SDSs must be freely available to lab personnel to examine at any time. These data sheets describe the chemicals and summarize information on the hazard and toxicity of specific chemical compounds. They also provide information on the proper handling of compounds, first aid for accidental exposure, and procedures to remedy spills or leaks.

Read the MSDS or SDS for each chemical you use. Store and handle all chemicals in accordance with standard safety procedures. Always wear protective gloves and safety glasses when you use solvents or corrosives. Also, contain waste streams, use proper ventilation, and dispose of all laboratory reagents according to the directions in the MSDS or SDS.

Table 11. Chemicals, tools, and equipment (Sheet 1 of 2)

Description	Part number
Chemicals	
Detergent (for example, Liquinox™)	(Liquinox) Fisher Scientific: <ul style="list-style-type: none"> • 50-821-299 (1 quart) • 50-821-298 (1 gallon)
Methanol, UHPLC/MS-grade	Fisher Scientific A458-1
Nitrogen gas, clean and dry	–
Water, UHPLC/MS-grade	Fisher Scientific W8-1
Tools	
Ion transfer tube removal tools ^a	
<ul style="list-style-type: none"> • TSQ Endura MS • TSQ Quantiva MS 	70111-20258 70005-20972
Screwdriver, Phillips #2 (M3)	–
(Optional) Toothbrush, soft (or similar tool)	–
(Optional) Tweezers, plastic (or similar tool)	–
Equipment	
Beaker or graduated cylinder (for use with methanol)	–
Chamois-tipped swabs	00725-01-00028

Table 11. Chemicals, tools, and equipment (Sheet 2 of 2)

Description	Part number
Gloves, lint-free and powder-free	Fisher Scientific 19-120-2947 ^b
	<p>Unity Lab Services:</p> <ul style="list-style-type: none"> • 23827-0008 (size medium) • 23827-0009 (size large)
Industrial tissues, lint-free	–
Magnification device	–
MICRO-MESH™ polishing swabs, 6000 grit (light purple color), 2.25 in. long	00725-01-00027
Sonicator	–

^a Provided in the TSQ Source Installation Kit

^b Multiple sizes are available.

Maintaining the API Source Housing

Only Thermo Fisher Scientific service engineers can service the API source housing, while user maintenance is limited to cleaning the housing as necessary. Follow all safety precautions in the *Ion Max NG and EASY-Max NG Ion Sources User Guide* regarding the installation and removal of the API source. For any additional service, contact your local Thermo Fisher Scientific service engineer.

IMPORTANT Prevent damage: Remove or install the API source's drain insert by pressing a small, slotted screwdriver against the insert's tab.

❖ To clean the API source housing

1. After the API source cools to room temperature, remove it from the MS.
2. Put on appropriate personal protective equipment, in particular safety glasses and chemical resistant gloves.
3. Under an appropriate fume hood, rinse the interior of the housing with UHPLC/MS-grade methanol.
4. Allow the housing to dry before you install it on the MS.

Maintaining the API Source Interface

While you or the service engineer can remove and service the API source interface, only the service engineer may service the other internal components.

To maintain the API source interface, follow these procedures:

- [Cleaning the Ion Sweep Cone, Spray Cone, and Ion Transfer Tube](#)
- [Removing the API Source Interface](#)
- [Cleaning the RF Lens, Exit Lens, MP00 RF Lens, and Lens L0](#)
- [Reinstalling the API Source Interface](#)

Note Before you continue, read the precautions in [Special Notices, Symbols, and Cautions](#).

IMPORTANT

- Prepare a clean work surface by covering the area with lint-free paper.
- Put on a new pair of lint- and powder-free gloves before starting each of these removal, cleaning, and reinstallation procedures.



CAUTION To prevent corrosion, do not use nitric acid to clean metal parts.

Cleaning the Ion Sweep Cone, Spray Cone, and Ion Transfer Tube

Because buffer salts or high concentrations of sample can cause blockages, you must clean the bore of the ion transfer tube. If pressure in the ion transfer tube and RF lens region (as measured by the Source Pressure gauge) drops considerably below 1 Torr, a blocked ion transfer tube is likely the cause.

Tip You do not have to vent the system to remove the ion transfer tube.

Follow these procedures:

1. [To remove the ion sweep cone and the ion transfer tube](#)
2. [To clean the spray cone and O-ring](#)
3. [To clean the ion transfer tube](#)
4. [To clean the ion sweep cone](#)

❖ To remove the ion sweep cone and the ion transfer tube



CAUTION Hot surface. The external surface of the spray insert, API source housing, and entry to the ion transfer tube can become hot enough to burn your skin. Before you touch or remove heated parts, allow the part to cool to room temperature (approximately 20 minutes) before you touch it.

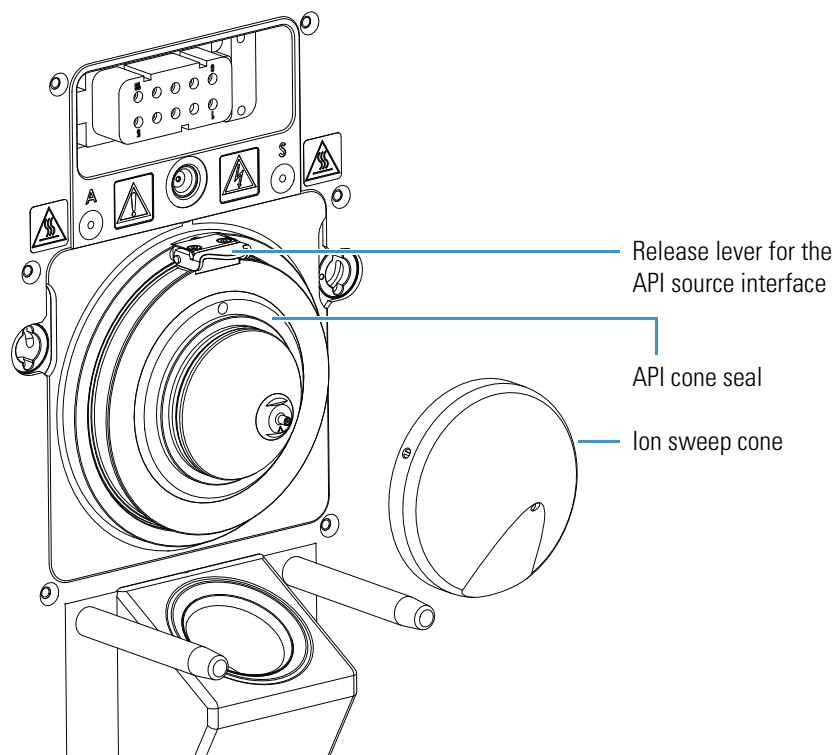
1. Turn off the liquid flow to the API source.
2. In the Tune application, place the MS in **Standby** mode.
3. In the Ion Source pane, set the Ion Transfer Tube Temperature and Vaporizer Temperature to 50 °C or less and observe the readback temperatures.
4. After the source cools to room temperature, remove it.
5. Remove the ion sweep cone by grasping its outer ridges and pulling it off (Figure 29).



