

**TSQ Series**

# **TSQ Quantum XLS Series**

**User Guide**

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December 2011

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EN 55011	2007; A2: 2007	EN 61000-4-5	2005
EN 61000-3-2	2006	EN 61000-4-6	2007
EN 61000-3-3	1995; A1: 2001; A2: 2005	EN 61000-4-11	2004
EN 61000-4-2	1995; A1: 1999; A2: 2001	EN 61326-1	2006
EN 61000-4-3	2006	FCC Class A	2008, CFR 47, Part 15
EN 61000-4-4	2004		

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## Preface

The Thermo Scientific TSQ Quantum XLS and TSQ Quantum XLS Ultra systems make up the TSQ Quantum XLS Series and are member of the TSQ Quantum™ family of mass spectrometers.

This *TSQ Quantum XLS Series User Guide* contains a description of the modes of operation and principle hardware components of your TSQ Quantum XLS Series system. In addition, this user guide provides step-by-step instructions for cleaning and maintaining your mass spectrometer.

### Contents

- [Related Documentation](#)
- [Safety and Special Notices](#)
- [Contacting Us](#)

### ❖ To suggest changes to documentation or to Help

- Complete a brief survey about this document by clicking the link below.  
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## Related Documentation

In addition to this guide, Thermo Fisher Scientific provides the following PDF document and Help for the TSQ Quantum XLS Series systems:

- *TSQ Quantum XLS Series Preinstallation Requirements Guide*
- Manuals that come with other modules of your system
- Help that is included with the software

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

Safety and special notices include the following:



**WARNING** Highlights hazards to humans. Each WARNING notice is accompanied by an appropriate hazard symbol.



**WARNING Burn Hazard.** The ion source, GC oven, injector, and transfer line are hot. Allow them to cool to room temperature before touching them.



**WARNING Shock Hazard.** Unplug the product-name mass spectrometer before proceeding.



**WARNING Material and Eye Hazard.** Wear impermeable laboratory gloves and eye protection when performing cleaning procedures.



**CAUTION** Highlights hazards to property or the environment.

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

**Note** Highlights information of general interest.

**Tip** Highlights helpful information that can make a task easier.

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# Introduction

The TSQ Quantum XLS Series systems are advanced analytical instruments that include a mass spectrometer, gas chromatograph, and the Xcalibur™ data system. See [Figure 1](#) and [Figure 2](#).

## Contents

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

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

The TSQ Quantum XLS Series mass spectrometers include an electron ionization/chemical ionization (EI/CI) ion source, ion optics, a triple-stage mass analyzer, and an ion detection system—all of which are enclosed in a vacuum manifold. Ionization of the sample takes place in the ion source. The specific process used to ionize the sample is known as the ionization mode. The ion optics transmit the ions produced in the ion source into the mass analyzer, where they are filtered according to their mass-to-charge ratio. The polarity of the potentials applied to the lenses in the ion source and ion optics determines whether positively charged ions or negatively charged ions are transmitted to the mass analyzer. You can configure the mass spectrometer to analyze positively or negatively charged ions (called the positive or negative ion polarity mode).

**Figure 1.** TSQ Quantum XLS Ultra mass spectrometer, TriPlus autosampler, and TRACE GC Ultra gas chromatograph



**Figure 2.** TSQ Quantum XLS mass spectrometer, TriPlus autosampler, and TRACE GC Ultra gas chromatograph



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

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

In a first stage of mass analysis, you can use the mass spectrometer to elucidate the structures of pure organic compounds and the structures of the components within mixtures.

Furthermore, in a second stage of mass analysis, the mass spectrometer can fragment and separate each ionic fragment of a molecule formed in the ion source to build up an entire structure for the molecule, piece by piece. As a result, the TSQ Quantum XLS Series systems make investigating all pathways for the formation and fragmentation of each ion in the mass spectrum possible.

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

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

## Ionization Modes

The specific process used to ionize the analyte is referred to as the ionization mode. You can operate the TSQ Quantum XLS Series mass spectrometers in either of two ionization modes:

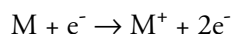
- [Electron Ionization Mode](#)
- [Chemical Ionization Mode](#)

---

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

## Electron Ionization Mode

In electron ionization (EI) mode, electrons are emitted by a heated, wire filament that has electric current running through it, by thermionic emission. The filament and its reflector are typically maintained at a  $-70$  V potential relative to the ion source block. This potential accelerates the electrons through the ionization space, called the ion volume. These energetic electrons interact with neutral, gas-phase analyte molecules present in the ion volume and cause the analyte to lose an electron and produce a radical cation:



Frequently, numerous cleavage reactions give rise to fragment ions, which provide structural information about the analyte.

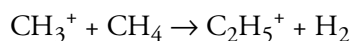
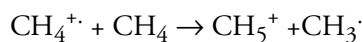
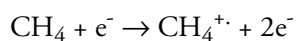
EI positive-ion mode is the only commonly used EI mode.

## Chemical Ionization Mode

In chemical ionization (CI) mode, ionization of the sample molecules is a multi-step process:

1. Reagent gas is introduced into the CI ion volume at a flow (for methane) of about 2 mL/min, along with sample vapors typically present at partial pressures of less than one-thousandth that of the reagent gas.
2. The energetic (typically 100 eV) electrons emitted by the heated filament interact to ionize the reagent gas and form a plasma. This reaction also produces thermal electrons.
3. Reagent gas ions react with reagent gas molecules to form a variety of secondary ions that are stable with respect to further reaction with reagent gas.

For example, for methane:



4. Positive sample ions are formed by one of the following:
  - The transfer of a proton from a secondary reagent gas ion to a sample molecule
  - The abstraction of an electron by a reagent gas ion
  - An ion association reaction where an adduct ion is formed between a reagent gas ion and a sample molecule

In methane positive ion mode CI, the relevant peaks observed are  $MH^{+}$ ,  $[M+CH_5]^{+}$ , and  $[M+C_2H_5]^{+}$ ; but mainly  $MH^{+}$ .



In isobutane positive ion mode CI, the main peak observed is  $MH^+$ .

In ammonia positive ion mode CI, the main peaks observed are  $MH^+$  and  $[M+NH_4]^+$ .

Negative sample ions are most commonly formed by one of the following:

- Sample molecules that capture the secondary thermal electrons present in the ion source
- Electron transfer from ionized reagent gas (for example,  $NH_2^-$ )
- Proton abstraction

Molecular ions observed in negative ion chemical ionization mass spectra are usually  $M^-$  or  $[M-H]^-$ .

## Ion Polarity Modes

You can operate the TSQ Quantum XLS Series mass spectrometers in either of two ion polarity modes: positive or negative. Both positively charged and negatively charged ions form in the ion source of the mass spectrometer. The mass spectrometer controls whether positive ions or negative ions are transmitted to the mass analyzer for mass analysis by changing the polarity of the potentials applied to the ion source and ion optics. The ion optics deliver the ions produced in the ion source, in a collimated beam, to the mass analyzer. The mass spectrometer can switch between positive and negative polarity modes in under 95 ms.

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

## Scan Modes

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

- MS scan modes: Q1MS and Q3MS scan modes
- MS/MS scan modes: Product scan mode, Parent scan mode, Neutral Loss scan mode
- Data-dependent scan mode

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

The mass analyzer or the mass spectrometer has three rod assemblies.<sup>2</sup> The first and third rod assemblies, Q1 and Q3, are quadrupoles, and the second rod assembly, Q2, is a square-profile quadrupole.

Rod assemblies can operate in either of two capacities:

- As ion transmission devices
- As mass analyzers

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

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

On the TSQ Quantum XLS Series mass spectrometers, the quadrupole rod assemblies can operate with rf and dc voltages or with only rf voltage. That is, Q1 and Q3 can act either as mass analyzers or ion transmission devices. The Q2 rod assembly operates exclusively with rf voltage. As a result, Q2 is always an ion transmission device. Surrounding Q2 is a collision cell where fragmentation can take place if the argon collision gas is present in the cell. For a summary of how the rod assemblies function in several of the major scan modes, see [Table 1](#).

**Table 1.** Summary of scan modes

Scan mode	Q1 quadrupole	Q2 collision cell	Q3 quadrupole
Q1MS	Scan <sup>a</sup>	Pass all ions <sup>b</sup>	Pass all ions
Q3MS	Pass all ions	Pass all ions	Scan
Product	Set <sup>c</sup>	Fragment ions <sup>d</sup> , then pass all fragments	Scan
Parent	Scan	Fragment ions, then pass all fragments	Set
Neutral loss	Scan	Fragment ions, then pass all fragments	Scan

<sup>a</sup>Scan = full scan or transmission of selected ions

<sup>b</sup>Pass all ions or fragments = pass ions or fragments within a wide range of mass-to-charge ratios

<sup>c</sup>Set = set to pass ions of a single mass-to-charge ratio or a set of mass-to-charge ratios

<sup>d</sup>Fragment ions = collisions with argon gas cause ions to fragment

<sup>2</sup> A rod assembly is a regular array of metal rods. For a discussion of the rod assemblies used on the TSQ Quantum XLS Series instruments, see [“Mass Analyzer”](#) on [page 31](#).

## Q1MS and Q3MS Scan Modes

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

## Product Scan Mode

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

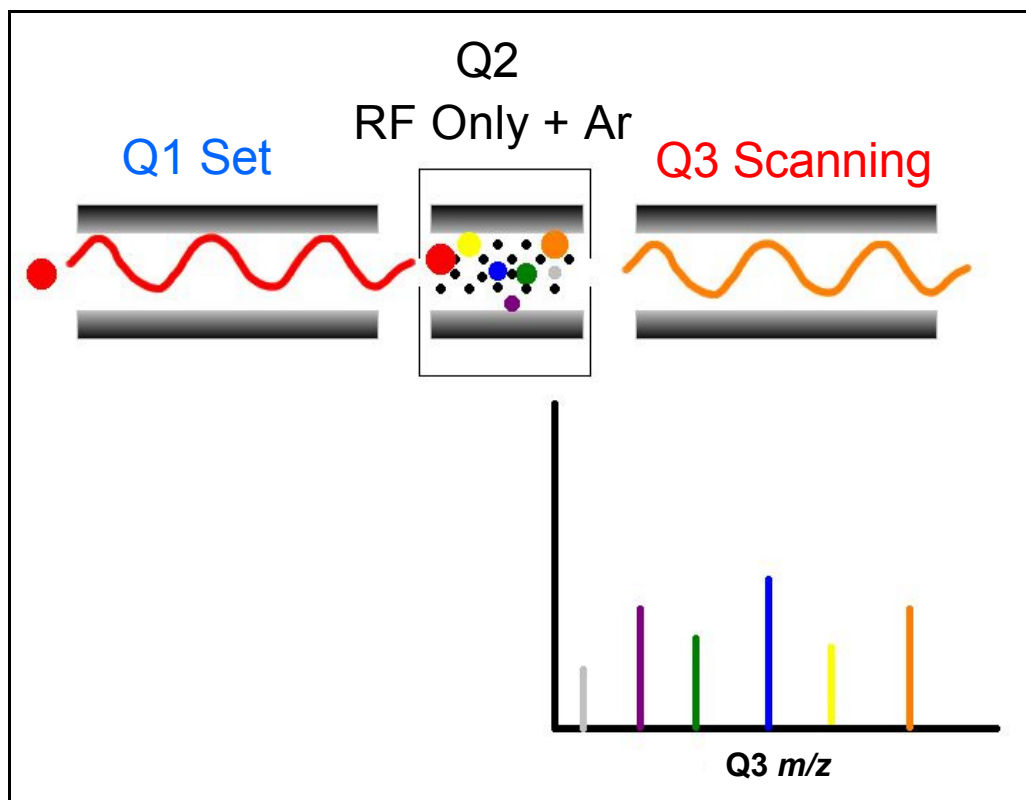
**Note** For convenience, when referring to the first, second, and third rod assemblies as pieces of hardware, you call them Q1, Q2, and Q3, respectively. However, for clarity in discussing their function in MS/MS scan modes, you refer to them as the parent mass analyzer, collision cell (ion transmission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

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

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

Figure 3 illustrates the Product scan mode.

**Figure 3.** Illustration of Product scan mode



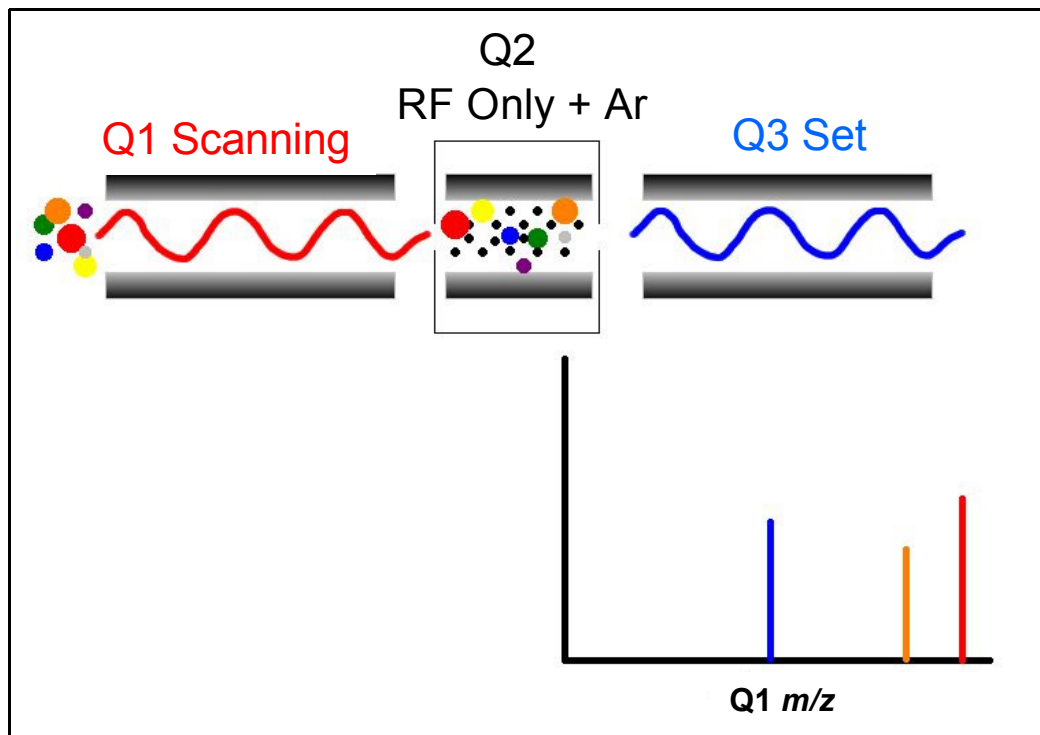
## Parent Scan Mode

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

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

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

Figure 4 illustrates the Parent scan mode.

**Figure 4.** Illustration of the Parent scan mode

You can perform experiments that use the parent scan mode (parent experiments) in structure and fragmentation studies as well as in survey analyses of mixtures. In general, parent experiments detect all compounds that decompose to a common fragment. The experiments are useful for the rapid detection of a series of structural homologs that have a common fragment ion (for example,  $m/z$  149 for the phthalates).

## Neutral Loss Scan Modes

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

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

In the second stage of analysis, ions admitted to the collision cell can fragment further by metastable ion decomposition or by CID to produce product ions. The product mass analyzer then separates these product ions by mass-to-charge ratio. [Figure 5](#) illustrates the Neutral Loss scan mode. Examples of compounds with a common neutral loss fragment appear in [Figure 6](#) on [page 11](#).

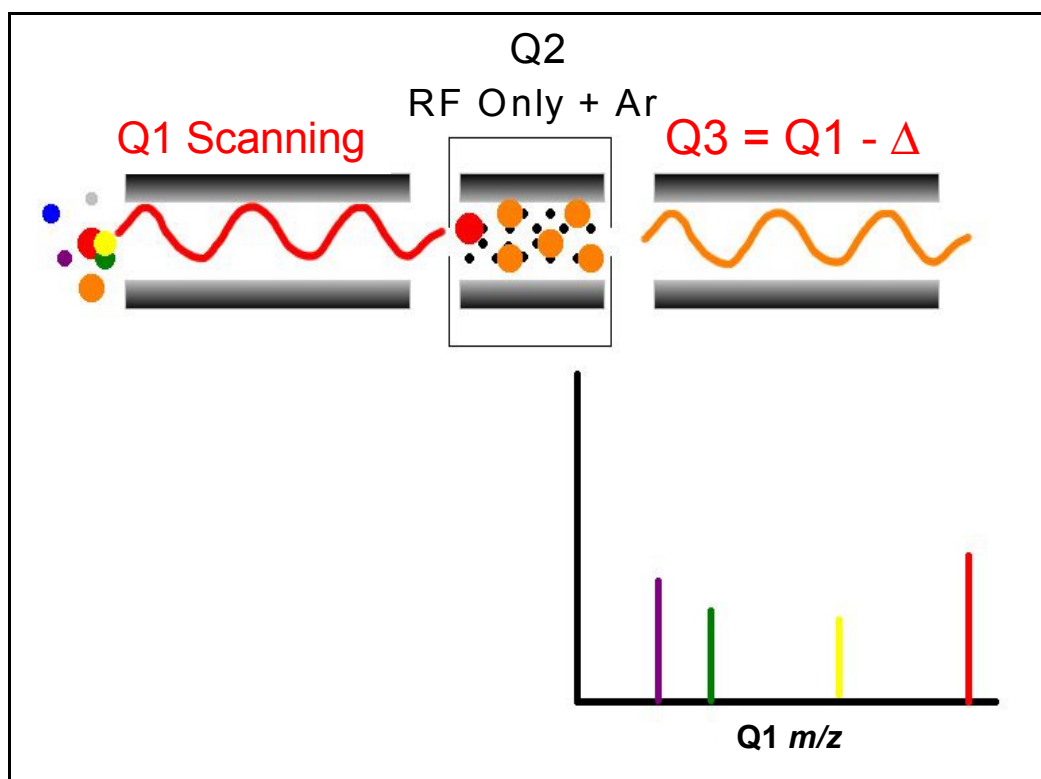
To detect an ion, between the time the ion leaves Q1 and enters Q3, it must lose a neutral moiety whose mass (the neutral loss mass) is equal to the difference in the mass ranges that the two mass analyzers scan. A neutral loss mass spectrum, then, is a spectrum showing all the parent ions that lose a neutral species of a selected mass.

Note that 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.