CAUTION

- Make sure that you do not accidentally lift the release lever that is located above the API source interface, which will vent the MS.
- To avoid contaminating the ion transfer tube, do not touch its exposed entrance.

Figure 29. Ion sweep cone removed from the MS mount assembly

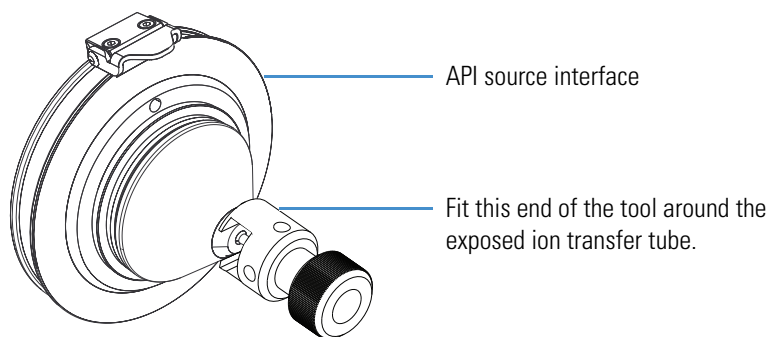


8 Maintenance

Maintaining the API Source Interface

6. Align the flat edges of the custom removal tool with the flat edges on the exposed tip of the ion transfer tube, and then do one of the following:
 - (TSQ Endura MS) Rotate the tool (Figure 30) counterclockwise. When the tube is free of the spray cone, use the hook (flat edges) on the tool to slowly pull it out of the API source interface.

Figure 30. Ion transfer tube removal tool (TSQ Endura MS)

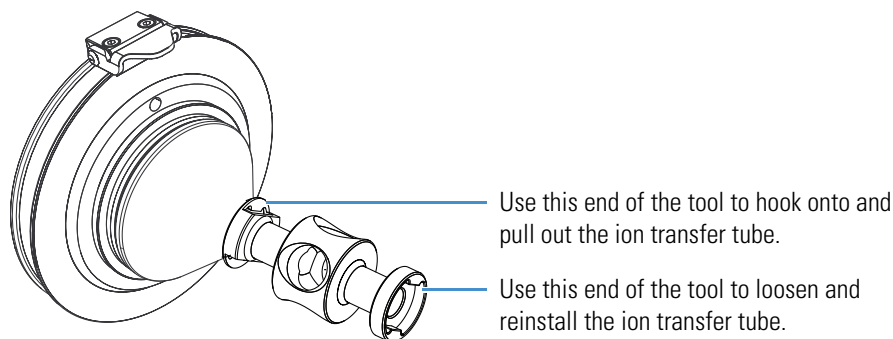


—or—

- (TSQ Quantiva MS) Using the correct end of the custom removal tool (Figure 31), rotate the ion transfer tube only 1/4-turn counterclockwise. Then, use the other end of the tool to remove the tube from the API source interface.

Tip If necessary, insert a hex key through a side hole for leverage.

Figure 31. Ion transfer tube removal tool (TSQ Quantiva MS)

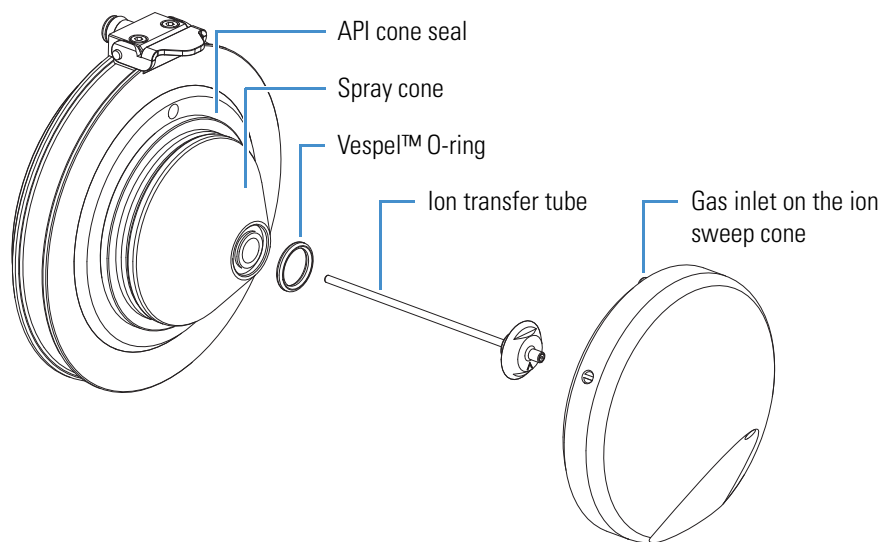


❖ **To clean the spray cone and O-ring**

Note The TSQ Quantiva MS does not have an O-ring behind its ion transfer tube.

1. Soak the lint-free tissues or chamois-tipped swabs in a 50:50 solution of methanol/water, and then clean the exterior surface of the spray cone.
2. (TSQ Endura MS) Remove and inspect the O-ring located in the spray cone under the entrance end of the ion transfer tube (Figure 32).

Figure 32. Spray cone, O-ring, ion transfer tube, and ion sweep cone (TSQ Endura MS)



3. (TSQ Endura MS) Clean the O-ring with methanol or replace it if necessary.
4. Using a magnification device, inspect the components for any residual lint or particulates.

Note Inspect the inside surfaces and edges for the presence of lint or particulates. If present, use plastic tweezers or a similar tool to remove them.

5. (TSQ Endura MS) Reinstall the O-ring in the spray cone.

❖ **To clean the ion transfer tube**

IMPORTANT Always use UHPLC/MS-grade methanol and water.

1. For extreme contamination, follow these steps. Otherwise, start with [step 2](#).
 - a. Overnight, sonicate the component in a 10% solution of Liquinox in water.
 - b. Rinse the component with water, and then for 2 minutes force a strong stream of water through the orifice.
 - c. For 30 minutes, sonicate the component in water.
2. For 30 minutes, sonicate the component in a 50:50 solution of methanol/water that contains 20% formic acid.

3. Rinse the component thoroughly with water.
4. For 15 minutes, sonicate the component in deionized water.
5. Rinse the component with methanol.
6. For 15 minutes, sonicate the component in methanol.
7. Dry the component thoroughly with nitrogen gas.

Replace the ion transfer tube if the bore becomes corroded or blocked.



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

- Put on a new pair of lint- and powder-free gloves.
- Verify that everything is properly aligned to prevent stripping the threads on the ion transfer tube.
- Rotate—do not bend—the ion transfer tube upon insertion.

❖ To clean the ion sweep cone

1. Soak lint-free tissues or chamois-tipped swabs in a 50:50 solution of methanol/water, and then clean both sides of the ion sweep cone.
2. For 10 minutes, sonicate the component in either a 50:50 solution of methanol/water or a 1% solution of Liquinox in water.
3. Rinse the component thoroughly with water.
4. Sonicate the component in water for 10 minutes.
5. Sonicate the component in methanol for 10 minutes.
6. Rinse the component with methanol.
7. Dry the component thoroughly with nitrogen gas.
8. Using a magnification device, inspect the component for any residual lint or particulates.

After you clean and reinstall these components, turn on the nonvacuum system voltages by placing the MS's electronics service switch in the Operating Mode (up) position.

Tip If you successfully unblocked the ion transfer tube, check that the Source Pressure reading has increased to a normal value (below 2 Torr for the TSQ Endura MS or below 4.5 Torr for the TSQ Quantiva MS). If trying this method does not clear the blockage, replace the ion transfer tube.

Removing the API Source Interface

❖ To remove the API source interface



CAUTION To avoid an electrical shock, be sure to follow the instructions in [Shutting Down the Mass Spectrometer Completely](#) before continuing with this procedure.

1. Shut down and vent the system, and let it cool to room temperature.

Venting the MS can take several minutes.



CAUTION Hot surface. Allow heated components to cool to room temperature (approximately 20 minutes) before you touch or service them.

2. Unplug the MS's power supply cord from the electrical outlet.



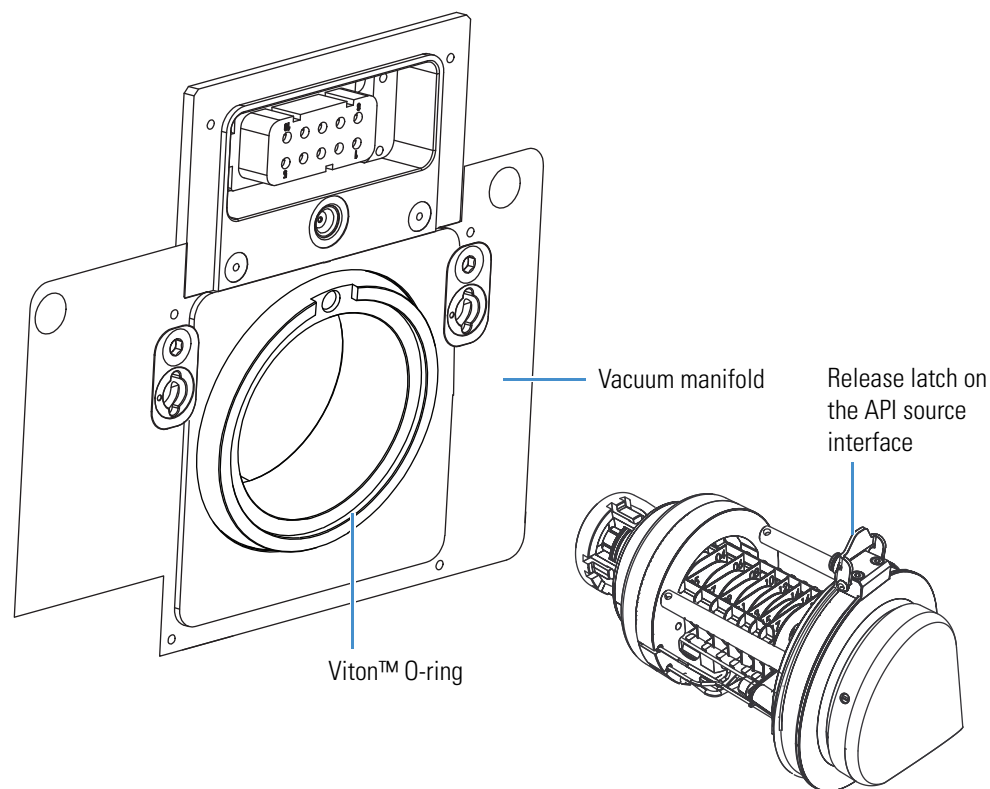
CAUTION Do not disconnect the power supply cord from the MS while the other end is still plugged into the electrical outlet.

3. Remove the API source housing.
4. Lift up the release latch, grasp the API source interface with your fingers, and then carefully pull it out of the vacuum manifold ([Figure 33](#)).

8 Maintenance

Maintaining the API Source Interface

Figure 33. API source interface removed from the vacuum manifold (TSQ Endura MS)



Cleaning the RF Lens, Exit Lens, MP00 RF Lens, and Lens L0

Chemicals can accumulate on the surfaces of the RF lens, exit lens, MP00 RF lens, and lens L0. However, the use of an RF lens that incorporates an RF electric field minimizes the harmful effects of this contamination. The lenses require cleaning less often than the ion sweep cone and the ion transfer tube. How frequently you clean these lenses depends on the type and quantity of the compounds that you analyze. Remove the lenses from the API source interface cage before cleaning them. No tools are needed to remove or install these components.

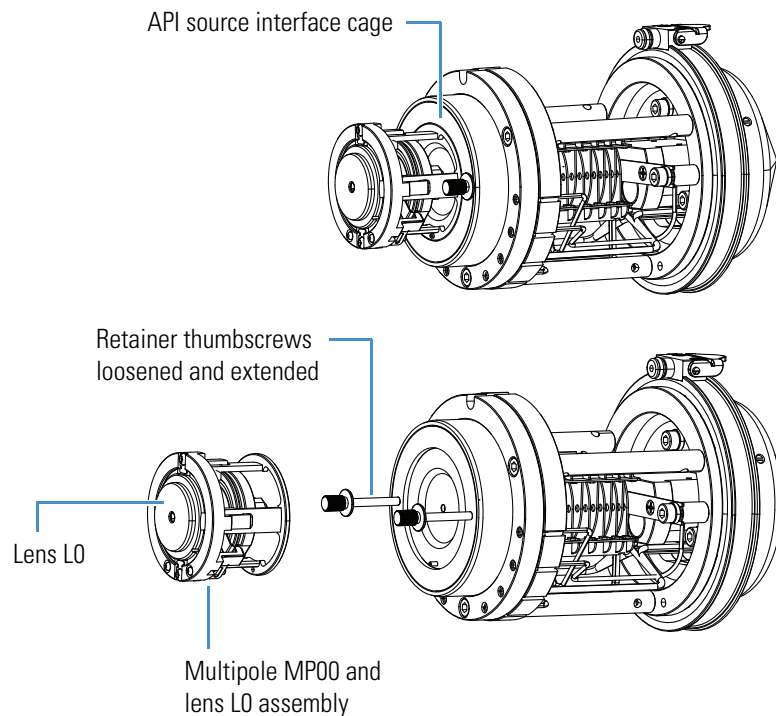
To clean the RF lens, exit lens, MP00 RF lens, and lens L0, follow these procedures:

1. To remove the RF lens, exit lens, MP00 RF lens, and lens L0
2. To clean the RF lens, exit lens, MP00 RF lens, and lens L0
3. To reinstall the RF lens, exit lens, multipole MP00, and lens L0
4. To reinstall the API source interface

❖ **To remove the RF lens, exit lens, MP00 RF lens, and lens L0**

1. Remove the API source interface (see [page 67](#)).
2. Wearing clean, lint- and powder-free gloves, loosen and extend the two captive thumbscrews that secure the RF lens, exit lens, multipole MP00, and lens L0 to the cage.
3. Pull the multipole MP00 and lens L0 assembly off of the API source interface cage. See [Figure 34](#). Place them on a clean, lint-free surface.