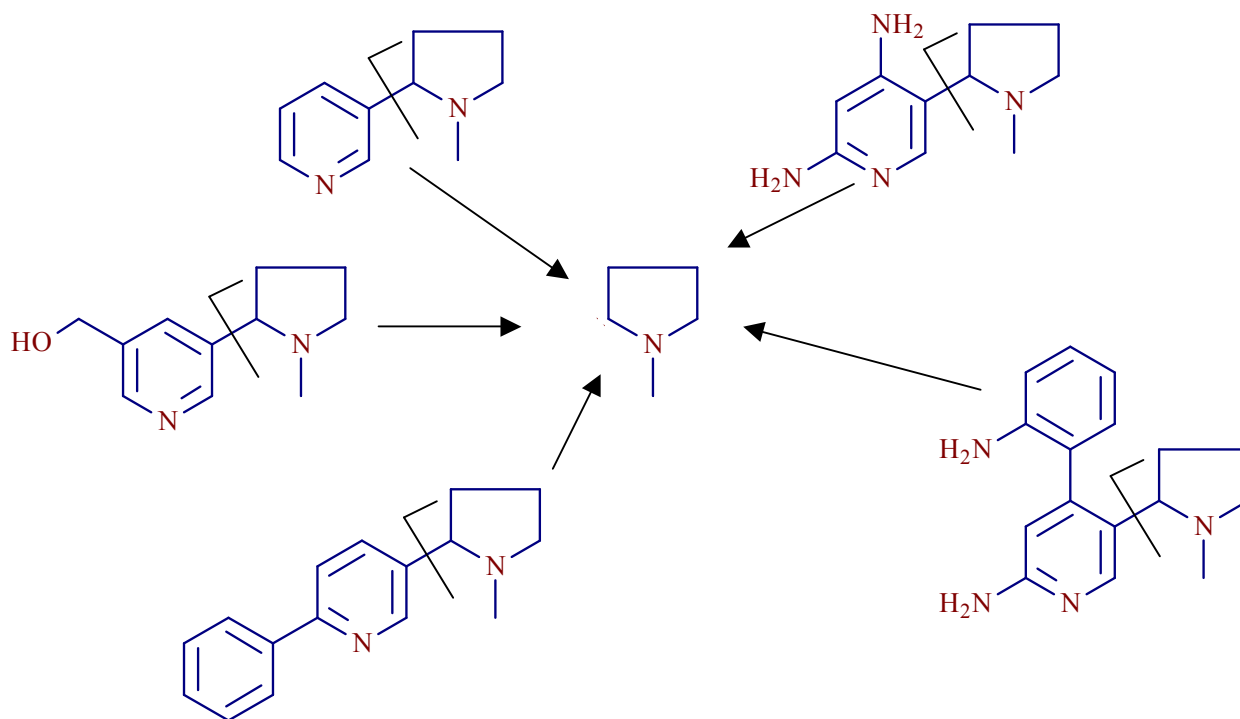
For a neutral loss (or neutral gain) mass spectrum, as for a parent mass spectrum, data for the mass-to-charge ratio axis is obtained from Q1 (the parent ion), whereas data for the ion intensity axis is obtained from Q3 (the product ion being monitored).

You can perform experiments that use the Neutral Loss scan mode (neutral loss experiments) when a large number of compounds are being surveyed for common functionality. Neutral moieties are frequently lost from substituent functional groups (for example,  $\text{CO}_2$  from carboxylic acids, CO from aldehydes, HX from halides, and  $\text{H}_2\text{O}$  from alcohols).

**Figure 5.** Illustration of the Neutral Loss scan mode



**Figure 6.** Examples of compounds with a common neutral-loss fragment



## Data-Dependent Scan Mode

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

- If you have some idea of what the parent ion is, or if you expect a certain kind of parent ion, you can set up a list of possible parent ions. Then, when one of the parent ions you specified is detected, you can acquire product spectra and analyze the information. Conversely, you can also set up a list of ions that you do *not* want selected for fragmentation.
- If you have little information about your compound, you can set up the parameters of a data-dependent experiment so that if the intensity of the ion signal is above a specified threshold, the mass spectrometer generates product spectra. Later, you can decide if the information is useful.

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

## Scan Types

You can operate the TSQ Quantum XLS Series systems with a variety of scan types. The most common scan types are as follows:

- [Full Scan](#)
- [Selected Ion Monitoring \(SIM\)](#)
- [Selected Reaction Monitoring \(SRM\)](#)
- [Intelligent Selected Reaction Monitoring \(iSRM\)](#)
- [Quantitation-Enhanced, Data-Dependent MS \(QED MS\)](#)
- [AutoSIM](#)

### Full Scan

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

You use full-scan experiments to determine or confirm the identity of unknown compounds or the identity of each component in a mixture of unknown compounds. (Generally, you need a full mass spectrum to determine the identity of an unknown compound.)

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

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

### Selected Ion Monitoring (SIM)

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



Because SIM monitors only a few ions, it can provide lower detection limits and greater speed than the full-scan modes. SIM achieves lower detection limits because more time is spent monitoring significant ions that are known to occur in the mass spectrum of the target analyte. SIM can achieve greater speed because it monitors only a few ions of interest; SIM does not monitor regions of the spectrum that are empty or have no ions of interest.

SIM can improve the detection limit and decrease analysis time, but it can also reduce specificity. Because SIM monitors only specific ions, any compound that fragments to produce those ions appear as the target compound, which can result in a false positive.

## Selected Reaction Monitoring (SRM)

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

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

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

## Highly-Selective Reaction Monitoring (HSRM)

Highly-selective reaction monitoring (HSRM) is SRM performed at higher Q1 resolution (0.4 u fwhm [less for TSQ Quantum XLS Ultra mass spectrometers] versus 0.7 u fwhm for SRM).

## Intelligent Selected Reaction Monitoring (iSRM)

In intelligent selected reaction monitoring (iSRM) experiments, the mass spectrometer performs multiple “primary” selected reaction monitoring (SRM) scans for each analyte (parent ion) of interest. The mass spectrometer uses for quantification the sum of the intensities of an analyte’s primary SRM scans.

You specify a trigger threshold for each primary SRM scan. If the intensities of all the listed primary SRM reactions for an analyte are above their trigger thresholds, and if all these scans are within a specified retention time window, then the mass spectrometer performs “secondary” SRM scans to confirm the identity of the analyte. The maximum number of secondary SRM reactions is 12 400.

The mass spectrometer uses reference SRM scans to adjust the acquisition time window of subsequent SRM scans. It uses the time difference between the expected and observed retention times of reference SRM reactions to correct the retention times that it uses to make procedural decisions. The mass spectrometer still records data with the true retention times. You should specify two to four reference reactions spaced throughout the LC run. The mass spectrometer uses the preceding two retention time corrections to calculate a piecewise linear retention time correction for the primary SRM scans that follow. As with primary SRM scans, reference SRM scans might trigger secondary SRM scans.

The maximum number of primary plus reference SRM transitions is 3600.

## Quantitation-Enhanced, Data-Dependent MS (QED MS)

The quantitation-enhanced, data-dependent MS (QED MS) scan type provides simultaneous quantitation (SRM) and structural confirmation (full-scan MS/MS product ion spectra). If the intensity of an SRM reaction that you specify for a parent ion is above its trigger threshold, the mass spectrometer performs a full-scan MS/MS product ion scan to confirm the identity of the analyte. You can perform retention time correction with QED MS.

## AutoSIM

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

## Data Types

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

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

### Profile Data Type

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

## Centroid Data Type

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

## Mass/Charge Range

The TSQ Quantum XLS and TSQ Quantum XLS Ultra mass spectrometers can operate in a mass/charge range of 10 to 3000 Da, and 10 to 1500 Da, respectively.



## Functional Description

This chapter describes the principal components of the TSQ Quantum XLS Series systems and their respective functions.

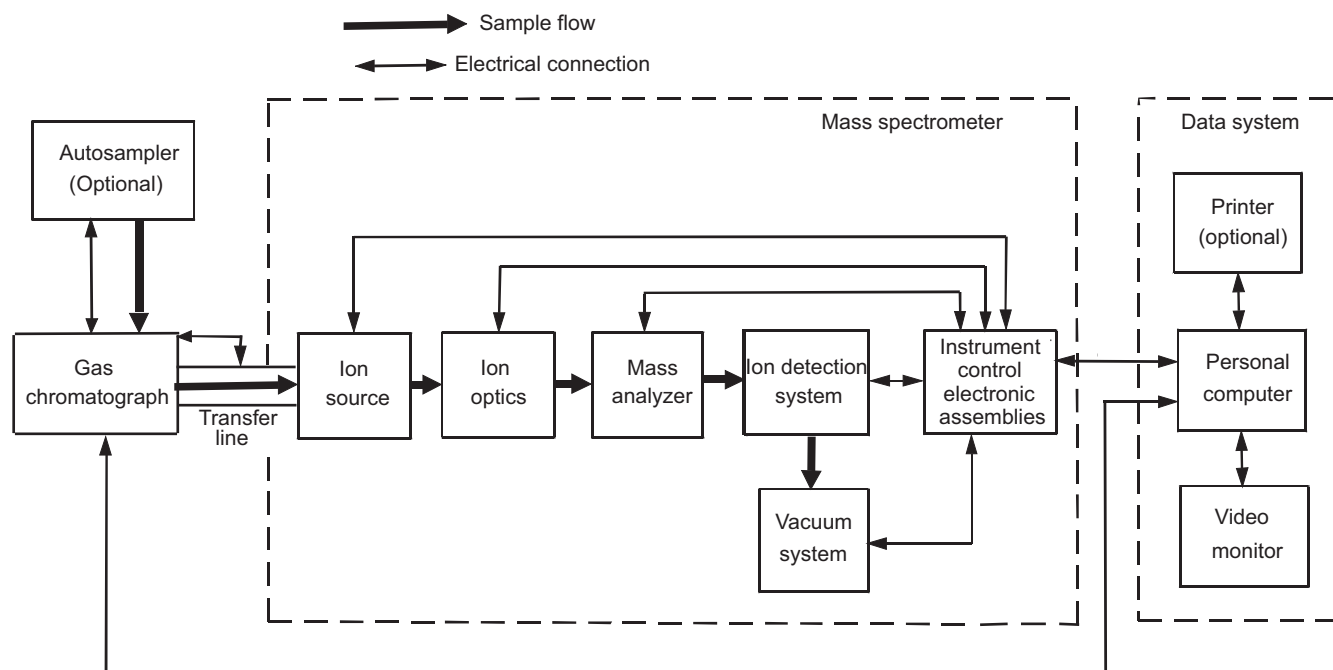
### Contents

- Autosampler (optional)
- Gas Chromatograph
- Direct Sample Probes (optional)
- Transfer Line
- Mass Spectrometer
- Data System

A functional block diagram of the TSQ Quantum XLS Series system is shown in [Figure 7](#). A sample transfer line connects the gas chromatograph (GC) to the mass spectrometer. The autosampler and GC are installed on the left side of the mass spectrometer.

In analysis by GC/MS, you inject a sample into a GC column. The sample then separates into its various components. The components elute from the GC column and pass through the transfer line into the mass spectrometer where they are analyzed. You can also use a direct sample probe to introduce sample into the mass spectrometer.

Electron ionization (EI) or chemical ionization (CI) ionizes sample molecules upon entering the mass spectrometer. The ion optics focus and accelerate the resulting sample ions into the mass analyzer where they are filtered according to their mass-to-charge ratios. An ion detection system then produces a signal proportional to the number of ions detected. The system electronics receive and amplify the ion current signal from the ion detection system. That signal is then passed on to the data system for further processing, storage, and display. The data system provides the primary mass spectrometer user interface.

**Figure 7.** Functional block diagram of the TSQ Quantum XLS Series system

## Autosampler

You can use the optional Thermo Scientific TriPlus™ autosampler to inject samples automatically into the GC inlet. With an autosampler, you can automate your GC/MS/MS analyses. The TriPlus autosampler is shown in [Figure 1](#) and [Figure 2](#) on [page 2](#).

Autosampler Start/Stop signals with the mass spectrometer are provided by contact closure.

You configure the TriPlus autosampler from the data system computer. Select the TriPlus instrument button in the Instrument Configuration window, available from the Microsoft™ Windows™ taskbar by choosing **Start > All Programs > Thermo Foundation 2.0 > Instrument Configuration**. For a description of TriPlus configuration options, refer to the Xcalibur Help.

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

For maintenance procedures, refer to the documentation provided with the autosampler.

## Gas Chromatograph

The Thermo Scientific TRACE GC Ultra™ gas chromatograph (GC) separates a sample mixture into its chemical components by gas chromatography. In gas chromatography, the sample mixture is partitioned between a solid stationary phase and a mobile gas. The stationary phase is adhered to the inside of a small-diameter glass tube: the capillary column. The molecular structure of each component of the mixture determines in which order each component elutes from the GC and enters the mass spectrometer. The TRACE GC Ultra gas chromatograph is shown in [Figure 1](#) and [Figure 2](#) on [page 2](#).

Gas chromatography is widely used in analytical chemistry, though the high temperatures used in GC make it unsuitable for high molecular weight biopolymers, frequently encountered in biochemistry. It is well suited for use in the petrochemical, environmental monitoring, and industrial chemical fields. It is also used extensively in chemistry research.

You configure the TRACE GC Ultra gas chromatograph from the data system computer. Click the **TRACE GC Ultra** instrument button in the Instrument Configuration window, available from the Microsoft Windows taskbar by choosing **Start > All Programs > Thermo Foundation 2.0 > Instrument Configuration**. For a description of TRACE GC Ultra configuration options, refer to the Xcalibur Help.

The TSQ Quantum XLS Series data system computers can directly control the TRACE GC Ultra. Choose **Start > All Programs > Thermo Xcalibur > Xcalibur** and click **Instrument Setup** to open the Instrument Setup window. Click the **TRACE GC Ultra** icon to open the TRACE GC Ultra page. For instructions to operate the TRACE GC Ultra, refer to the Help.

For front-panel (keypad) operation of the GC and maintenance procedures for the GC, refer to the documentation provided with the GC. To replace the GC capillary column, see [“Removing and Installing a GC Capillary Column”](#) on [page 107](#).

## Direct Sample Probes

With the optional direct sample probes, you can introduce compounds directly into the ion source without GC column separation. See [Figure 8](#). The direct sample probes are ideal for qualitative or semi-quantitative analysis of materials that do not require a GC column separation or are difficult, if not impossible, to elute chromatographically, as with solids. The direct sample probes introduce samples directly into the ion source via a vacuum interlock. A single controller box ([Figure 8](#)) with interchangeable probe tools makes it easy to select the best method of sample introduction.

The direct sample probe system includes two probe tools:

- Direct exposure probe
- Direct insertion probe

The direct exposure probe (DEP) has a heated filament that rapidly vaporizes liquids or solutions. The DEP is ideal for rapid molecular weight confirmation of liquids or solids dissolved in a suitable solvent. The DEP can vaporize compounds with a high boiling point.

The direct insertion probe (DIP) has a temperature-controlled, heated capillary tube that slowly vaporizes solid samples. You can use the DIP for rapid analysis of solids or trace components in solid matrices, such as forensic samples or tissue.

**Figure 8.** Direct sample probe and controller

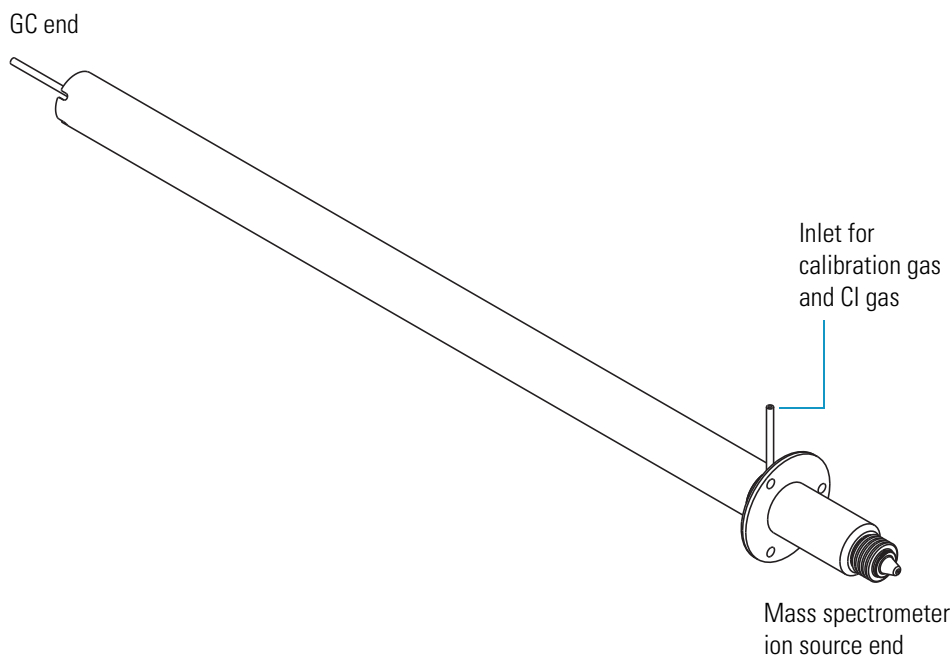


## Transfer Line

The transfer line is the interface between the GC and mass spectrometer. The transfer line heats the capillary column as it passes from the GC into the ion source in the mass spectrometer. This prevents the sample from condensing. The transfer line includes an inlet for calibration gas and chemical ionization gas. See [Figure 9](#).



**Figure 9.** Transfer line



## Mass Spectrometer

The TSQ Quantum XLS Series mass spectrometers provides sample ionization and mass analysis of samples introduced from a gas chromatograph or direct insertion probe. The mass spectrometer uses a triple-quadrupole mass analyzer with an ion source external to the mass analyzer. Several important features of the TSQ Quantum XLS Series mass spectrometers are as follows:

- High sensitivity and resolution
- $m/z$  10 to 3000 mass range for the TSQ Quantum XLS, and  $m/z$  10 to 1500 mass range for the TSQ Quantum XLS Ultra
- EI and CI ionization modes
- Positive and negative ion polarity modes
- MS and MS/MS scan modes
- Full-scan, SIM, SRM, iSRM, QED MS, AutoSIM, and data-dependent scan types

The mass spectrometer includes the following components:

- [Controls and Indicators](#)
- [EI/CI Ion Source](#)
- [Ion Optics](#)

- [Mass Analyzer](#)
- [Ion Detection System](#)
- [Vacuum System and Inlet Gasses Hardware](#)
- [Electronic Assemblies](#)
- [Data System](#)

## Controls and Indicators

Five light-emitting diodes (LEDs) are located in the upper right of the front panel of the mass spectrometer. See [Figure 10](#) and [Figure 11](#).

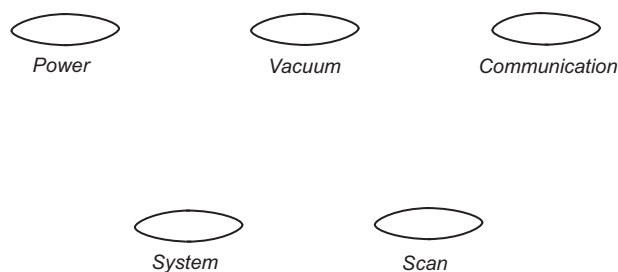
The Power LED illuminates green whenever power is supplied to the vacuum system and electronic assemblies of the mass spectrometer.

The Vacuum LED illuminates yellow when the turbomolecular pump is nearly at speed (80 percent of its operating speed of 750 MHz), and it is safe to turn on the ion gauge. The Vacuum LED is off if the turbomolecular pump is not at speed. The Vacuum LED illuminates green whenever the pressure in the analyzer chamber, as measured by the ion gauge, is at or below the value required to enable high voltages to the mass analyzer. See [Table 2](#).

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



**Figure 11.** Front panel LEDs of the TSQ Quantum XLS mass spectrometer



**Table 2.** Maximum allowed pressure to turn on high voltages

Carrier gas	Ar collision gas	Maximum pressure (Torr)
He	Off	$8 \times 10^{-6}$
He	On	$5 \times 10^{-5}$

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

The System LED illuminates yellow whenever the mass spectrometer is in standby—that is, high voltage is not supplied to the ion source, mass analyzer, or ion detection system, but the mass spectrometer power is on. The System LED illuminates green whenever the high voltage is enabled and the system is in the On state. High voltage is enabled if the pressure of the analyzer chamber is below the values listed in [Table 2](#).

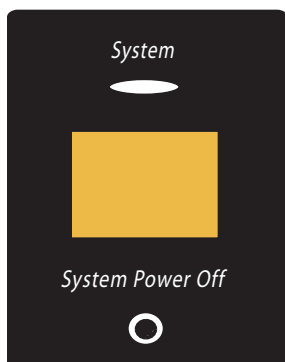
The Scan LED flashes blue whenever the mass spectrometer is on and is scanning ions.

The System Power Off button, located on the front of the electronics module, turns off power to the mass spectrometer, gas chromatograph, and autosampler. See [Figure 12](#). To restore power to the mass spectrometer, gas chromatograph, and autosampler, you must use the main power circuit breaker, located on the back of the electronics module.



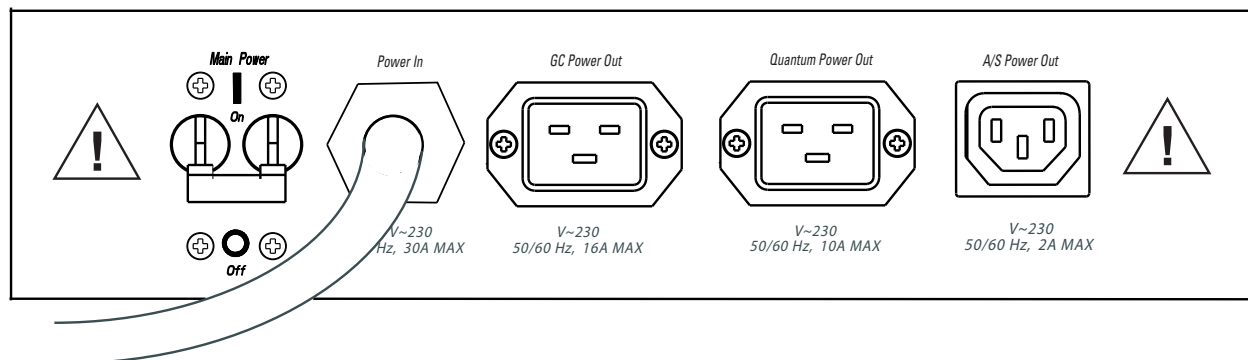
**CAUTION** In an emergency, to shut off all power to the mass spectrometer, gas chromatograph, and autosampler, press the System Power Off button located at the front of the instrument.

**Figure 12.** Front panel System Power Off button



The main power circuit breaker switch (labeled Main Power) is located on the power panel at the back of the electronics module. See [Figure 13](#). In the Off (O) position, the circuit breaker removes all power to the mass spectrometer, gas chromatograph, and autosampler. In the On (I) position, power is supplied to the mass spectrometer, gas chromatograph, and autosampler. In the standard operational mode, the circuit breaker is kept in the On (I) position.

**Figure 13.** Back power panel of the electronics module



The mass spectrometer main power circuit breaker switch (labeled Main Power) is located on the instrument power panel in the lower corner of the right-side panel of the mass spectrometer. See [Figure 14](#). In the Off position, the circuit breaker removes all power to the mass spectrometer, including the vacuum pumps. In the On position, power is supplied to the mass spectrometer. For the standard operational mode, the circuit breaker is in the On position.

The electronics service switch (labeled Electronics) is located next to the main power circuit breaker on the mass spectrometer power panel ([Figure 14](#)). In the Service Mode position, the switch removes power to all components of the mass spectrometer other than the vacuum system. The Operating Mode position supplies power to all non-vacuum system components of the mass spectrometer.

The vacuum service switch (labeled Vacuum) is located next to the electronics service switch on the instrument power panel ([Figure 14](#)). In the Service Mode position, the switch removes power to all components of the vacuum system, including the forepump, turbomolecular pump, and turbomolecular pump controller. The switch in the Operating Mode position supplies power to all vacuum system components of the mass spectrometer.

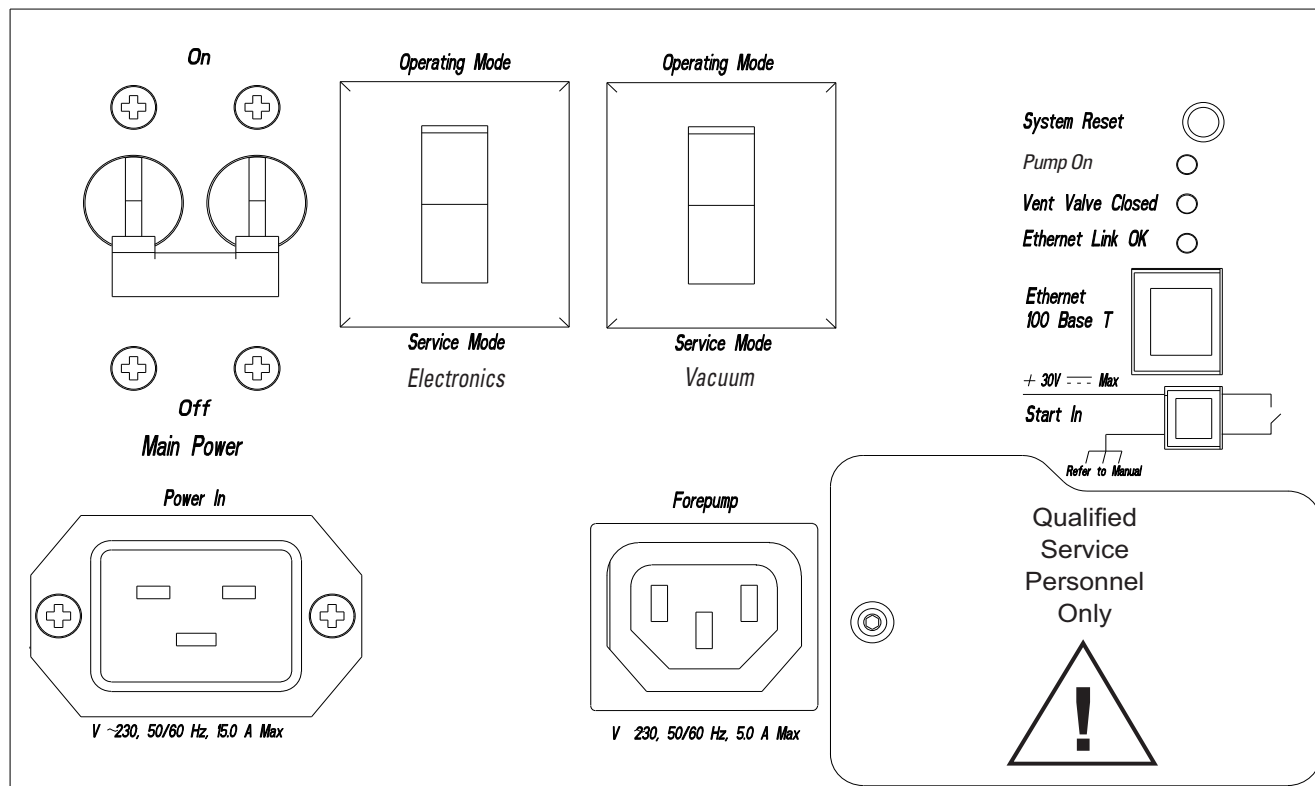
The System Reset button is also located on the mass spectrometer power panel. Pressing the System Reset button takes the 5 V logic to ground and causes the embedded computer on the System Control printed circuit board (PCB) to restart. For information on how to reset the mass spectrometer software is then reloaded from the data system, see [“Resetting the Data System” on page 57](#). For information on how to reset the mass spectrometer, see [“Resetting the Mass Spectrometer” on page 57](#).

Three LEDs are located on the power panel: The Pump On LED is green when the rough pump current sensor detects current to the forepump. The LED is off when the forepump current sensor does not detect current to the forepump. If the current sensor detects a loss of current when the mass spectrometer is on, the vacuum system vents.

The Vent Valve Closed LED is green whenever the vent valve current sensor detects current through the vent valve and the vent valve is closed. The LED is off when the vent valve is open.

The Ethernet Link OK LED is green when the System Control PCB is communicating with the data system computer. The LED is off when there is no communication between the System Control PCB and the data system computer.

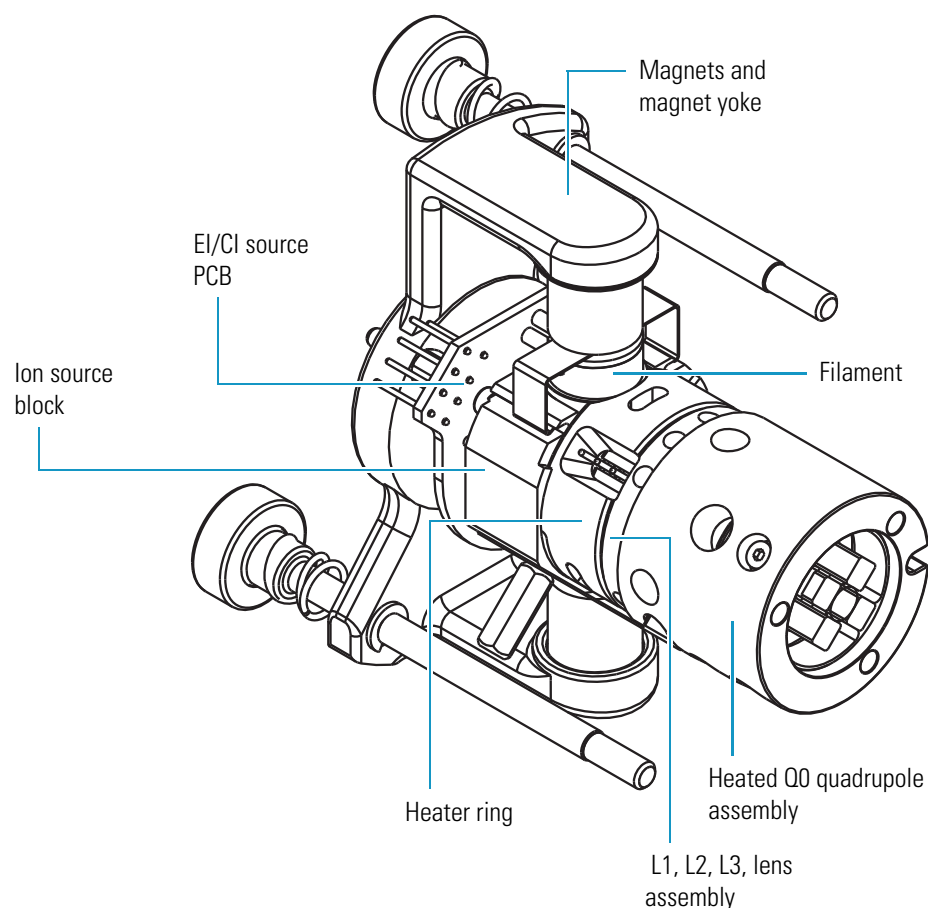
**Figure 14.** Right-side power panel of the mass spectrometer



## EI/CI Ion Source

The EI/CI ion source forms gas phase sample ions from sample molecules that elute from the GC or are introduced by the direct sample probe. See [Figure 15](#). You can operate the ion source in either the electron ionization (EI) or chemical ionization (CI) mode. See “[Ionization Modes](#)” on [page 3](#).

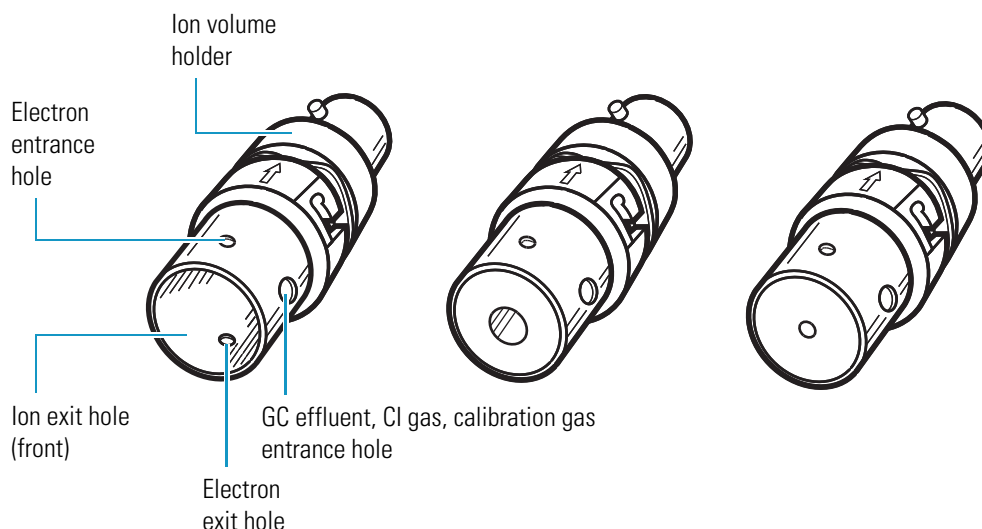
**Figure 15.** Ion source of the TSQ Quantum XLS Series mass spectrometer



The ion volume, located in the center of the ion source, is the site where electrons interact with sample or reagent gas molecules to form ions. Three exchangeable ion volumes and ion volume holders are available for use in the ion source. See [Figure 16](#). The choice of ion volume depends on the ionization mode. The open EI ion volume is open on the analyzer end, with a relatively large electron entrance hole. The closed EI ion volume has a smaller ion exit hole than the EI ion volume. This results in a higher pressure of analyte and greater sensitivity, but less dynamic range. The CI ion volume is closed on the analyzer end, except for a small ion exit hole and a relatively small electron entrance hole. In the CI mode, you must maintain a relatively high reagent gas pressure.

The ion source block holds the ion volume in its center. Samples are introduced from the GC capillary column through an aperture on the side of the ion source block and then into the ion volume. Gases for calibration or chemical ionization enter the ion volume through the transfer line.

**Figure 16.** EI (left), closed EI (center), and CI (right) ion volumes and holders



Cartridge heaters heat the ion source block and lens assemblies to minimize the rate at which deposits form on the ion source block, ion volume, and lens assemblies. The ion source block is also heated to assist in the rapid temperature equilibration of the ion source block and ion volume after the filament is turned on. In EI mode, the ion source is typically maintained at 150 °C to 220 °C. However, you can sometimes use lower or higher temperatures for certain applications. In the CI mode, the ion source is typically maintained at 180 °C to 200 °C. The ion source heater is feedback controlled.

The filament assembly, positioned in a recess at the top of the ion source block, contains the filament, reflector, and electron lens. The filament is a rhenium wire that is electrically heated to produce electrons by thermionic emission. The reflector repels electrons emitted by the filament away from the filament toward the ion volume. The filament and its reflector are maintained at a negative potential relative to the ion volume. The electron lens prevents positive ions from traveling up the electron beam. In turn, this prevents positive ions from leaving the ion volume through the electron entrance hole. The difference in potential between the filament and the ion volume determines the electron energy.

Two permanent magnets are held in a magnet yoke in the proper position above and below the ion source block. The permanent magnets collimate the electron beam and cause the beam to spiral through the ion volume. This ensures optimum ionization of the sample.

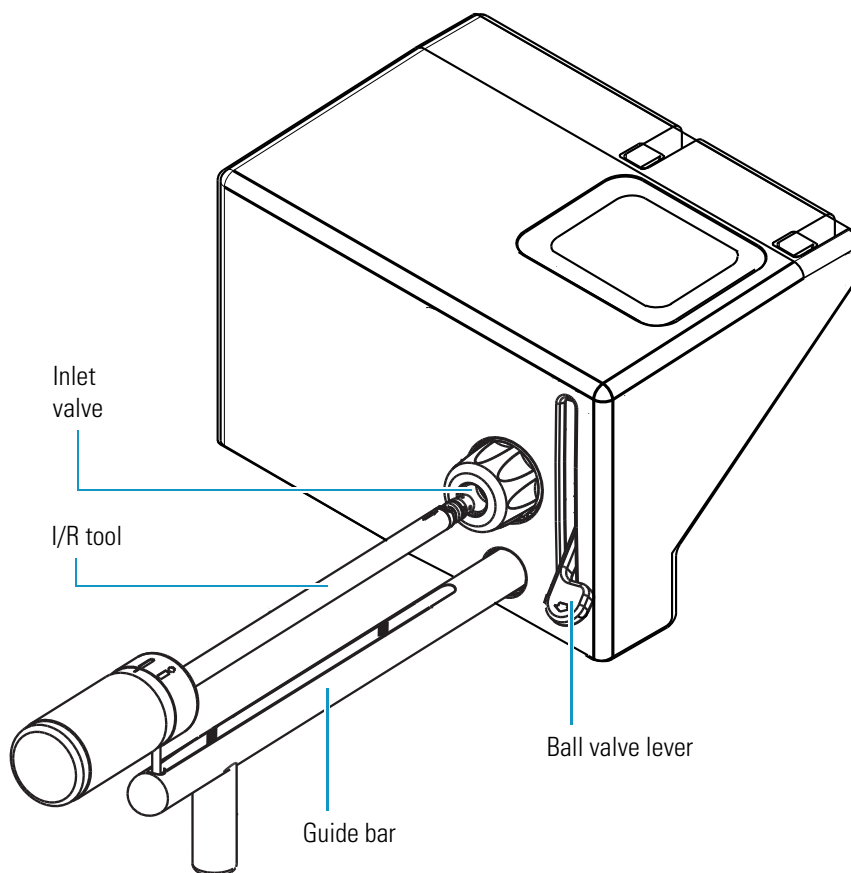
The ion source of the TSQ Quantum XLS Series mass spectrometer has two ion source lens assemblies, called the L1, L2, and L3 lens assembly and the heated Q0 quadrupole assembly. The lenses extract the ions formed in the ion source and transmit them to the ion optics. The lens L1 voltage is mass dependent. The rods of the heated Q0 quadrupole contact the rods of the Q0 quadrupole and share their rf and dc voltages.