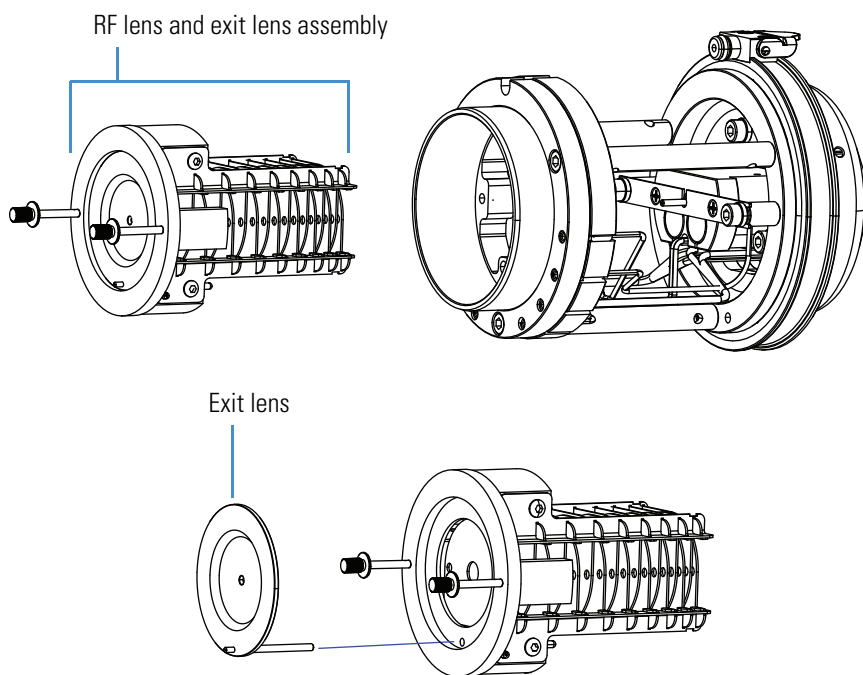
Figure 34. Removing the multipole MP00 and lens L0 assembly



4. Grasp the two retainer thumbscrews and carefully pull the RF lens ([Figure 35](#)) with the exit lens straight out of the API source interface cage.

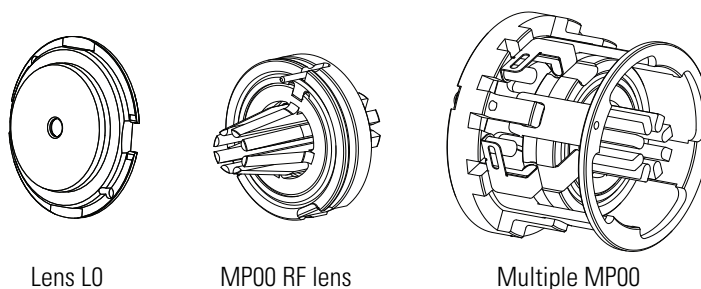
5. Remove the exit lens off of the RF lens. Place both on a clean surface.

Figure 35. Removing the RF lens and exit lens (TSQ Endura MS)



6. Using the lens L0 removal tool (or plastic tweezers), rotate the lens counterclockwise to remove it, and then push out the multipole MP00 from the MP00-L0 mount cage. Place the components on a clean surface.

Figure 36. Removing the lens L0 and multipole MP00 from the MP00-L0 mount cage



❖ **To clean the RF lens, exit lens, MP00 RF lens, and lens L0**



CAUTION Do not clean the lenses with abrasives, acidic or caustic substances, or detergents not specified in this chapter.

IMPORTANT Always use UHPLC/MS-grade methanol and water.

1. Using a magnification device, inspect the components for any lint, particulates, and sample buildup or coatings.
2. For 10 minutes, sonicate the components in either a 50:50 solution of methanol/water or a 1% solution of Liquinox in water.
3. If a sonicator is not available, do the following:
 - To clean the RF lens, use chamois-tipped swabs with a 1% solution of Liquinox in water. To clean the areas that you cannot reach with the swab, use the 6000 grit MICRO-MESH polishing swabs.
 - To clean the exit lens, use a soft toothbrush with a 1% solution of Liquinox in water.
4. For the exit lens, MP00 RF lens, and lens L0, use the 6000 grit MICRO-MESH polishing swabs to clean the bore.
5. Rinse the components thoroughly with water.
6. Sonicate the components in water for 10 minutes.
7. Sonicate the components in methanol for 10 minutes.
8. Rinse the components with methanol.
9. Dry the components thoroughly with nitrogen gas.
10. Using a magnifying device, inspect the components for any residual lint or particulates.

Note Inspect the bore of the orifices for the presence of lint or particulates. If present, use plastic tweezers or a similar tool to remove them.

❖ **To reinstall the RF lens, exit lens, multipole MP00, and lens L0**

1. Attach the exit lens to the RF lens, and then reinsert the RF lens into the API source interface cage (Figure 35).
2. Reassemble the multipole MP00 and lens L0 assembly.
3. Attach the MP00-L0 assembly to the API source interface cage, and then attach lens L0 (Figure 34).

Reinstalling the API Source Interface

❖ To reinstall the API source interface

1. Orient the API source interface with the release latch at the top (Figure 33).
2. Carefully insert the API source interface into the vacuum manifold.
3. Reinstall the API source housing.
4. Start up the system as described in [Starting the System After a Complete Shutdown](#).

Maintaining the Forepumps

Maintaining the forepumps requires inspecting, adding, purging, and changing the pump oil. Refer to the manufacturer's manual for instructions.

Check the forepump oil often. New oil has a translucent, light amber color. During normal operation, oil must always be visible in the oil level sight glass between the MIN and MAX marks. If the oil level is below the MIN mark, add oil. If the oil is cloudy or discolored, purge the oil to decontaminate dissolved solvents. If the pump oil is still discolored, change it. Plan to change the pump oil every 10 000 hours (or about every 12–13 months) of operation.



CAUTION To minimize the risk of oil contamination in the vacuum system, make sure that the purging ballast is closed when you vent the system to atmosphere.

Maintaining the Air Filter

Clean the air filter located behind the MS's front cover every four months, or sooner if it is dirty.

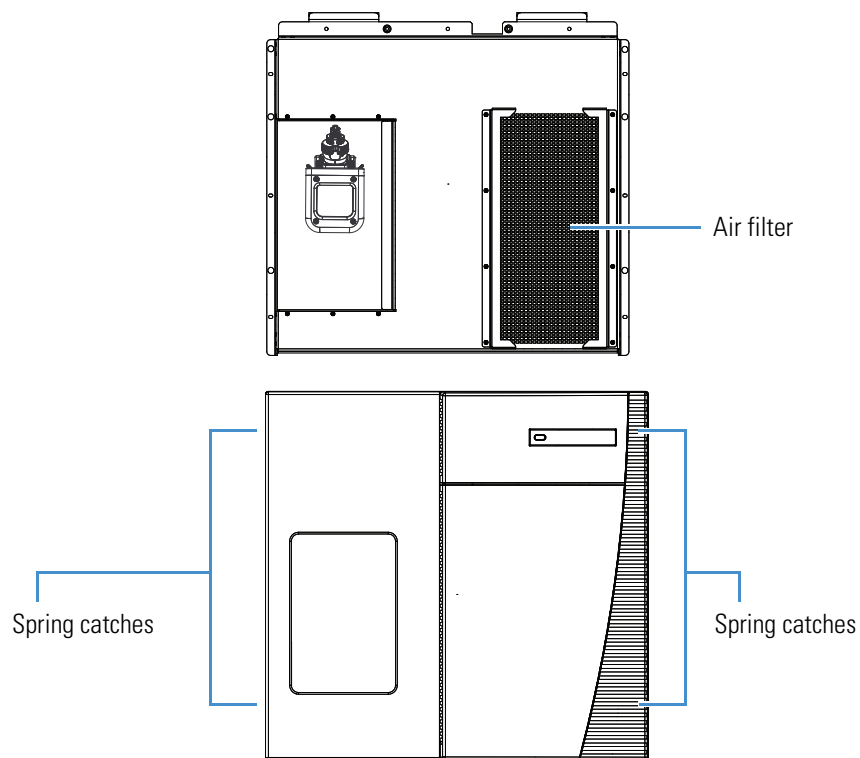
Note You do not need to remove the API source to remove the front cover of the MS.

❖ To clean the air filter

1. Remove the air filter as follows:
 - a. Remove the front cover of the MS as follows:
 - i. Disconnect the plumbing tubing to the API source.
 - ii. Depress the four spring catches that are located on either side of the front cover.
 - iii. Pull the front cover off at an angle to clear the API source.

b. Remove the filter from the filter bracket (Figure 37).

Figure 37. Air filter location in the MS with the front cover removed



2. Wash the air filter in a solution of soap and water.
3. Rinse the filter with tap water, and then allow it to air dry.
4. Reinstall the air filter and front cover.
5. Reconnect the plumbing tubing.

Pumping Down the Mass Spectrometer

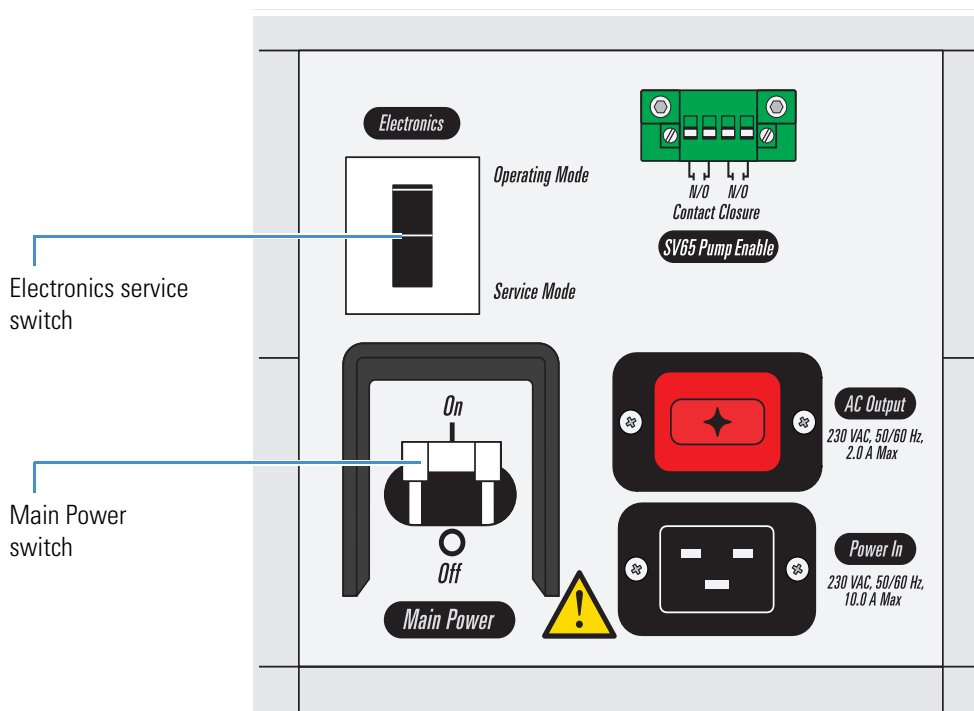
After first installing the MS or if it was turned off for an extended period of time, pump down the MS vacuum system for at least 15 hours.

❖ To pump down the MS

1. Check that the forepumps' exhaust tubing connects to the exhaust system and that any valves in the exhaust path are open.
2. (TSQ Quantiva MS only) Do the following:
 - a. Wearing a new pair of lint- and powder-free gloves, remove the API source and the ion sweep cone.
 - b. Follow the procedure "To remove the ion transfer tube" in Chapter 8 of the *TSQ Endura and TSQ Quantiva Hardware Manual*.
 - c. Reinstall the ion sweep cone and the API source.
3. Turn on the Main Power switch (Figure 38), wait 15 minutes, and then place the electronics service switch in the Operating Mode (up) position.

When the MS enters operating mode, the restart sequence begins. The Power LED on the front panel turns green, and the Vacuum, Communication, and System LEDs remain off. When the MS startup process is complete, the Vacuum and Communication LEDs are green and the System LED is yellow. The MS is now in standby mode.

Figure 38. Power entry module (right side of the instrument)



4. Wait at least 15 hours.

- In the Tune window, open the Status pane, double-click **Vacuum**, and then verify that the Source Pressure and Analyzer Pressure readback values are below the operating threshold limits (see Table 12). Normal readback measurements show a green square (■).

Table 12. Threshold limits for the vacuum pressure gauges

Instrument	Source pressure (Torr)	Analyzer pressure (Torr)
TSQ Endura	2.5	9.0×10^{-6}
TSQ Quantiva	4.5	

- (TSQ Quantiva MS only) When the pressure readback values are normal, carefully reinstall the ion transfer tube into the heater block.



CAUTION Take these precautions when reinstalling the ion transfer tube:

- Wearing a new pair of lint- and powder-free gloves, verify that everything is properly aligned to prevent stripping the threads on the ion transfer tube.
- Do not bend the ion transfer tube. Rotate it as you insert it.

8 Maintenance

Pumping Down the Mass Spectrometer

Diagnostics and PCB and Assembly Replacement

The TSQ Endura and TSQ Quantiva system diagnostics can test many instrument components. For example, they can help you locate a problem with the instrument electronics. Usually, replacing a faulty PCB or assembly can correct the problem. After applying the fix, run the diagnostic tests again to verify that the instrument is functioning properly.

Contents

- [Running the System Diagnostics](#)
- [Replacing Fuses, PCBs, and Power Supplies](#)

Running the System Diagnostics

The system diagnostics test the major electronic circuits within the MS and indicate whether the circuits pass or fail the tests.

The 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, the person running the diagnostics must be familiar with system operation and basic hardware theory as well as the details of the diagnostics.

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

- 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 question, a hardware failure is possible, and running the diagnostics is appropriate.

9 Diagnostics and PCB and Assembly Replacement

Replacing Fuses, PCBs, and Power Supplies

If the answer is yes to either of the last two questions, the problem is probably mechanical, not electrical. Verify again that alignment, configurations, and cable connections are correct before you call the 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 email 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.