## Inlet Valve

The inlet valve, which is attached to the front of the vacuum manifold, is a vacuum-sealed valve that allows you to change ion volumes or insert the direct exposure probe without venting the mass spectrometer to atmosphere. You use the insertion/removal (I/R) tool to insert or remove ion volumes. See [Figure 17](#). The forepump evacuates the inlet valve.

The ball valve is a ball with a hole in it, and it is located between the vacuum manifold and the inlet valve block. The ball valve is open when the hole in the ball is aligned with the opening between the vacuum manifold and the inlet valve. The ball valve lever opens and closes the ball valve. When the ball valve is closed, it prevents the vacuum manifold from venting to atmosphere.

**Figure 17.** Inlet valve, I/R tool, guide bar, and ball valve lever





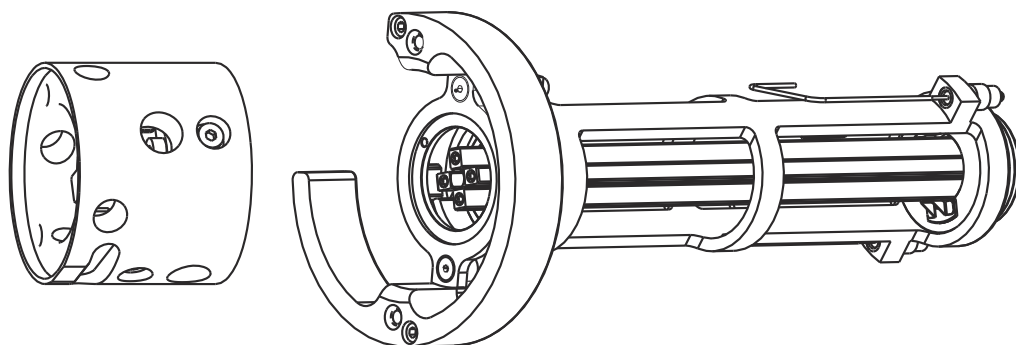
## Ion Optics

The ion optics focus the ions produced in the ion source and transmit them to the mass analyzer. The ion optics includes the Q0 quadrupole and lenses L11 and L12.

The Q0 quadrupole is a square array of square-profile rods that act as an ion transmission device. See [Figure 18](#). An rf voltage applied to the rods gives rise to an electric field that guides the ions along the axis of the quadrupole. The Q0 offset voltage increases the translational kinetic energy of ions emerging from the ion source.

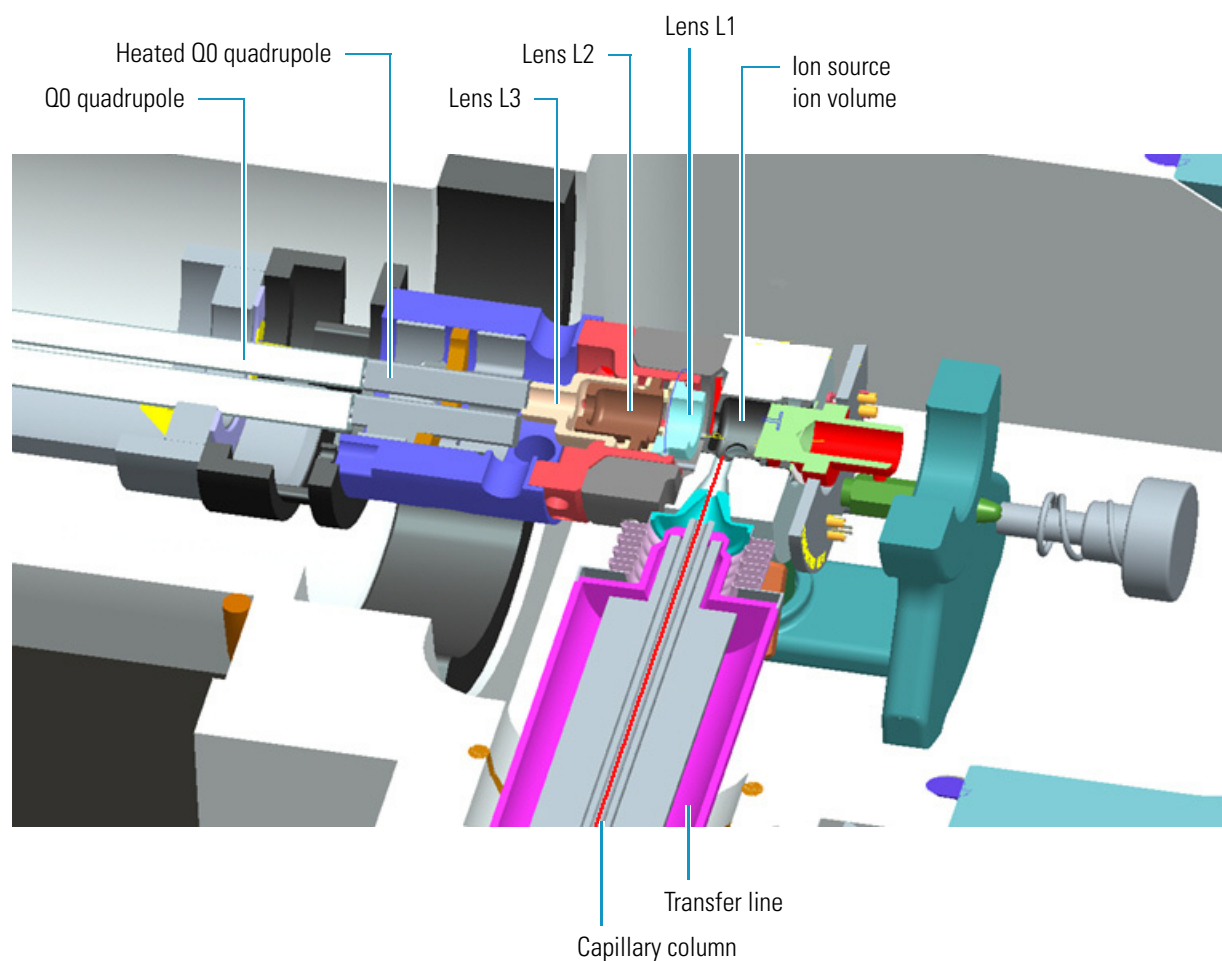
The Q0 quadrupole is split into two sections. See [Figure 18](#). The smaller, heated Q0 quadrupole assembly attaches to the ion source, which heats it with the cartridge heaters. The rods of the heated Q0 quadrupole make electrical contact with the rods of the larger Q0 quadrupole.

**Figure 18.** Heated Q0 quadrupole (left) and Q0 quadrupole (right)



[Figure 19](#) gives a cross-sectional view of the transfer line, ion source, heated Q0 quadrupole, and Q0 quadrupole.

**Figure 19.** Cross-sectional view of the transfer line, ion source, heated Q0 quadrupole, and Q0 quadrupole of the TSQ Quantum XLS Series mass spectrometer



The L11 and L12 lenses are metal disks with a circular hole in the center that the ion beam can pass through. Together they act as a two-element cone lens. You can apply an electrical potential to the lens to accelerate (or decelerate) ions as they approach the lens and focus the ion beam as it passes through the lens. The value ranges between 0 and  $\pm 300$  V. Lenses L11 and L12 also act as a vacuum baffle between the Q0 quadrupole chamber and the mass analyzer chamber.

## Mass Analyzer

The mass analyzer separates ions according to their mass-to-charge ratio and then passes them to the ion detection system. The mass analyzers on the TSQ Quantum XLS Series mass spectrometers consist of three quadrupole rod assemblies (Q1, Q2, and Q3) and three lens sets.

The mass analyzer is discussed in detail in the following subtopics:

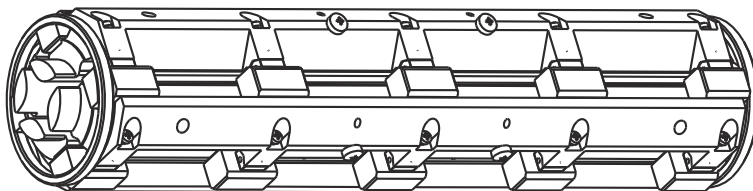
- [Quadrupole Rod Assemblies](#)
- [Rf and dc Fields Applied to the Quadrupoles](#)
- [Mass Analysis](#)
- [Collision Cell and CID Efficiency](#)
- [Quadrupole Offset Voltage](#)
- [Mass Analyzer Lenses](#)

### Quadrupole Rod Assemblies

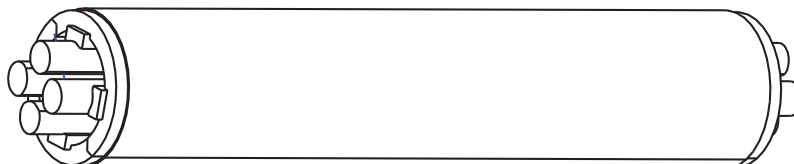
The three rod assemblies used in the mass spectrometer are numbered from the ion source end of the manifold and are designated Q1, Q2, and Q3. Q1 and Q3 are quadrupoles that enable high-resolution scans without signal loss.

Q1 and Q3 are square arrays of precision-machined and precision-aligned, true hyperbolic quadrupoles, called hyperquads (TSQ Quantum XLS Ultra mass spectrometer) or hyperbolic-profile round rods (TSQ Quantum XLS mass spectrometer). See [Figure 20](#) and [Figure 21](#). Quartz spacers act as electrical insulators between adjacent rods.

**Figure 20.** Q1 or Q3 hyperquad of the TSQ Quantum XLS Ultra mass spectrometer

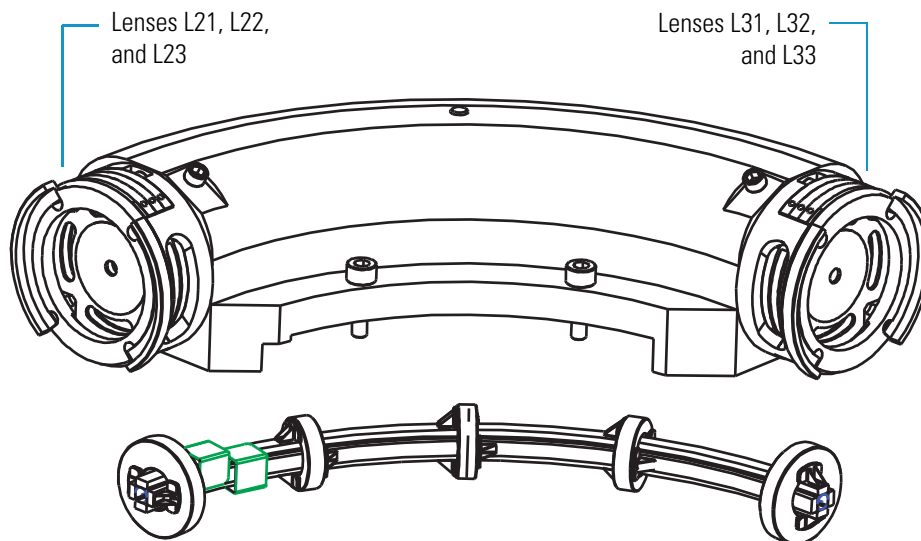


**Figure 21.** Q1 or Q3 quadrupole of the TSQ Quantum XLS mass spectrometer



Q2 is a square-profile quadrupole rod assembly. Q2 always acts as an ion transmission device. The Q2 quadrupole rods are bent through a 90-degree arc. In addition to reducing the footprint of the instrument, this prevents the transmission of unwanted neutral species to the detector and dramatically lowers the noise level in the data. Q2 has become synonymous with the term *collision cell*. Technically, the collision cell is the chamber that encloses Q2 where collision-induced dissociation can take place if the argon collision gas is present. See [Figure 22](#).

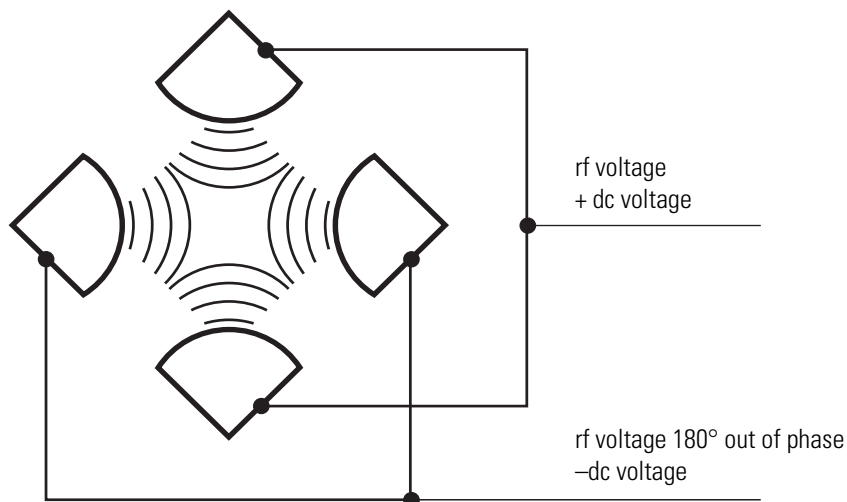
**Figure 22.** Collision cell, Q2 quadrupole, and lenses



### Rf and dc Fields Applied to the Quadrupoles

In a quadrupole rod assembly, because rods opposite each other in the array connect electrically, you can consider the four rods as two pairs of two rods each. Ac and dc voltages are applied to the rods and these voltages are ramped during the scan. Voltages of the same amplitude and sign are applied to the rods of each pair. However, the voltages applied to the different rod pairs are equal in amplitude but opposite in sign. See [Figure 23](#).

**Figure 23.** Polarity of the rf and dc voltages applied to the rods of the Q1 and Q3 mass analyzers



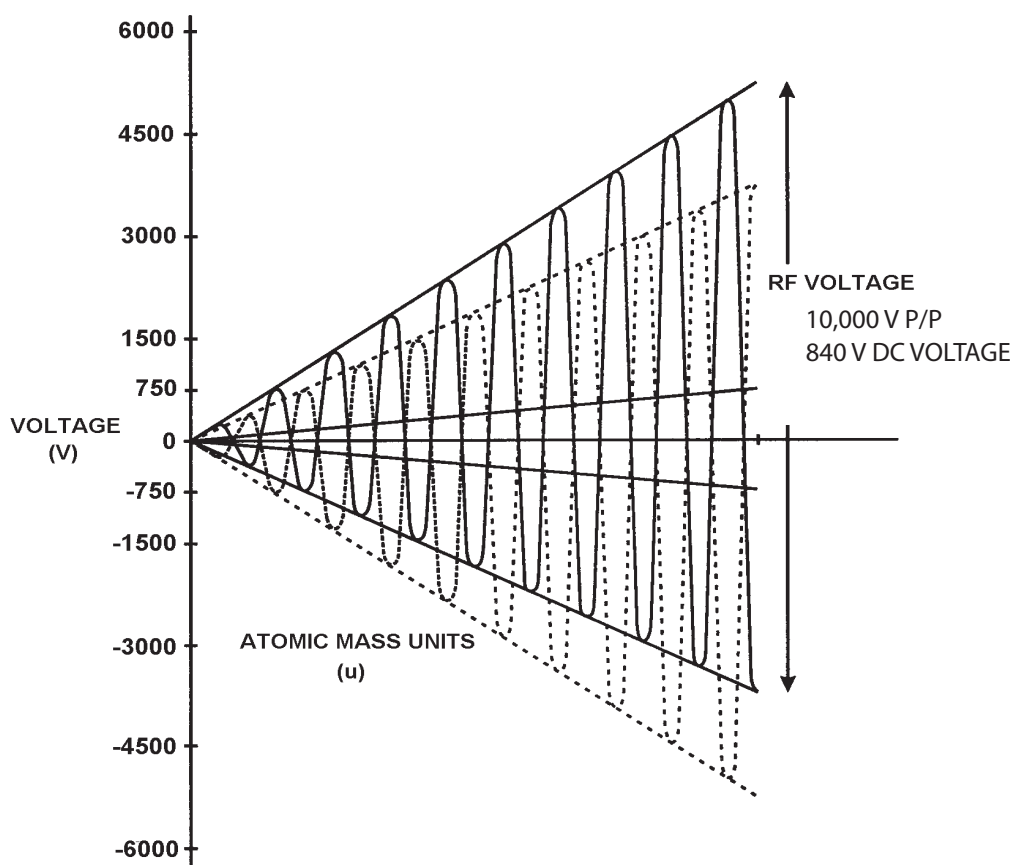
The ac voltage applied to the quadrupole rods is of constant frequency (1.123 MHz). The ac voltage applied to the rods varies from 0 to 10 000 V peak-to-peak, and the dc voltage varies from 0 to  $\pm 840$  V. Voltages of the same amplitude and sign are applied to each rod pair. However, the voltages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

Because the frequency of this ac voltage is in the radio frequency range, you refer to it as rf voltage. In [Figure 24](#), the solid line represents the combined rf and dc voltage applied to one rod pair, and the dashed line represents the combined rf and dc voltage applied to the other rod pair. The ratio of rf voltage to dc voltage determines the ability of the mass spectrometer to separate ions of different mass-to-charge ratios.

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

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

**Figure 24.** Magnitude of the rf and dc voltages applied to the rods of the Q1 and Q3 mass analyzers



## Mass Analysis

The Q1 and Q3 rods are charged with a variable ratio of rf voltage and dc voltage (Figure 24). These potentials give rise to an electrostatic field that gives stable oscillations to ions with a specific mass-to-charge ratio and unstable oscillations to all others.

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

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

The precision quadrupole rods of the mass spectrometer provide excellent sensitivity, peak shape, resolution, and high mass transmission.

## Collision Cell and CID Efficiency

In the MS/MS scan modes, the mass spectrometer applies a large voltage of opposite polarity to the Q2 rod pairs between scans, which empties the collision cell. This process ensures that no ions remain in the collision cell from scan to scan.

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

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

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

Three expressions convey the efficiency of the CID process:

- Collection efficiency
- Fragmentation efficiency
- Overall CID efficiency

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

**Fragmentation efficiency:** The fraction of the ion flux at the exit of the collision cell that results from fragmented ions. Fragmentation efficiency depends directly on the stability of the ion and indirectly on the mass of the ion. The more stable the ion, the less likely a given collision will fragment the ion. Typically, low mass ions require a higher collision energy to dissociate than high mass ions. To compensate for this, you can use the data system to specify a mass-dependent collision energy ramp.

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

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

## Quadrupole Offset Voltage

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

In general, for a given experiment, the mass spectrometer 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 mass spectrometer automatically computes the Q3 quadrupole offset voltage necessary 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 parent ions are formed) and Q2 (where they collide with collision gas). As the offset voltage on Q2 increases, the TKE of the parent ions also increases. As a result, increases in the Q2 offset voltage increase the energy of ion/Ar collisions. The collision energy is usually ramped downward with  $m/z$  to promote the fragmentation of low mass ions.