Note A subset of the diagnostic tools targets specific functions of the entire MS. In general, these system evaluation tools do not contain pass or fail criteria nor do they rate the performance. Instead, they provide data that can be interpreted by a service engineer. Because the system evaluations examine complex interactions, the service engineer uses the data in conjunction with other tools and tests to form a diagnosis.

❖ To run diagnostics

Note Some diagnostic tests require that you infuse calibration solution.

1. Open the Tune window.
2. Click the **Diagnostics** icon () to open the Diagnostics pane.
3. Select which diagnostics you want to run and click **Start**.

The data system displays the status of the diagnostics in the Tune window.

Replacing Fuses, PCBs, and Power Supplies

Fuses protect the various circuits by opening whenever an overcurrent condition occurs. On the MS, an open fuse indicates a failed board or electronic module that a service engineer must replace.

The electronic assemblies that control the operation of the MS 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 MS.



CAUTION To prevent electric shock, do not attempt to replace parts or to make any repairs to the electronic assemblies.



CAUTION Thermo Fisher Scientific service is required. Because the electronic assemblies are close-packed to minimize the size of the instrument, only a service engineer can replace electrical components (that is, fuses, PCBs, power supplies, and so on).

Replaceable Parts

The TSQ Endura MS and TSQ Quantiva MS arrive with the following kits and replaceable parts. The exception is the Chemical Kit, which arrives separately as part of the preinstallation kit. Use the provided part numbers when ordering replacement parts.

Contents

- Chemical Kit
- Calibration Kit
- MS Setup Kit
- Performance Specification Kit
- Single Mechanical Pump Kit
- Dual Mechanical Pumps Kit
- TSQ Source Installation Kit
- API Source Interface
- Miscellaneous Parts

Chemical Kit

Chemical Kit	80100-62006
Polytyrosine 1-3-6 standard, solid (CS Bio Company Inc., CS0272S) . . .	00301-22925
TSQ Reserpine Solution Kit.	80100-62033
LCMS Functionality Test Kit (for field service use only).	HAZMAT-01-00044

Calibration Kit

Calibration Kit	80000-62013
Source LC Connection Kit (Table 13)	80000-62057
Syringe, gas tight, 500 µL	00301-19016
Syringe Adapter Kit (Table 14)	70005-62011

Table 13. Source LC Connection Kit (P/N 80000-62057)

Item	Part number
Fitting, fingertight, two-piece, one wing, 10-32 (Upchurch Scientific™ F-200, 2 provided)	00101-18195
Grounding union, zero-dead-volume (ZDV), stainless steel, 1/16 in. orifice, 0.010 in. (0.25 mm) thru-hole, 10-32 (Upchurch Scientific U-435)	00101-18182
Tubing, natural PEEK, 1/16 in. OD, 0.0025 in. ID, 28 cm (11 in.) long	80000-22032
Tubing, red PEEK, 1/16 in. OD, 0.005 in. ID, 18 cm (7.1 in.) long (2 provided)	80000-22053

Table 14. Syringe Adapter Kit (P/N 70005-62011)

Item	Part number
Ferrule, fingertight, natural PEEK (Upchurch Scientific F-142, 2 provided)	00101-18196
Fitting, fingertight, one-piece, natural PEEK, 10-32 (Upchurch Scientific F-120, 16 provided)	00109-99-00016
Fitting, fingertight, two-piece natural PEEK, two wings, 10-32 (Upchurch Scientific F-300, 2 provided)	00101-18081
Tubing, red PEEK, 1/16 in. OD, 0.005 in. ID, 0.6 m (2 ft) long (Upchurch Scientific 1535XL)	00301-22912
Tubing, Teflon FEP, 1/16 in. OD, 0.030 in. ID, 3 cm (1.2 in.) long (Upchurch Scientific 1522)	00301-22915
Union, HPLC, black PEEK, 10-32, 0.01 in. thru-hole (Upchurch Scientific P-742)	00101-18202

MS Setup Kit

MS Setup Kit	80100-62003
Drain hose adapter with O-ring	70111-20971
Connector plug, MINI-COMBICON™, 8-pin, 26.67 mm (1.05 in.) long, rated 160 V, 8 A (contact closure, 2 provided)	00004-21512
Container, Nalgene™, 4 L heavy-duty; filling/venting cap	80100-20265
Ethernet cables, shielded Category 5e, 2.1 m (7 ft) long (2 provided)	00302-99-00036
Ethernet power supply (rated 100–240 Vac, 50/60 Hz, 0.6/0.3 A input; 18 W, 12 Vdc, 1.5 A output)	00012-01-00039
Ethernet switch, 5-port Gigabit	00825-01-00111
Ferrule, brass, front, 1/4 in. ID (2 provided)	00101-10000
Ferrule, brass, front, 1/8 in. ID (2 provided)	00101-08500
Ferrule, brass, back, 1/4 in. ID (2 provided)	00101-04000
Ferrule, brass, back, 1/8 in. ID (2 provided)	00101-02500
Swagelok™-type nut, brass, 1/4 in. ID (2 provided)	00101-12500
Swagelok-type nut, brass, 1/8 in. ID (2 provided)	00101-15500
Tubing, precleaned copper, 1/8 in. OD, 0.030 in. thick, 4.6 m (15 ft) long (for the UHP argon and nitrogen gases)	00301-22701
Tubing, Teflon PFA, 1/4 in. (6.35 mm) OD, 0.062 in. (1.57 mm) thick, 4.6 m (15 ft) long (for the HP nitrogen gas)	00101-50100
Tubing, Tygon™, 1-3/8 in. OD, 1 in. ID, 3 m (10 ft) (for the drain/waste line)	00301-01-00020

Performance Specification Kit

Performance Specification Kit	80100-62008
Column, HPLC, 20 × 2.1 mm ID, Hypersil GOLD AQ™ C18, 1.9 µm particles	00109-01-00013
Fitting, fingertight, one-piece, natural PEEK, 10-32 (Upchurch Scientific F-120, 10 provided)	00109-99-00016
Needle port, PEEK (Rheodyne 9013)	00110-22030
Sample loop, 2 µL, PEEK	00110-16012
Syringe, gas tight, 500 µL	00301-19016
Tubing, red PEEK, 1/16 in. OD, 0.005 in. ID, 3 m (10 ft) long (Upchurch Scientific 1535XL)	00301-22912
Union Tee, HPLC, PEEK, 1/16 in. orifice, 0.020 in. (0.5 mm) thru-hole, 10-32 (provided with fingertight fittings) (Upchurch Scientific P-727)	00101-18204

Single Mechanical Pump Kit

Single Mechanical Pump Kit	80100-62004
Forepump, Oerlikon Leybold Vacuum™, SOGEVAC™ SV 65 BI, single-phase 230 Vac, 50/60 Hz	00108-01-00032
Forepump oil tray, stainless steel, caster wheels	00201-99-00549
Accessories Single Mechanical Pump Kit (Table 15)	80100-62015

Table 15. Accessories Single Mechanical Pump Kit (P/N 80100-62015)

Item	Part number
90-Degree Elbow Installation Kit (2 provided, Table 16)	97055-62036S
Relay control cable, single pump, 2.4 m (8 ft) long (preassembled)	80000-63139
Single pump vacuum hose assembly, KF40, 2.4 m (8 ft) long (preassembled)	80000-60229
Tubing, Tygon, 3/4 in. (19.1 mm) OD, 0.5 in. (12.7 mm) ID, 3 m (10 ft) long	00301-22920

Table 16. 90-Degree Elbow Installation Kit (P/N 97055-62036S)

Item	Part number
Centering ring with O-ring, nitrile and aluminum, NW40	00108-02-00005
Elbow, aluminum, NW40, 90 degree	00108-02-00010
Swing clamp, aluminum, NW32/40	00108-02-00004

Dual Mechanical Pumps Kit

Dual Mechanical Pumps Kit	80100-62013
Forepump, Oerlikon Leybold Vacuum, SOGEVAC SV 65 BI, single-phase 230 Vac, 50/60 Hz (2 provided)	00108-01-00032
Forepump oil tray, stainless steel, caster wheels (2 provided)	00201-99-00549
Accessories Dual Mechanical Pump Kit (Table 17)	80100-62016

Table 17. Accessories Dual Mechanical Pump Kit (P/N 80100-62016)

Item	Part number
90-Degree Elbow Installation Kit (3 provided, Table 16)	97055-62036S
Dual relay control cable, 2.4 m (8 ft) long (preassembled)	80100-63146
Dual pump vacuum hose assembly (preassembled)	80100-60049
Fitting Tee, barbed, nylon, for 0.5 in. (12.7 mm) ID tubing	00103-01-00012
Tubing, Tygon, 3/4 in. (19.1 mm) OD, 0.5 in. (12.7 mm) ID, 6 m (20 ft) long	00301-22920

TSQ Source Installation Kit

TSQ Source Installation Kit

Ion transfer tube removal tool, TSQ Endura	70111-20258
Ion transfer tube removal tool, TSQ Quantiva	70005-20972
L0 lens removal tool	70005-20900
Viper™ Capillary Kit (5 provided)	00109-99-00068

API Source Interface

TSQ Endura MS

API source interface assembly	
Exit lens	80100-20070
Ion sweep cone	80000-20895
Ion transfer tube	70005-20606
Lens L0	80100-20548
O-ring, Vespel, graphite, 0.325 in. ID, 0.046 in. thick (under ion transfer tube)	97055-20442
SRIG lens stack (S-lens)	80000-60136

TSQ Quantiva MS

API source interface assembly	
Exit lens	80100-20070
Ion sweep cone	80100-20646
Ion transfer tube (vertical orifice)	80100-20641
Lens L0	80100-20548
SRIG lens stack (ion funnel)	80100-60036

Miscellaneous Parts

Divert/Inject Valve and Syringe Pump Assembly

Divert/inject valve, Rheodyne MX Series II	00109-99-00046
Holder, divert valve and syringe pump	80100-60258
Syringe pump, Chemyx Fusion 100T	00109-99-00045

Air Filter

Air filter, metal mesh	80000-10355
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Forepump Accessories

Internal demister (exhaust) filter	00108-01-00041
Lubricant oil, 1 L	HAZMAT-01-00063

Power Supply Cords

Mass Spectrometer

- North American locations: NEMA 6-15 plug, rated 250 Vac, 15 A,
2.5 m (8 ft) long 96000-98035
- International locations: CEE (3-pole) plug, rated 250 Vac, 16 A,
2.5 m (8 ft) long 80000-63188

Forepump

- North American locations: NEMA 6-15 plug, rated 250 Vac, 15 A,
2.5 m (8 ft) long Provided with the forepump
- International locations: CEE (3-pole) plug, rated 250 Vac, 16 A,
2.5 m (8 ft) long 80000-63186

Sample Loop

- 2 μ L, Peek 00110-16012

Glossary

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

A

API ion transfer tube A tube assembly that assists in desolvating ions that are produced by the ESI, APCI, or NSI nozzle.

API ion transfer tube offset voltage A DC voltage applied to the ion transfer tube. The voltage is positive for positive ions and negative for negative ions.

API source The sample interface between the liquid chromatograph (LC) and the mass spectrometer (MS).

API stack Consists of the components of the API source that are held under vacuum and includes the ion spray cone, ion transfer tube, exit lens, and ion transfer tube mount.

atmospheric pressure chemical ionization (APCI) A soft ionization technique operating at atmospheric pressure. Electrons from a corona discharge initiate the process by ionizing the mobile phase vapor molecules, forming a reagent gas. Charged species are generated in the gas phase.

atmospheric pressure ionization (API) Ionization performed at atmospheric pressure by using atmospheric pressure chemical ionization (APCI), heated-electrospray (H-ESI), or nanospray ionization (NSI).

atmospheric pressure photoionization (APPI) A soft ionization technique that shows an ion generated from a molecule when it interacts with a photon from a light source.

auxiliary gas The outer-coaxial gas (nitrogen) that assists the evaporation of the sample solution as it exits the ESI, APCI (optional), or APPI (optional) spray insert. The mass spectrometer heats this gas to the user-specified vaporizer temperature.

C

centroid data Data used to represent mass spectral peaks in terms of two parameters: the centroid (the weighted center of mass) and the intensity. The data is displayed as a bar graph. The normalized area of the peak provides the mass intensity data.

charge state The imbalance between the number of protons (in the nuclei of the atoms) and the number of electrons that a molecular species (or adduct ion) possesses. If the species possesses more protons than electrons, its charge state is positive. If it possesses more electrons than protons, its charge state is negative.

collision energy The energy used when ions collide with the collision gas.

collision gas A neutral gas used in the collision cell to undergo collisions with ions.

collision-induced dissociation (CID) A method of fragmentation where ions are accelerated to high-kinetic energy and then allowed to collide with neutral gas molecules such as helium. The collisions break the bonds and fragment the ions into smaller charged product ions and neutral fragments.

contact closure connection The cable connection is from the external peripheral device to the mass spectrometer contact closure pins (Start In and Ground). The external device sends the contact closure (start) signal to the mass spectrometer.

conversion dynode A highly polished metal surface that converts ions from the mass analyzer into secondary particles, which enter the electron multiplier.

D

divert/inject valve A valve on the mass spectrometer that can be plumbed as a divert valve or as a loop injector.

E

electron multiplier A device used for current amplification through the secondary emission of electrons. Electron multipliers can have a discrete dynode or a continuous dynode.

electrospray (ESI) A soft ionization technique operating at atmospheric pressure. Ions are generated in solution and a high voltage is applied to generate small droplets that are then evaporated until all ions are in the gas phase.

F

flow rate, syringe pump status The syringe pump injection flow rate in milliliters per minute (mL/min) or microliters per minute (μ L/min) for the current sample, as defined in the current experiment method.

forepump The pump that evacuates the foreline. A rotary-vane pump is a type of forepump. It might also be referred to as a backing, mechanical, rotary-vane, roughing, or vacuum pump.

fragment ion A charged dissociation product of an ionic fragmentation. Such an ion can dissociate further to form other charged molecular or atomic species of successively lower formula weights.

full-scan type Provides a full mass spectrum within a defined mass range.