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



## Mass Analyzer Lenses

The TSQ Quantum XLS Series mass analyzers have three lens sets. See [Figure 22](#) on [page 32](#). Those between Q1 and Q2 are designated L21, L22, L23; those between Q2 and Q3 are designated L31, L32, L33; and the lens between Q3 and the ion detection system is designated the exit lens. All of the lenses have circular holes in their centers that the ion beam passes through.

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

The L2 $x$  lens set (between Q1 and Q2), where  $x=1,2,3$ , and the L3 $x$  lens set (between Q2 and Q3) serve these functions:

- To minimize the amount of collision gas that enters the mass analyzers (Q1 and Q3) from the collision cell (Q2). Lenses L22 and L21 on one side of Q2 and lenses L32 and L33 on the other side of Q2 act as baffles. (For high-mass transmission, be sure to maintain a low pressure in the mass analyzers.)
- To retain the collision gas. Lenses L23 and L3 form two of the walls of the collision cell, so they tend to hold the collision gas in the collision cell. The collision gas escapes, however, through the same lens holes that the ion beam passes through.
- To shield Q1 from the rf voltage applied to Q2 and vice versa (L2 $x$  lens set) and to shield Q3 from the rf voltage applied to Q2 and vice versa (L3 $x$  lens set).
- To focus the ion beam. The three lenses between Q1 and Q2 (and those between Q2 and Q3) together form a three-element aperture lens. The first and third lenses are generally set to similar or identical values and the central lens is set to a value different (either higher or lower) from the other two.

The voltage applied to each of the lenses can vary from about  $-300$  to  $+300$  V. Typically, however, the voltage applied to the first and third elements of the L2 $x$  lens set is somewhat greater than the quadrupole offset voltage applied to Q1. Because the Q1 quadrupole offset voltage is generally set to about  $\pm 5$  V (depending on the charge of the ions of interest), the voltage applied to lenses L21 and L23 is typically about  $-10$  V for positive ions and  $+10$  V for negative ions. The voltage applied to the central lens of the L2 $x$  lens set is typically about  $\pm 225$  V.

In the Q3MS scan mode, the voltage applied to the lenses of the L3 $x$  lens set is about the same as that applied to the corresponding lens in the L2 $x$  lens set. Note, however, that in the MS/MS scan modes, the voltage applied to the L3 $x$  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.

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

## Ion Detection System

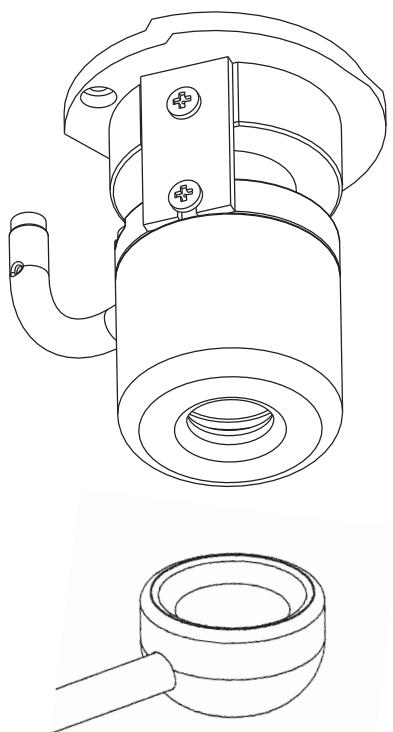
The TSQ Quantum XLS Series mass spectrometers are equipped with a high-sensitivity, off-axis ion detection system. See [Figure 25](#). This system produces a high signal-to-noise ratio and provides for voltage polarity switching between positive ion and negative ion modes of operation. The ion detection system includes a 10 kV conversion dynode and a channel electron multiplier. The ion detection system is located on the back of the vacuum manifold behind the mass analyzer.

The conversion dynode is a concave metal surface located at a right angle to the ion beam. The mass spectrometer applies to the conversion dynode a potential of +10 kV for negative ion detection or –10 kV for positive ion detection. When an ion strikes the surface of the conversion dynode, one or more secondary particles are produced. These secondary particles can include positive ions, negative ions, electrons, and neutrals. When positive ions strike a negatively charged conversion dynode, the secondary particles of interest are negative ions and electrons. When negative ions strike a positively charged conversion dynode, the secondary particles of interest are positive ions. The curved surface of the conversion dynode focuses these secondary particles and a voltage gradient accelerates the particles into the electron multiplier.

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

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

**Figure 25.** Ion detection system, showing the electron multiplier (top) and conversion dynode (bottom)



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

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

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

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

## Vacuum System and Inlet Gasses Hardware

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

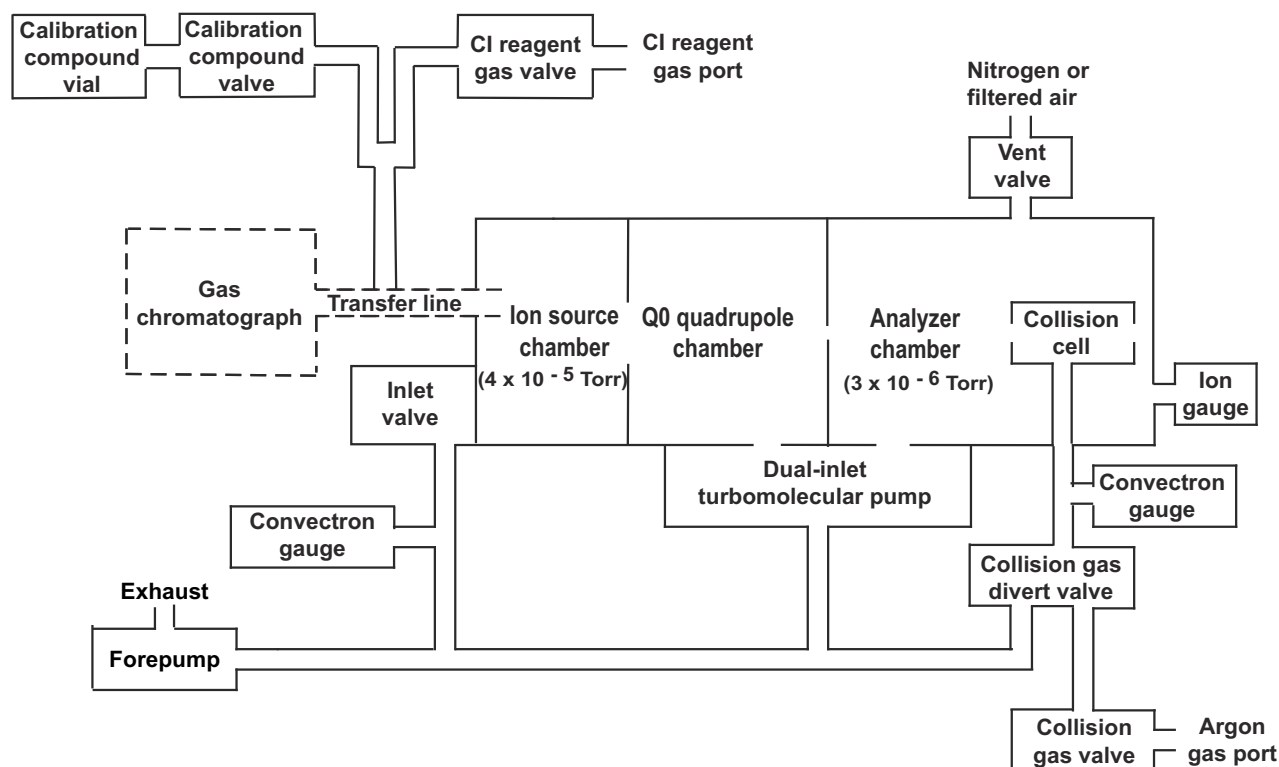
- Vacuum Manifold
- Turbomolecular Pump
- Forepump
- Convectron Gauges
- Ion Gauge

The inlet gasses hardware controls the flow of collision gas, CI reagent gas, calibration compound, and air (during venting) into the mass spectrometer. The hardware for the inlet gasses includes the following components:

- Vent Valve
- Collision Gas Flow Control Valves
- Calibration Compound and CI Reagent Gas Flow Control

Figure 26 shows a functional block diagram of the vacuum system and inlet gasses hardware.

**Figure 26.** Functional block diagram of the vacuum system and inlet gasses hardware



## Vacuum Manifold

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

The main vacuum manifold is divided into two chambers by a baffle. See [Figure 27](#). The high vacuum port of the turbomolecular pump evacuates the region inside the first chamber, called the analyzer region, to less than  $10^{-5}$  Torr. The turbomolecular pump then discharges into the forepump through the foreline.

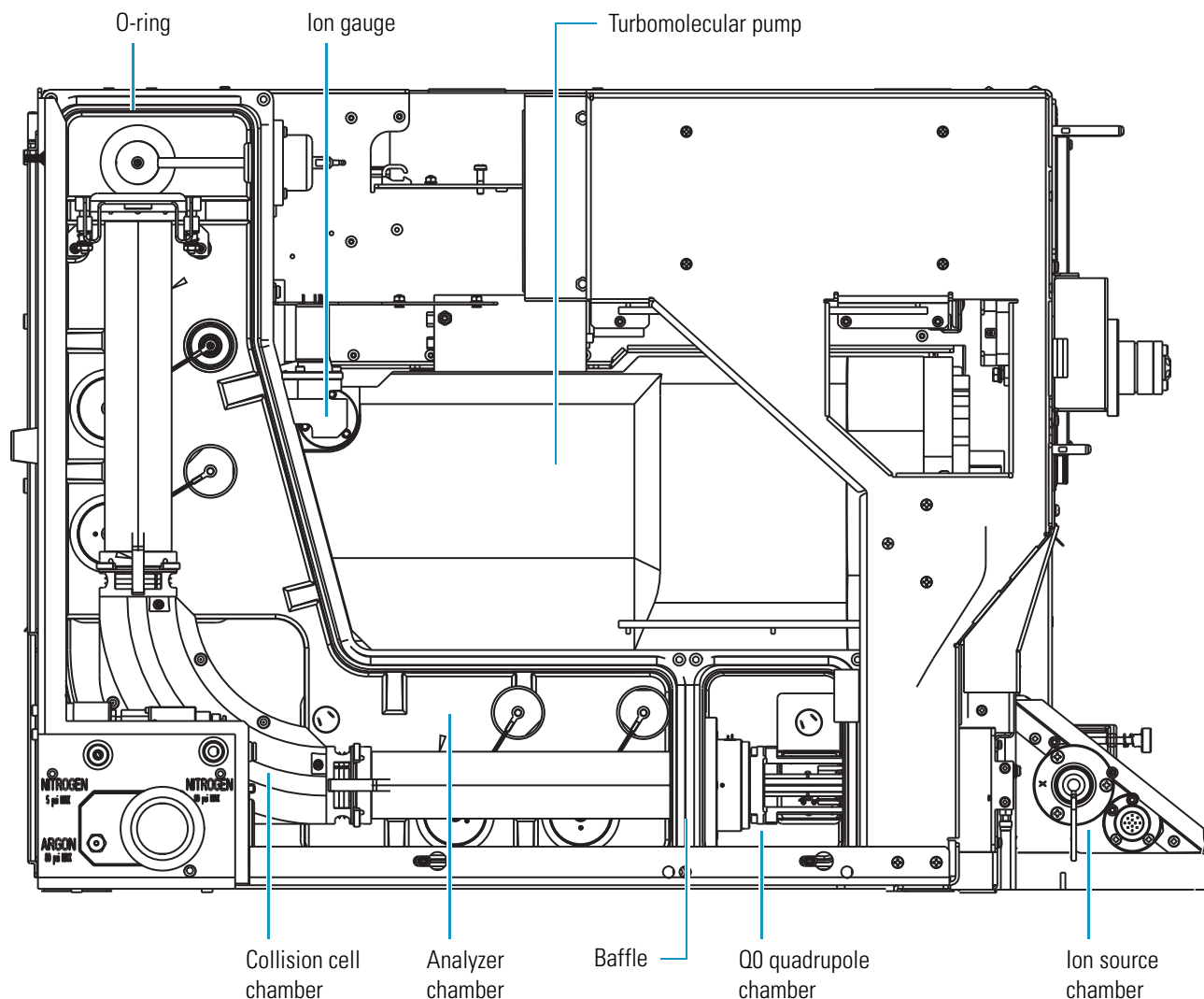
The region inside the second chamber, called the Q0 quadrupole region, is evacuated to 1 mTorr by the interstage port of the turbomolecular vacuum pump.

A second vacuum manifold houses the ion source, which is open to the Q0 quadrupole chamber. The interstage port of the turbomolecular pump also evacuates the ion source region.

When CID is turned on, the collision cell chamber, inside the analyzer chamber, has a user-controlled argon pressure of between 1 and 4 mTorr. The forepump evacuates the argon in the collision cell when CID is turned off.

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

**Figure 27.** Vacuum manifold (interior)



## Turbomolecular Pump

A Leybold TW220/150/15S double-inlet turbomolecular pump provides the vacuum for the ion source, Q0 quadrupole region, and analyzer region of the vacuum manifold. The turbomolecular pump mounts onto the top of the vacuum manifold ([Figure 27](#)).

The turbomolecular pump has two pumping inlets:

- A high-vacuum inlet at the top of the rotor stack, which evacuates the analyzer chamber
- An interstage inlet about halfway down the rotor stack, which evacuates the ion source and Q0 quadrupole chambers

The turbomolecular pump is controlled by a Leybold TDS controller and powered by a +24 V dc (250 W) power supply. The mass spectrometer circuit breaker switch and the vacuum service switch, but not the electronics service switch, turn power for the turbomolecular pump off and on. A fan draws air in from the front of the instrument to cool the pump.

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

## Forepump

An Edwards™ E2M30 forepump (or roughing pump) establishes the vacuum necessary for the proper operation of the turbomolecular pump. The forepump also evacuates the inlet valve and the collision cell. The pump has a maximum displacement of 650 L/min and maintains a minimum pressure of approximately 0.01 Torr (1 Pa).

The forepump is connected to the turbomolecular pump by a section of reinforced PVC tubing. The power cord of the forepump is plugged into the outlet labeled *Forepump* on the power panel (see [Figure 14](#) on [page 25](#)). This outlet supplies power to the pump and is controlled by the main power circuit breaker switch and vacuum service switch, not by the electronics service switch.



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

## Convectron Gauges

A Convectron gauge measures the pressure in the inlet valve and the foreline, which connects the turbomolecular pump and the forepump. A second Convectron gauge measures the pressure of argon collision gas in the collision cell.

The Convectron gauge uses a Wheatstone bridge with a temperature dependent resistor to measure pressure down to a fraction of a mTorr. The voltage present at the top of the bridge depends on how fast the resistor can radiate heat, which is related to the pressure. The pressure that the Convectron gauge measures is monitored by vacuum protection circuitry on the Source PCB, which in turn is monitored by the embedded computer on the System Control PCB. The vacuum protection circuitry detects whether the foreline pressure is too high for the proper operation of the turbomolecular pump.

## Ion Gauge

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

## Vent Valve

The vent valve, located in the area of Q2, allows the vacuum manifold to be vented with nitrogen, if you have a nitrogen cylinder connected, or else with air that has been filtered through a sintered nylon filter. The vent valve is a solenoid-operated valve, which is controlled by the Vent Delay PCB. When the solenoid is energized, the vent valve closes. If the power fails or the main power circuit breaker is placed in the Off (O) position, a 4-farad capacitor located in the Power Entry Module keeps the solenoid in the closed position for several minutes. If power is not restored in this time, then the solenoid opens and the system is vented with nitrogen or filtered air. The vent valve closes after power is restored to the mass spectrometer.

## Collision Gas Flow Control Valves

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

Ions enter the Q2 collision cell, collide with the argon collision gas, and then, because of the collision, dissociate into smaller fragments. See [“Collision Cell and CID Efficiency” on page 35](#).

Argon enters the mass spectrometer through a 1/8 in. port on the left side of the mass spectrometer.

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

## Calibration Compound and CI Reagent Gas Flow Control

The calibration compound gas flow control valve controls the flow of calibration compound gas into the ion source, via the transfer line. The calibration gas flow can be either high or low. Normally, you use low flow, but high flow might be necessary for negative ion CI calibration.

The CI gas flow control valve controls the flow of chemical ionization reagent gas into the ion source, via the transfer line. The maximum CI gas flow rate is about 4 mL/min, depending on the gas.



## Electronic Assemblies

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

The Power Entry Module provides the following:

- Mass spectrometer power control
- A contact closure interface
- Vent valve control
- An Ethernet 100 base-T connection from the System Control PCB to the data system PC
- A mechanical pump failure protection circuit (linked to vent valve control)
- A system reset button
- Status LEDs
- Service ports

The right-side power panel, shown in [Figure 14](#) on [page 25](#), is part of the Power Entry Module.

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

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

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

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

The rf voltage generation electronic assemblies produce the Q0, Q1, Q2, and Q3 rf voltages that enable ion transmission and mass analysis. All rf voltages are controlled by the Analyzer Control PCB and the System Control PCB.

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

The rf voltage generation electronic assemblies include the following components:

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

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

The ion detection system electronic assemblies include the following:

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

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

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

## Data System

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

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

## Computer Hardware

These are the major features of the data system computer:

- Intel™ Pentium™, Core™ 2 Duo, or Xeon™ processor
- High-capacity hard disk drive
- Primary Ethernet port (data system to mass spectrometer)
- Secondary Ethernet port (data system to local area network)
- High-performance video graphics card
- CDRW drive
- DVD drive
- 1280 × 1024 resolution color monitor
- Keyboard and mouse

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

## Data System/Mass Spectrometer/GC Interface

The data system computer contains a 100 base-T Ethernet adapter (called the primary Ethernet adapter) that is dedicated to data system/mass spectrometer/GC communication. This primary Ethernet adapter communicates with the mass spectrometer and GC modules via a 10/100 base-T Ethernet switch. The Ethernet adapter on the mass spectrometer resides on the System Control PCB. A twisted pair, Ethernet cable connects the primary Ethernet adapter of the data system to the Ethernet switch, which is connected to the Ethernet connector on the power panel of the mass spectrometer and to the GC.

## Data System/Local Area Network Interface

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



## System Shutdown, Startup, and Reset

Many maintenance procedures for the TSQ Quantum XLS Series systems require that the mass spectrometer be shut down completely. In addition, you can place the mass spectrometer in Standby mode if you plan to not use the system for 12 hours or more.

### Contents

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

## Shutting Down the System in an Emergency

You can turn off all power to the mass spectrometer, gas chromatograph, and autosampler by pressing the System Power Off button, located on the front of the electronics module (see [Figure 28](#)), or the main power circuit breaker, located on the back of the electronics module (see [Figure 29](#)). You can turn on the system power only with the main power circuit breaker on the back of the electronics module and not the System Power Off switch.

### ❖ To turn off the mass spectrometer in an emergency



**CAUTION** Press the System Power Off button located on the front of the electronics module. See [Figure 28](#). The System Power Off button turns off all power to the mass spectrometer (including the vacuum pumps), gas chromatograph, and autosampler. Although removing power abruptly does not harm components within the system, under normal conditions do not shut down the system using the System Power Off button. For the recommended procedure, see “[Shutting Down the System Completely](#)” on [page 51](#).

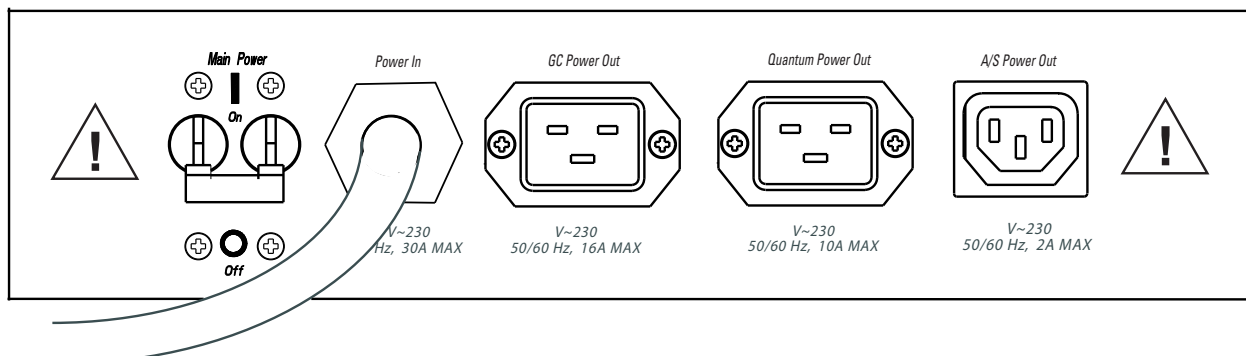
### 3 System Shutdown, Startup, and Reset

Shutting Down the System in an Emergency

**Figure 28.** System Power Off button on the front of the electronics module



**Figure 29.** Power panel on the back of the electronics module



## Placing the System in Standby Mode

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

### ❖ To place the system in Standby mode



1. Wait until data acquisition, if any, is complete.
2. From the TSQ EZ Tune window, choose **Control > Standby** (or click the **On/Standby** button) to put the mass spectrometer in standby.

When you choose Control > Standby, the TSQ Quantum XLS Series system turns off the electron multiplier, the conversion dynode, the ion source filament and lenses (but not the heater), and the mass analyzer and ion optics rf voltages. See [Table 4 on page 59](#) for the On/Off status of mass spectrometer components when the mass spectrometer is in Standby mode. The System LED on the front panel of the mass spectrometer illuminates yellow when the system is in standby.

3. Leave the mass spectrometer power on.
4. Leave the GC power on with column flow.
5. Leave the autosampler power on.
6. Leave the data system power on.

## Shutting Down the System Completely

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

### ❖ To shut down the system completely

1. Cool the GC oven, injector, transfer line, and ion source:
  - GC oven: **30 °C** (from the Oven page of the TRACE GC Ultra Setup view)
  - Injector: **off** (from the SSL page of the TRACE GC Ultra Setup view)
  - Transfer line: **off** (from the Aux Zones page of the TRACE GC Ultra Setup view)
  - Ion source: **30 °C** (from the TSQ EZ Tune window)

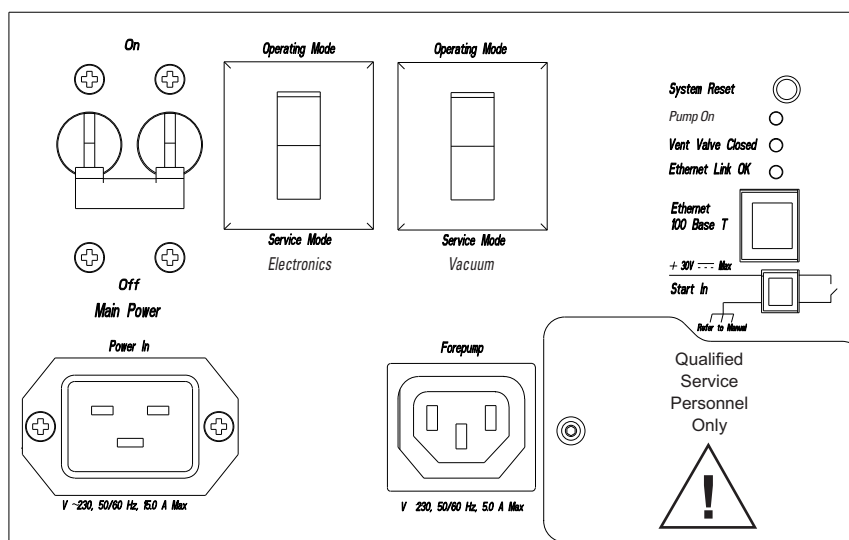
**Note** If you do not plan to change the column or perform maintenance on the gas chromatograph, you do not have to lower the injector temperature.

### 3 System Shutdown, Startup, and Reset

#### Shutting Down the System Completely

2. From the TSQ EZ Tune window, choose **Control > Standby** (or click the **On/Standby** button) to put the mass spectrometer in standby.
3. Place the electronics service switch, located on the right-side power panel, in the Service Mode. See Figure 30.

**Figure 30.** Right-side power panel of the mass spectrometer



4. Place the vacuum service switch, located on the right-side power panel, in the Service Mode position.
5. Place the mass spectrometer main power circuit breaker switch, located on the right-side power panel, in the Off position. When you place the main power circuit breaker switch in the Off position, the following occurs:
  - All power to the mass spectrometer is turned off. (All LEDs on the front panel of the mass spectrometer are off.)
  - A capacitor on the Vent Delay PCB provides power to the vent valve for two to four minutes (to allow the turbomolecular pump to spin down). After the capacitor discharges, power to the vent valve solenoid shuts off. When power to the vent valve solenoid shuts off, the vent valve opens and the vacuum manifold vents with nitrogen, if you have a nitrogen cylinder connected, or else with filtered air.
  - After about two minutes, the pressure of the vacuum manifold reaches atmospheric pressure.
6. Unplug the power cord for the mass spectrometer.



**WARNING Burn Hazard.** Allow heated components to cool before servicing them.



**Note** If you plan to perform routine or preventive system maintenance on the mass spectrometer only, you can leave the argon, data system, GC, and autosampler on. In this case, the shutdown procedure is complete. However, if you do not plan to operate your system for an extended period of time, Thermo Fisher Scientific recommends that you turn off the GC, data system, and autosampler as described in [step 7](#) through [step 12](#) below.

7. Turn off the GC. Follow the procedure described in the manual that came with the GC.
8. Turn off the autosampler by using the main power on/off switch.
9. Press the System Power Off button ([Figure 28](#) on [page 50](#)) to remove all power from the TSQ Quantum XLS Series system.
10. If you do not plan to use the system for an extended period, turn off the argon collision gas supply at the tank.
11. Turn off the data system:
  - a. Choose **Start > Shut Down** from the Windows task bar. The Shut Down Windows dialog box appears.
  - b. To start the Windows shutdown procedure, select **Shut down** and click **OK**.
12. Turn off the (optional) printer by using the on/off switch.



**WARNING Burn Hazard.** The ion source, GC oven, injector, and transfer line are hot. Allow them to cool to room temperature before touching them.

## Starting Up the System after a Complete Shutdown

Starting the TSQ Quantum XLS Series system after it has been shut down requires completion of these tasks:

- [Restoring Power to the TSQ Quantum XLS Series System](#)
- [Starting Up the GC](#)
- [Starting Up the Data System](#)
- [Starting Up the Mass Spectrometer](#)
- [Starting Up the Autosampler](#) (autosampler is optional)
- [Setting Up Conditions for Operation](#)

## Restoring Power to the TSQ Quantum XLS Series System

To restore power to the TSQ Quantum XLS Series system, place the main power circuit breaker, located on the back of the electronics module ([Figure 29](#) on [page 50](#)), in the On position.

## Starting Up the GC

To start the gas chromatograph (GC), follow the startup procedure described in the manual that came with the GC. Verify that the gas chromatograph is on and there is carrier gas flowing through the column into the mass spectrometer.

## Starting Up the Data System

### ❖ To start the data system

1. Turn on the monitor, computer, and printer.
2. Observe the Windows startup procedure on the monitor. At the prompt, press CTRL+ALT+DELETE.
3. Click **OK** or enter your password (if you have one) in the Logon Information dialog box.

## Starting Up the Mass Spectrometer

### ❖ To start the mass spectrometer



**CAUTION** Do not turn on the mass spectrometer without GC capillary column flow. Air can damage the GC column and contaminate the ion source.

1. Turn on the flow of argon at the tank if it is off.

**IMPORTANT** Make sure that the data system is running before you start the mass spectrometer. The mass spectrometer can not operate until it receives software from the data system.

2. Make sure that the mass spectrometer main power circuit breaker switch, on the right side power panel ([Figure 30](#) on [page 52](#)), is in the Off (O) position, and the electronics service switch and the vacuum service switch are both in the Service Mode position.
3. Plug in the power cord for the mass spectrometer.

4. Place the mass spectrometer main power circuit breaker switch in the On (I) position.  
Placing the main power circuit breaker switch in the On (I) position supplies power to those mass spectrometer components that are not affected by the vacuum service switch and the electronics service switch.
5. Place the vacuum service switch in the Operational position.
6. Place the electronics service switch in the Operational position. The following occurs:
  - The Power LED on the mass spectrometer front panel illuminates green to indicate that power is provided to the mass spectrometer electronics. (The electron multiplier, conversion dynode, ion source, and mass analyzer and ion optics rf voltages remain off.) See [Figure 31](#) and [Figure 32](#).
  - The embedded computer restarts. After several seconds the Communication LED on the front panel illuminates yellow to indicate that the data system and the mass spectrometer have started to establish a communication link.
  - After several more seconds, the Communication LED illuminates green to indicate that the data system and the mass spectrometer have established a communication link. Software for the operation of the mass spectrometer is then transferred from the data system to the mass spectrometer.
  - After three minutes, the System LED illuminates yellow to indicate that the software transfer from the data system to the mass spectrometer is complete and that the instrument is in standby.
  - The Vacuum LED on the front panel of the mass spectrometer remains off until the turbomolecular pump reaches 80 percent of its operational speed of 750 Hz. At this time the ion gauge is turned on and the Vacuum LED illuminates yellow. The Vacuum LED illuminates green, and the high voltage can be turned on, only if the pressure in the mass analyzer region of the vacuum manifold is less than the appropriate value listed in [Table 3](#).

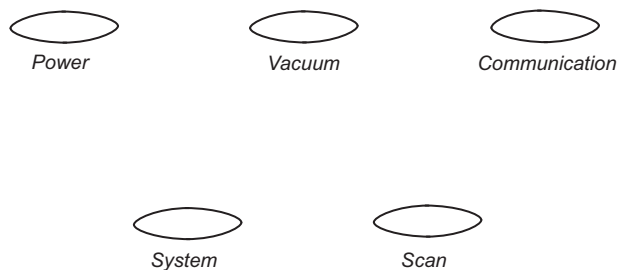
**Table 3.** Maximum allowed pressure to turn on high voltage

Carrier gas	Ar collision gas	Maximum pressure (Torr)
He	Off	$8 \times 10^{-6}$
He	On	$5 \times 10^{-5}$

**Figure 31.** Front panel LEDs of the TSQ Quantum XLS Ultra mass spectrometer



**Figure 32.** Front panel LEDs of the TSQ Quantum XLS mass spectrometer



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

## Starting Up the Autosampler

To start the autosampler, place the main power switch on the autosampler in the On position. If necessary, configure the autosampler.

For procedures for placing sample vials, preparing solvent and waste bottles, installing syringes, and so on, refer to the manual that came with the autosampler.

## Setting Up Conditions for Operation

### ❖ To set up your TSQ Quantum XLS Series mass spectrometer for operation

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

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

3. In the TSQ EZ Tune window, choose **View > Instrument Status**. Look at the Status view. Check that the pressure measured by the ion gauge is below about  $3 \times 10^{-6}$  Torr with the collision gas turned off.

**Note** You do not need to calibrate and tune the mass spectrometer each time you restart the TSQ Quantum XLS Series system. To tune and calibrate the mass spectrometer, see [Chapter 4, “Tuning and Calibrating.”](#)

## Resetting the Mass Spectrometer

If communication between the mass spectrometer and data system computer is lost, it might be necessary to reset the mass spectrometer using the System Reset button on the right-side power panel. Pressing the System Reset button creates an interrupt in the embedded computer. This causes the embedded computer to restart in a known (default) state. For the location of the System Reset button, see [Figure 30](#) on [page 52](#).

The procedure given here assumes that the mass spectrometer and data system computer are both powered on and operational. If the mass spectrometer, data system computer, or both are off, go to [“Starting Up the System after a Complete Shutdown”](#) on [page 53](#).

### ❖ To reset the mass spectrometer

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

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

## Resetting the Data System

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

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

1. Choose **Start > Shut Down** from the Windows task bar. The Shut Down Windows dialog box appears.
2. Select **Restart** and click **OK** to start the Windows shutdown and restart procedure.
3. Observe the Windows shutdown and restart procedure on the monitor. At the prompt, press CTRL+ALT+DELETE.
4. Click **OK** or enter your password (if you have one) in the Logon Information dialog box.

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



## Turning Off Selected Mass Spectrometer Components

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

- Turn off individual mass spectrometer components from the TSQ EZ Tune window. Turning off individual mass spectrometer components might be necessary when you are troubleshooting or when you are running certain diagnostic procedures.
- Place the mass spectrometer in Standby mode. Standby is the normal state for the mass spectrometer when it is not in use. To place the mass spectrometer in standby, choose **Control > Standby** (or toggle the On/Standby button) from the TSQ EZ Tune window.
- Place the mass spectrometer in the Off condition. The Off condition is similar to Standby, except all high voltage components of the mass spectrometer are turned off. To place the mass spectrometer in the Off condition, choose **Control > Off** from the TSQ EZ Tune window.
- Place the electronics service switch in the Service Mode position. The electronics service switch turns off all components in the mass spectrometer other than the +24 V power supply, forepump, turbomolecular pump, Vent Delay PCB, and fans.
- Place the vacuum service switch in the Service Mode position. The vacuum service switch turns off all vacuum system components, including the +24 V power supply, forepump, turbomolecular pump, Vent Delay PCB, and fans.
- Place the right-side power panel circuit breaker switch in the Off position. Placing the right-side power panel circuit breaker switch in the Off position removes all power to the mass spectrometer, including the vacuum system.
- Press the System Power Off button. Pressing the System Power Off button removes all power to the mass spectrometer, gas chromatograph, and autosampler.

[Table 4](#) summarizes the on/off status of mass spectrometer components, voltages, and gas flows.

**Table 4.** On/Off status of mass spectrometer components and voltages

Mass spectrometer component	Standby 	Off 	Electronics service switch in Service Mode position	Vacuum service switch in Service Mode position	MS Main power circuit breaker switch in Off position
Electron multiplier	Off	Off	Off	Off	Off
Conversion dynode	Off	Off	Off	Off	Off
Mass analyzer rf voltage	Off	Off	Off	Off	Off
Mass analyzer dc offset voltage	Off	Off	Off	Off	Off
Q0 ion optics rf voltage	Off	Off	Off	Off	Off
Q0 ion optics dc offset voltage	Off	Off	Off	Off	Off
Ion source filament	Off	Off	Off	Off	Off
Ion source heater	<b>On</b>	Off	Off	Off	Off
Ion source lenses	Off	Off	Off	Off	Off
Argon collision gas	Off	Off	Off	Off	Off
Vent valve	Closed	Closed	Closed	<b>Open</b> (after 2 to 4 min)	<b>Open</b> (after 2 to 4 min)
Turbomolecular pump	<b>On</b>	<b>On</b>	<b>On</b>	Off	Off
Forepump	<b>On</b>	<b>On</b>	<b>On</b>	Off	Off
Vent Delay PCB	<b>On</b>	<b>On</b>	<b>On</b>	<b>On</b>	Off
Embedded computer	<b>On</b>	<b>On</b>	Off	<b>On</b>	Off
Turbomolecular pump controller	<b>On</b>	<b>On</b>	<b>On</b>	Off	Off
Power supply, electron multiplier, and conversion dynode	Off	Off	Off	<b>On</b>	Off
Power supply, 8 kV	Off	Off	Off	<b>On</b>	Off
PS1 power supply, +24 V	<b>On</b>	<b>On</b>	<b>On</b>	Off	Off
PS2 power supply, +5, ±15, ±24 V dc	<b>On</b>	<b>On</b>	Off	Off	Off
PS3 power supply, +36, –28 V dc	<b>On</b>	<b>On</b>	Off	Off	Off
Fan, turbomolecular pump	<b>On</b>	<b>On</b>	<b>On</b>	Off	Off
Fan, above manifold	<b>On</b>	<b>On</b>	<b>On</b>	Off	Off
Fan, center wall	<b>On</b>	<b>On</b>	<b>On</b>	Off	Off
Convectron gauge, foreline	<b>On</b>	<b>On</b>	<b>On</b>	<b>On</b>	Off
Convectron gauge, collision cell	<b>On</b>	<b>On</b>	Off	<b>On</b>	Off
Ion gauge	<b>On</b>	<b>On</b>	Off	Off	Off





## Tuning and Calibrating

Tune parameters are instrument parameters that affect the intensity of the ion signal. Calibration parameters are instrument parameters that affect the mass accuracy and resolution of the mass spectrum. Tuning and calibrating the TSQ Quantum XLS Series mass spectrometer automatically with TSQ EZ Tune uses perfluorotributylamine (FC-43) as the tuning and calibration compound. FC-43 resides in a vial inside the mass spectrometer.

### Contents

- [Displaying the FC-43 Mass Spectrum](#)
- [Running Auto Tune and Calibration](#)
- [Saving the Tune and Calibration Report](#)
- [Running Maintenance Tune](#)
- [Creating a Quality Control \(QC\) Tune Report](#)

Record the ion signal intensity of FC-43 (see [Figure 34](#)) just after you tune and calibrate the mass spectrometer. Periodically check the FC-43 ion signal. Retune and calibrate the mass spectrometer if the FC-43 ion signal falls below 50 percent of the tuned value. Also, retune and calibrate after switching between EI and CI modes or between positive and negative polarity modes.

**Note** You might need to calibrate more often if you operate in H-SRM mode (as opposed to SRM mode only).

[Table 5](#) lists typical peaks that are observed in the FC-43 mass spectrum in EI, positive polarity mode.

**Table 5.** Typically observed FC-43 peaks in EI, positive polarity mode

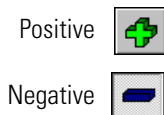
<i>m/z</i> 69	<i>m/z</i> 314
<i>m/z</i> 100	<i>m/z</i> 352
<i>m/z</i> 114	<i>m/z</i> 402
<i>m/z</i> 119	<i>m/z</i> 414
<i>m/z</i> 131	<i>m/z</i> 464
<i>m/z</i> 169	<i>m/z</i> 502
<i>m/z</i> 219	<i>m/z</i> 614
<i>m/z</i> 264	

## Displaying the FC-43 Mass Spectrum

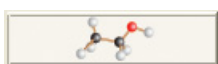
The first step in tuning and calibrating the mass spectrometer is to display the FC-43 mass spectrum.