H

heated-electrospray (H-ESI) Converts ions in solution into ions in the gas phase by using electrospray (ESI) in combination with heated auxiliary gas.

I

image current detection The detection of ion motion by the charge (current) induced on one or more capacitive plates (outer electrodes).

ion detection system A high sensitivity, off-axis system for detecting ions. It produces a high signal-to-noise ratio (S/N) and allows for switching of the voltage polarity between positive ion and negative ion modes of operation. The ion detection system includes two ± 12 kVdc conversion dynodes and a discrete dynode electron multiplier.

ion isolation A step in the quadrupole Q1 mass analysis where the mass analyzer ejects all ions except for the ions of interest.

ion isolation waveform voltage A waveform applied to the linear ion trap that ejects all ions except the SIM ion or precursor ion.

ion optics Focuses and transmits ions from the API source to the mass analyzer.

ion polarity mode The mass spectrometer can operate in either of two ion polarity modes: positive or negative.

ion sweep cone A removable cone-shaped metal cover that fits on top of the API ion transfer tube and acts as a physical barrier to protect the entrance of the tube.

L

lens A metal disk with a circular hole in the center that allows the ion beam to pass.

M

mass analysis A process that produces a mixture of ionic species that is then separated according to the mass-to-charge ratios (m/z) of the ions to produce a mass spectrum.

mass analyzer A device that determines the mass-to-charge ratios (m/z) of ions by one of a variety of techniques.

mass analyzer DC offset voltage A DC voltage that is applied to the mass analyzer electrodes to help draw ions in from the ion optics. This voltage defines the translational kinetic energy of the ions as they enter the mass analyzer. For the mass detector, the mass analyzer DC offset voltage is -10 Vdc for positive ions and $+10$ Vdc for negative ions.

mass spectrometer An instrument that ionizes sample molecules and then measures and analyses the ions according to their mass-to-charge ratio (m/z). The resulting mass spectrum is a characteristic pattern for the identification of a molecule.

mass spectrum A graphical representation (plot) of measured ion abundance versus mass-to-charge ratio. The mass spectrum is a characteristic pattern for the identification of a molecule and is helpful in determining the chemical composition of a sample.

mass-to-charge ratio (m/z) An abbreviation used to denote the quantity formed by dividing the mass of an ion (in Da) by the number of charges carried by the ion. For example, for the ion $C_7H_7^{2+}$, $m/z = 45.5$.

molecular ion An ion formed by the removal (positive ion) or addition (negative ion) of one or more electrons to/from a molecule without fragmentation of the molecular structure.

multipole A symmetrical, parallel array of (usually) four, six, or eight cylindrical rods that acts as an ion transmission device. An RF voltage and DC offset voltage are applied to the rods to create an electrostatic field that efficiently transmits ions along the axis of the multipole rods.

multipole DC offset voltage A DC voltage applied to a multipole rod assembly. The multipole DC offset voltage helps to define the translational kinetic energy of the ions within the assembly.

multipole RF voltage The amplitude of the RF voltage applied to the multipoles.

N

nanoelectrospray ionization (nanoESI or NSI) A type of electrospray (ESI) that accommodates very low flow rates of sample and solvent at $1-20$ nL/min (for static nanoelectrospray) or $100-1000$ nL/min (for dynamic nanoelectrospray, which is also called nanoESI nanoLC gradient separation).

neutral loss mass The mass of the neutral species that is lost by the precursor ion in a neutral loss experiment.

neutral loss scan mode A scan mode that links together an MS and MS/MS scan so that they are scanned at the same rate over scan ranges of the same width. However, the respective mass ranges are offset by a selected mass so that the MS/MS scan is a selected number of mass units lower than the MS scan.

P

peak threshold The minimum number of intensity counts per sampling interval that is required before a signal is recorded.

peak width The distance across a peak measured at a selected peak-height level, in minutes or mass units. The peak-height level is usually specified as a percentage of the maximum peak height.

peak width at half height The full width of a peak at half its maximum height, sometimes abbreviated FWHM.

precursor ion An electrically charged molecular species that can dissociate to form fragments. The fragments can be electrically charged or neutral species. A precursor ion can be a molecular ion or an electrically charged fragment of a molecular ion.

precursor mass The mass-to-charge ratio of a precursor ion. The location of the center of a target precursor-ion peak in mass-to-charge ratio (m/z) units.

product ion An electrically charged fragment of an isolated precursor ion.

product mass The mass-to-charge ratio of a product ion. The location of the center of a target production peak in mass-to-charge ratio (m/z) units.

profile data Data representing mass spectral peaks as point-to-point plots, with each point having an associated intensity value.

Q

qualitative analysis Chemical analysis designed to determine the identity of the components of a substance.

quantitative analysis Chemical analysis designed to determine the quantity or concentration of a specific substance in a sample.

R

retention time (RT) The time after injection at which a compound elutes. The total time that the compound is retained on the chromatograph column.

RF lens A multipole rod assembly that is operated with only radio frequency (RF) voltage on the rods. In this type of device, virtually all ions have stable trajectories and pass through the assembly.

RF voltage (linear ion trap) An AC voltage of constant frequency and variable amplitude that is applied to the quadrupole rods of a multipole. Because the frequency of this AC voltage is in the radio frequency (RF) range, it is referred to as RF voltage.

S

scan Comprised of one or more microscans. Each microscan is one mass analysis (ion injection and storage/scan-out of ions) followed by ion detection. After the microscans are summed, the scan data is sent to the data system for display and/or storage. The process of ramping the amplitude of the RF and DC voltages on the multipole rods in the mass analyzer to transmit ions from the lowest mass to the highest mass of a specified scan range.

selected ion monitoring (SIM) scan type A scan type where the mass spectrometer acquires and records ion current following the isolation of a range of mass-to-charge ratio values.

selected reaction monitoring (SRM) scan type A scan type with two stages of mass analysis and where a particular reaction or set of reactions, such as the fragmentation of an ion or the loss of a neutral moiety, is monitored. In SRM a limited number of product ions is monitored.

sheath gas The inner coaxial gas (nitrogen), which is used in the API source to help nebulize the sample solution into a fine mist as the sample solution exits the ESI or APCI nozzle.

signal-to-noise ratio (S/N) The ratio of the signal height (S) to the noise height (N). The signal height is the baseline corrected peak height. The noise height is the peak-to-peak height of the baseline noise.

sweep gas Nitrogen gas that flows out from the gap between the sweep cone and the ion transfer tube into the API source. Sweep gas aids in solvent declustering and adduct reduction.

syringe pump A device that delivers a solution from a syringe at a specified rate.

T

turbomolecular pump A vacuum pump that provides a high vacuum for the mass spectrometer and detector system.

V

vacuum manifold A thick-walled, aluminum chamber, with various electrical feedthroughs and gas inlets, which encloses the API stack, ion optics, mass analyzers, and ion detection system.

vacuum system Components associated with lowering the pressure within the mass spectrometer. A vacuum system includes the vacuum manifold, pumps, pressure gauges, and associated electronics.

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