### ❖ To display the FC-43 mass spectrum

1. Choose **Start > Programs > Thermo Instruments > TSQ > TSQ Tune** to open the EZ Tune window.
2. Choose a polarity mode. In this example the mass spectrometer is in positive polarity mode. If necessary, click the polarity button.

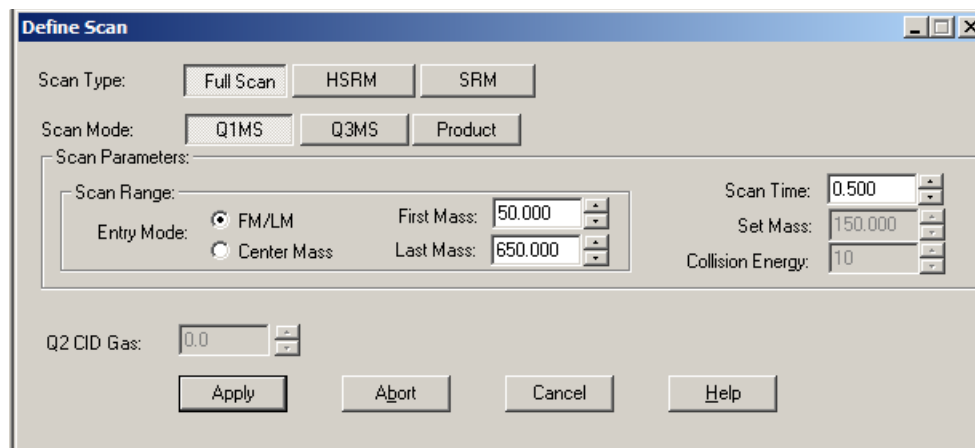


**Note** For EI negative polarity mode, you might have to set the calibration gas flow to high.



3. Click the **Define Scan** button to display the Define Scan dialog box. See [Figure 33](#).
4. In the Define Scan dialog box, select or enter the following settings:
  - Scan type: **Full Scan**
  - Scan mode: **Q1MS**
  - Scan range entry mode: **FM/LM**
  - First mass: **50**
  - Last mass: **650**
  - Scan time: **0.500**

**Figure 33.** Define Scan dialog box



5. Click **Apply** to apply the settings.

Cal Gas Off

Cal Gas On

Filament Off

Filament On

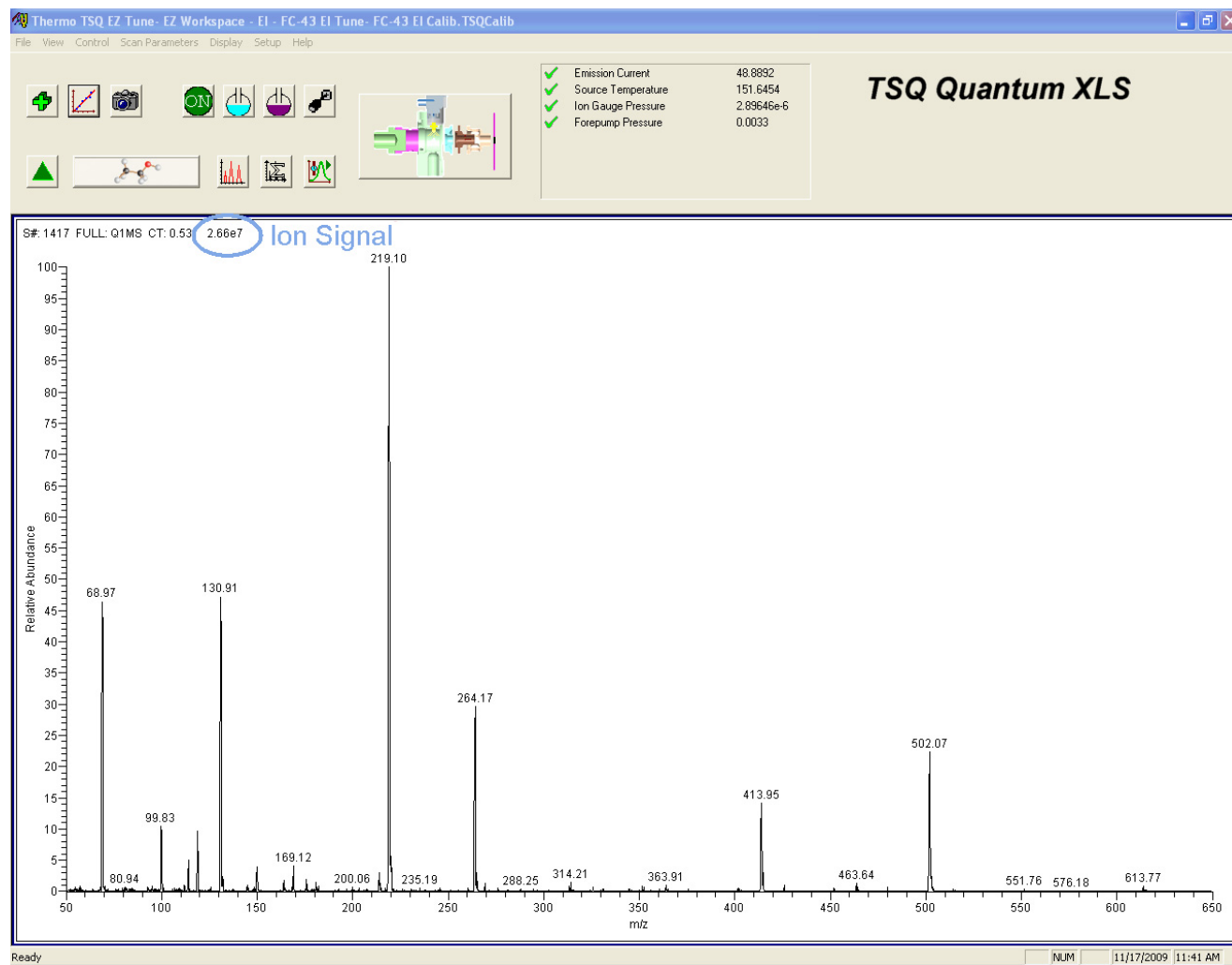
6. To turn on the flow of calibration gas into the ion source, click the **Calibration Gas** button in the EZ Tune toolbar.

7. To turn on the filament, click the **Filament** button in the EZ Tune toolbar to turn on the filament.

8. Choose **Control > On** to start the mass spectrometer scanning.

9. Observe the mass spectrum. If your mass spectrum looks very different from the one in [Figure 34](#), see “Diagnostics and Troubleshooting” on [page 113](#).

**Figure 34.** EZ Tune EZ Workspace, showing the FC-43 mass spectrum in EI, positive polarity mode before tuning and calibrating



## Running Auto Tune and Calibration

Run the tune and calibration procedure after you obtain a good FC-43 ion signal.

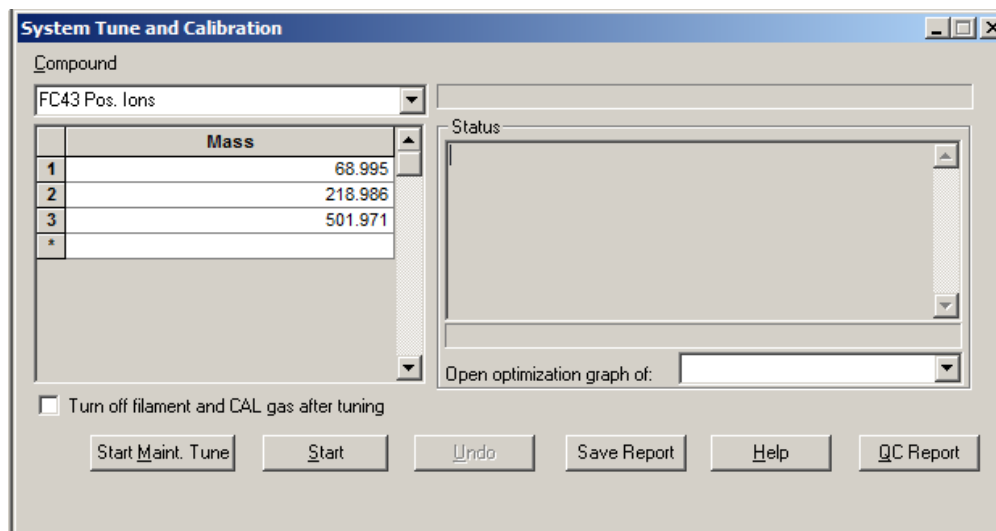
❖ **To tune and calibrate your mass spectrometer automatically in the EI, positive ion mode**

1. Display the FC-43 positive ion mass spectrum as described in the previous section.



2. Click the **System Tune and Calibration** button (or choose **Setup > System Tune and Calibration**) to display the System Tune and Calibration dialog box (see [Figure 35](#)).

**Figure 35.** System Tune and Calibration dialog box



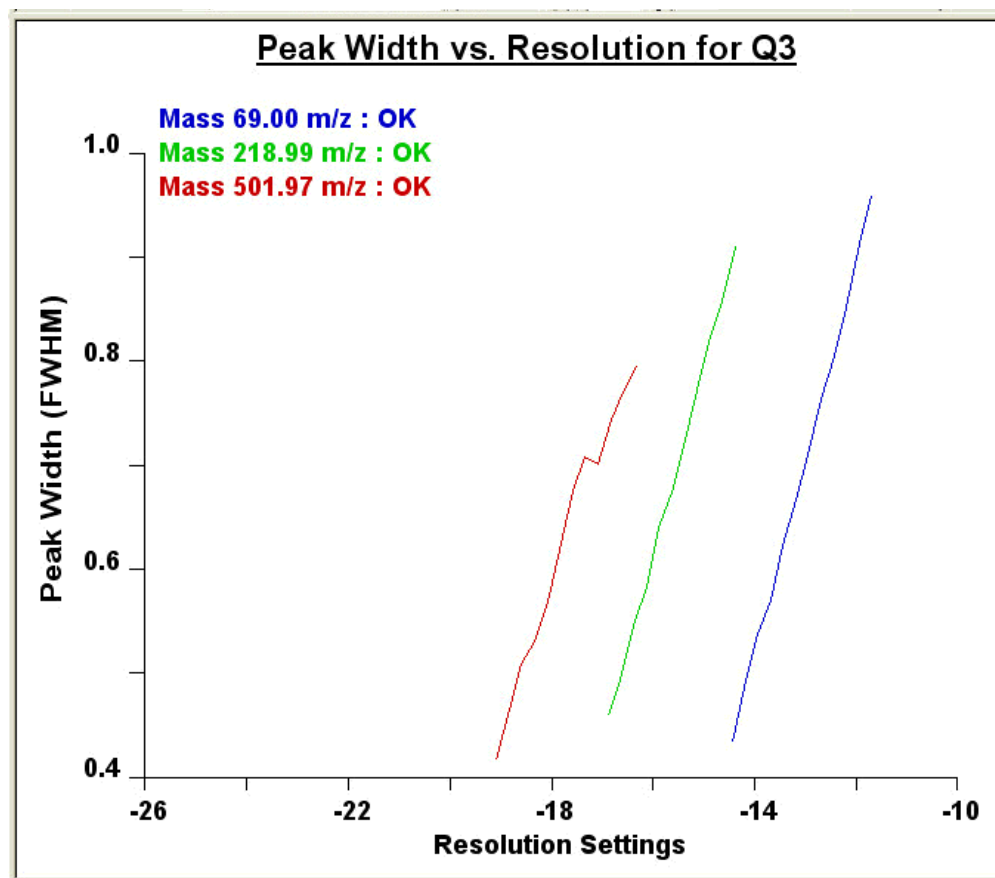
3. In the Compound list, select **FC43 Pos. Ions**. This automatically selects the positively charged FC-43 ions to be used for automatic tuning and calibrating.
4. To start the automatic tuning and calibration procedure, click **Start**.

The Status box displays real-time messages about the system tune and calibration so that you can monitor the progress of each subprocedure. After a subprocedure is complete, the system reports the result (for example, whether it passed or failed). At the end of the entire procedure, it displays a summary.

- If errors occur during the automatic tuning and calibration procedure, go to [step 5](#).
  - If the automatic tuning and calibration procedure finishes without errors, go to [step 6](#).
5. If errors occur during the automatic tuning and calibration procedure, restore the previous mass spectrometer device settings and perform the tuning and calibration procedure again by completing the following steps:
    - a. To restore the prior tuning and calibration settings, click **Undo**.
    - b. To reload the prior tuning and calibration settings to the mass spectrometer, click **Accept**.
    - c. Troubleshoot and correct the problem that caused the tuning and calibration procedure to fail. See “[Tuning Issues](#)” on [page 128](#).
    - d. Go to [step 4](#) and restart the tuning and calibration procedure.

[Figure 36](#) shows a typical parameter optimization plot.

**Figure 36.** Typical parameter optimization plot



6. To accept the results of the tuning and calibration procedure, click **Accept**.

After you accept the results of the tuning and calibration procedure, a message box prompts you to copy the positive ion tuning and calibration settings to the negative ion mode.

- If you have already tuned and calibrated the instrument successfully in the negative ion mode, click **No**. (Do not copy the positive ion mode parameters to the negative ion mode.)
- If you have not tuned and calibrated the instrument in the negative ion mode, click **Yes**.

**Note** If you intend to perform high-sensitivity, negative-ion mass spectrum analysis, Thermo Fisher Scientific recommends that you also perform a full tune and calibration of the instrument in the negative ion mode.

7. Save the calibration file as follows:
  - a. Click **Save Calib. As** to open the Save Calibration File dialog box.
  - b. In the File Name box, enter a name for your calibration file.
  - c. Click **Save** to save the calibration file. The Save As dialog box appears.
8. Save the tune method file as follows:
  - a. In the File Name box, enter a name for your tune method file.
  - b. Click **Save** to save the tune method file.

The mass spectrometer is now tuned and calibrated in the EI positive ion mode.

## Saving the Tune and Calibration Report

You can save the information that appears in the Status box and in the parameter optimization plots as a PDF file. Examples of status information and parameter optimization plots from the tune and calibration report follow in [Figure 37](#), and [Figure 38](#) on [page 69](#).

**Figure 37.** Tune and calibration report, status page

```
Results from System Tune and Calibration using FC43 Pos. Ions:

Q1 and Q3 Tuning & Calibrating

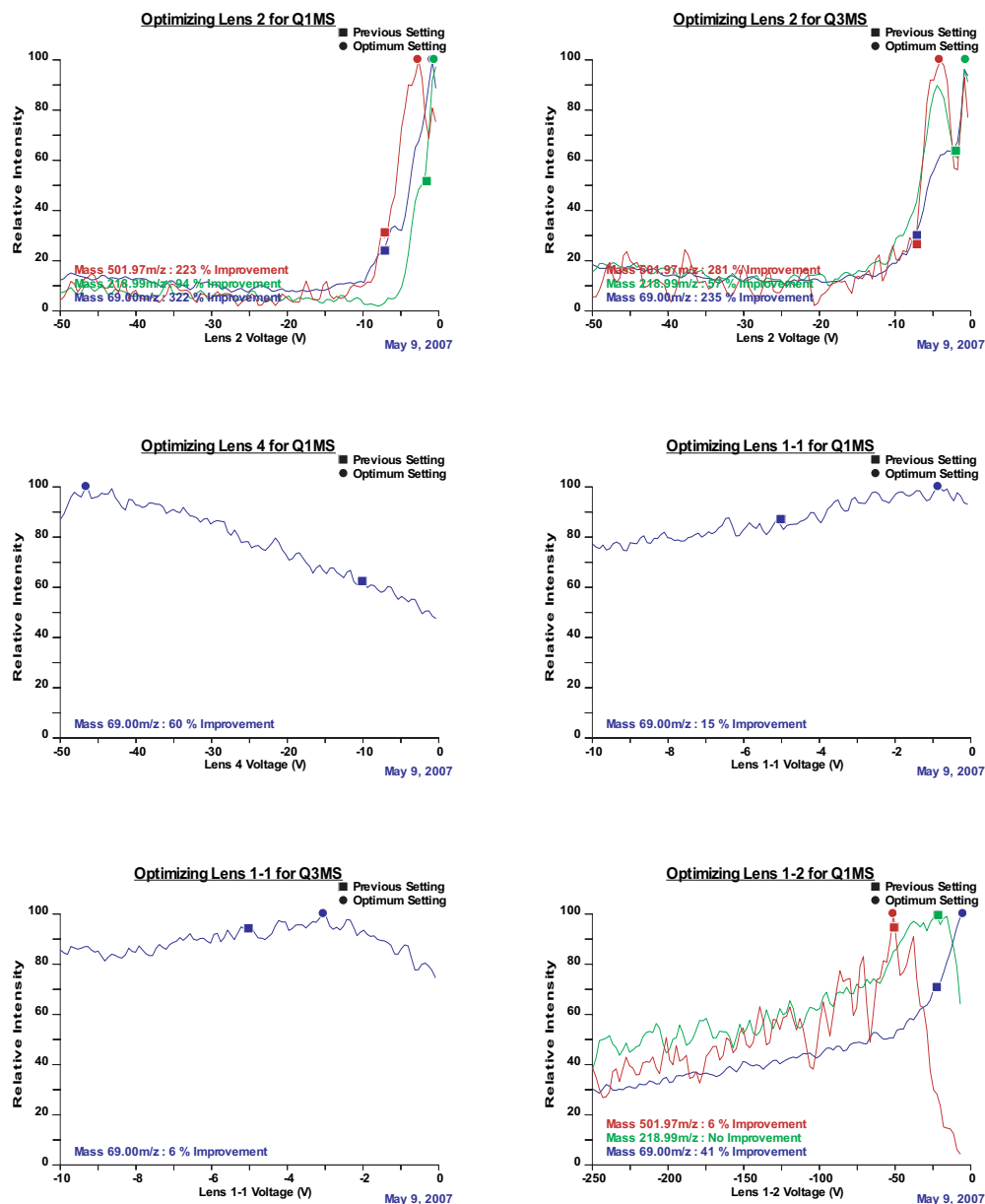
10:55:29:  Tuning and Calibrating Q1
10:55:39:  Tuning Q1MS at mass 69.00 m/z
10:55:41:    Opening resolution
10:55:42:    Adjusting resolution
10:56:02:    The adjusted resolution is -13.33 at the width 0.78
10:56:02:    Coarse resolution done - Quick calibration
10:56:07:    The adjusted calibration of mass 69.0 is -0.88
10:56:08:    Averaging Stopping Curve...
10:56:12:    Q1 Quadrupole Offset set to -0.85 for all reswidths
10:56:14:  Optimizing Lens 2 for ion 69.00 m/z
10:56:20:    Previous Setting = -7.00, New Setting = -0.80
10:56:20:    Maximum Intensity = 1.04e+06
10:56:20:    322 % Improvement
10:56:20:  Optimizing Lens 4 for ion 69.00 m/z
10:56:26:    Previous Setting = -10.00, New Setting = -46.55
10:56:26:    Maximum Intensity = 1.61e+06
10:56:26:    60 % Improvement
10:56:26:  Optimizing Lens 1-1 for ion 69.00 m/z
10:56:32:    Previous Setting = -5.00, New Setting = -0.86
10:56:32:    Maximum Intensity = 1.93e+06
10:56:32:    15 % Improvement
10:56:32:  Optimizing Lens 1-2 for ion 69.00 m/z
10:56:38:    Previous Setting = -21.90, New Setting = -5.00
10:56:38:    Maximum Intensity = 2.43e+06
10:56:38:    41 % Improvement
10:56:38:  Optimizing Lens 2-1 for ion 69.00 m/z
10:56:45:    Previous Setting = -8.45, New Setting = 3.92
10:56:45:    Maximum Intensity = 2.56e+06
10:56:45:    17 % Improvement
10:56:45:  Tuning Q1MS at mass 501.97 m/s
10:56:47:    Opening resolution
10:56:48:    Adjusting resolution
10:57:04:    The adjusted resolution is -14.38 at the width 0.78
10:57:04:    Coarse resolution done - Quick calibration
10:57:04:    The adjusted calibration of mass 502.0 is -0.16
10:57:11:    Averaging Stopping Curve...
10:57:16:    Q1 Quadrupole Offset set to -2.00 for all reswidths
10:57:18:  Optimizing Lens 2 for ion 501.97 m/z
10:57:24:    Previous Setting = -7.00, New Setting = -2.70
10:57:24:    Maximum Intensity = 2.97e+05
10:57:24:    223 % Improvement
10:57:24:  Optimizing Lens 1-2 for ion 501.97 m/z
10:57:30:    Previous Setting = -50.14, New Setting = -51.11
10:57:30:    Maximum Intensity = 4.35e+05
10:57:30:    6 % Improvement
10:57:30:  Optimizing Lens 2-1 for ion 501.97 m/z
```

Signature: \_\_\_\_\_



**Figure 38.** Tune and calibration report, parameter optimization plots

Quantum Tune Master - Tune and Calibration



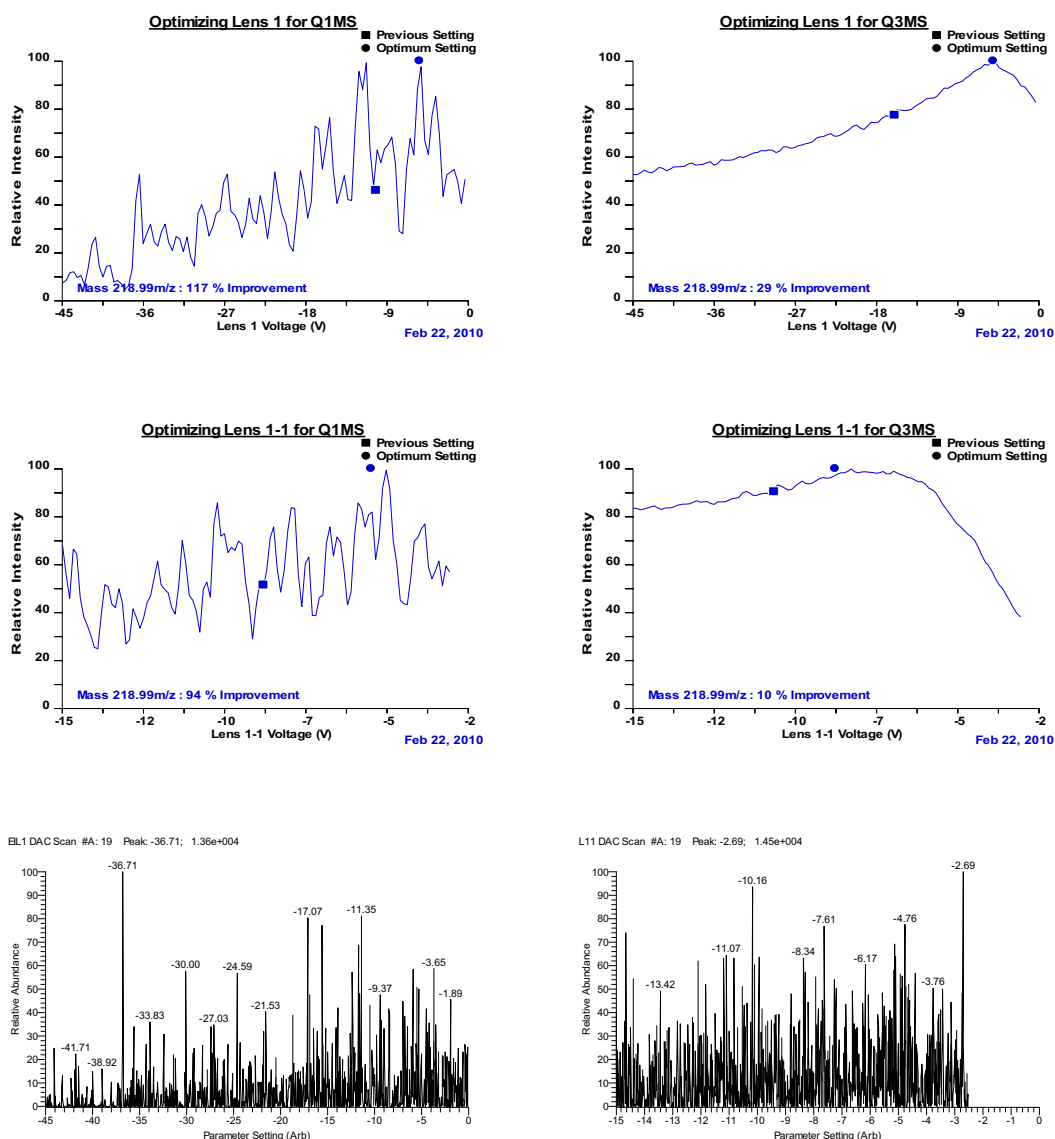
#### ❖ To save the tune and calibration report

1. In the System Tune and Calibration dialog box, click **Save Report**. The Save As dialog box appears.
2. Enter the name and the path of the report, and click **Save**.

## Running Maintenance Tune

Use the maintenance tune procedure in EZ Tune to quickly increase the ion signal of the mass spectrometer. The maintenance tune adjusts the lens L1 voltage and the lens L11 offset voltage to maximize the ion signal for, for example,  $m/z$  219 in FC-43 positive polarity mode. At the end of the procedure you can save the optimized lens L1 voltage to a tune file and the optimized lens L11 offset voltage to a calibration file. [Figure 39](#) shows a maintenance tune report.

**Figure 39.** Maintenance tune report, page 2



❖ **To run maintenance tune**

1. Display the FC-43 mass spectrum in positive or negative polarity mode as described in “Displaying the FC-43 Mass Spectrum” on page 62.



2. Click the **System Tune and Calibration** button (or choose **Setup > System Tune and Calibration**) to display the System Tune and Calibration dialog box. See Figure 35 on page 65.
3. Select the calibration compound
4. Click **Start Main. Tune** to start the maintenance tune procedure.
5. After the procedure terminates you can accept the maintenance tune and save the calibration, or undo the tune.

## Creating a Quality Control (QC) Tune Report

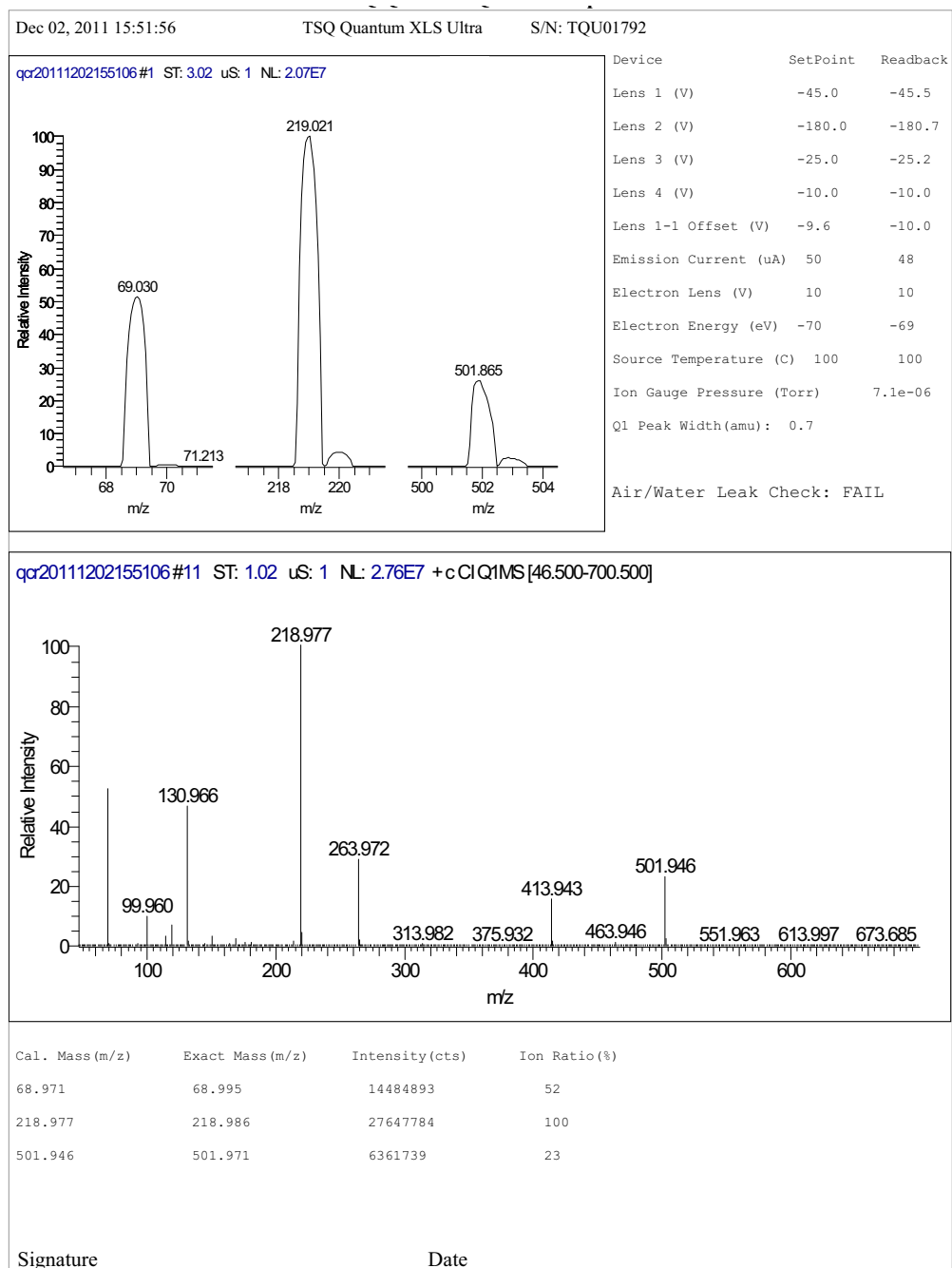
Use the TSQ QC (quality control) Report dialog box in EZ Tune to produce a report that displays tune parameters and mass spectra relevant to the performance of the mass spectrometer. You can save the report as a PDF file.

The TSQ QC tune report includes the following:

- Profile spectra of the three FC-43 peaks
- Setpoints and readbacks of the ion source lenses and L11 voltages
- Q1/MS full scan centroid spectrum from  $m/z$  50 to 650
- FC-43 peak positions and intensity ratios
- Results of a leak check (pass or fail)

Figure 40 shows a QC tune report.

**Figure 40.** QC tune report



❖ **To create and save a QC tune report**

1. Choose **View > QC Report** to open the TSQ QC Report dialog box.
2. Click **Start** to start the QC report procedure.
3. After the procedure terminates, click **View Report** to view the QC report as a PDF file.
4. Save the PDF file.

## Changing Ionization Modes

You can operate the TSQ Quantum XLS Series mass spectrometers in either EI or CI ionization mode. Changing ionization modes requires changing ion volumes. You do not need to shut down the mass spectrometer to change ion volumes.

The following sections describe how to change the ionization mode.

### Contents

- [Removing the Ion Volume](#)
- [Installing the Ion Volume](#)

## Removing the Ion Volume



### Tools needed

- Gloves, clean, lint- and powder-free
- Insert/removal (I/R) tool and guide bar



### Frequency

When you change ionization modes or as needed to clean the ion volume

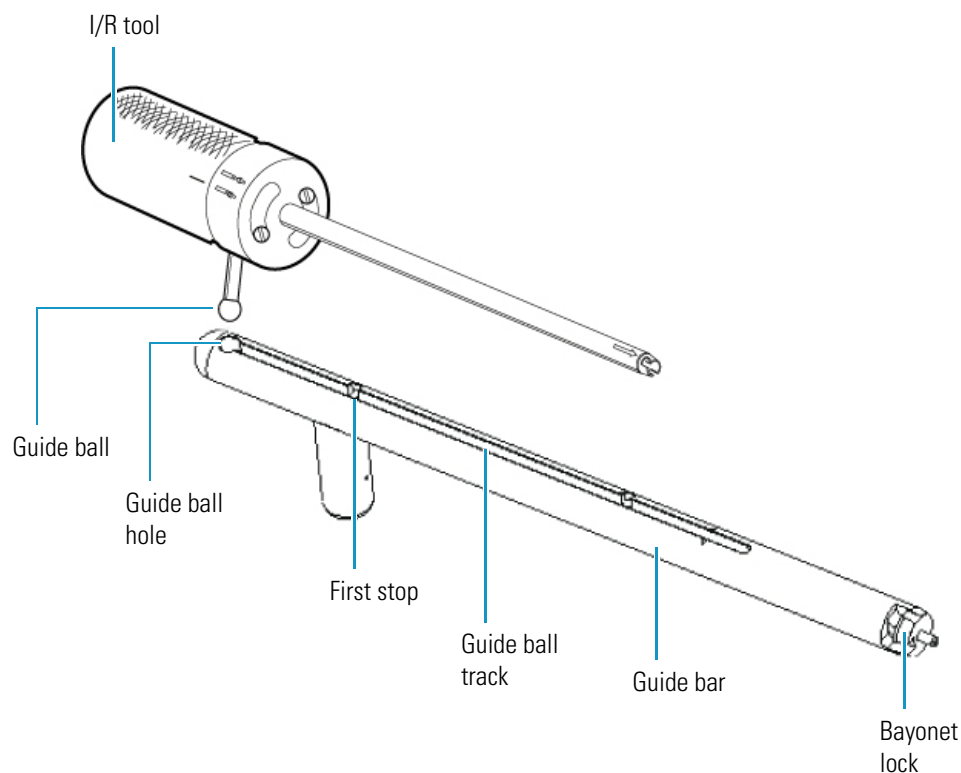
### ❖ To remove the ion volume

1. Install the guide bar:
  - a. With the guide ball track facing left, insert the guide bar into the entry housing. See [Figure 41](#).
  - b. Push the guide bar in as far as it can go; then, rotate it 90° clockwise to lock the guide bar in the entry housing.


## 5 Changing Ionization Modes

### Removing the Ion Volume

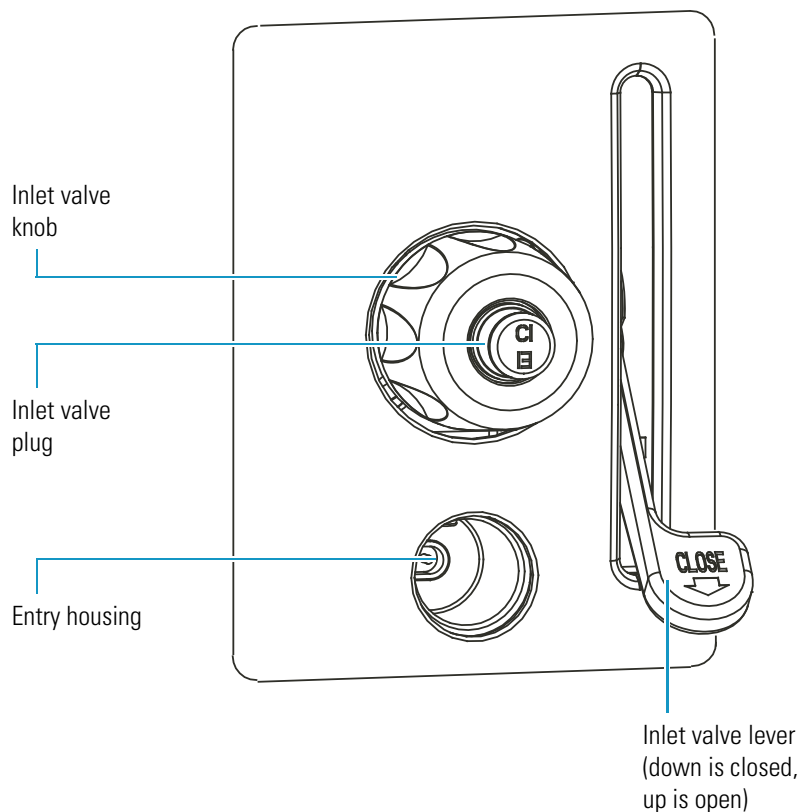
**Figure 41.** Insertion/removal (I/R) tool and guide bar




2. Prepare the inlet valve and I/R tool for insertion:

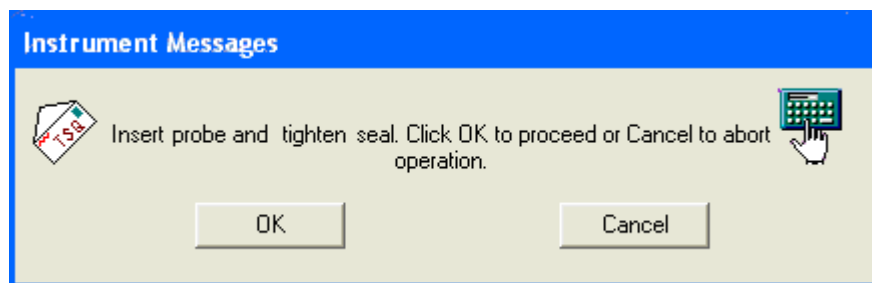
- a. Make sure the inlet valve is closed. [Figure 42](#) shows the inlet valve lever is down for closed.
- b. Loosen the inlet valve knob counterclockwise and remove the inlet valve plug. The inlet valve plug prevents air from entering the vacuum manifold in case the inlet valve is inadvertently opened.
- c. Turn the I/R tool to the unlock position , which indicates the I/R tool is in position to accept the ion volume.

**Figure 42.** Inlet valve components



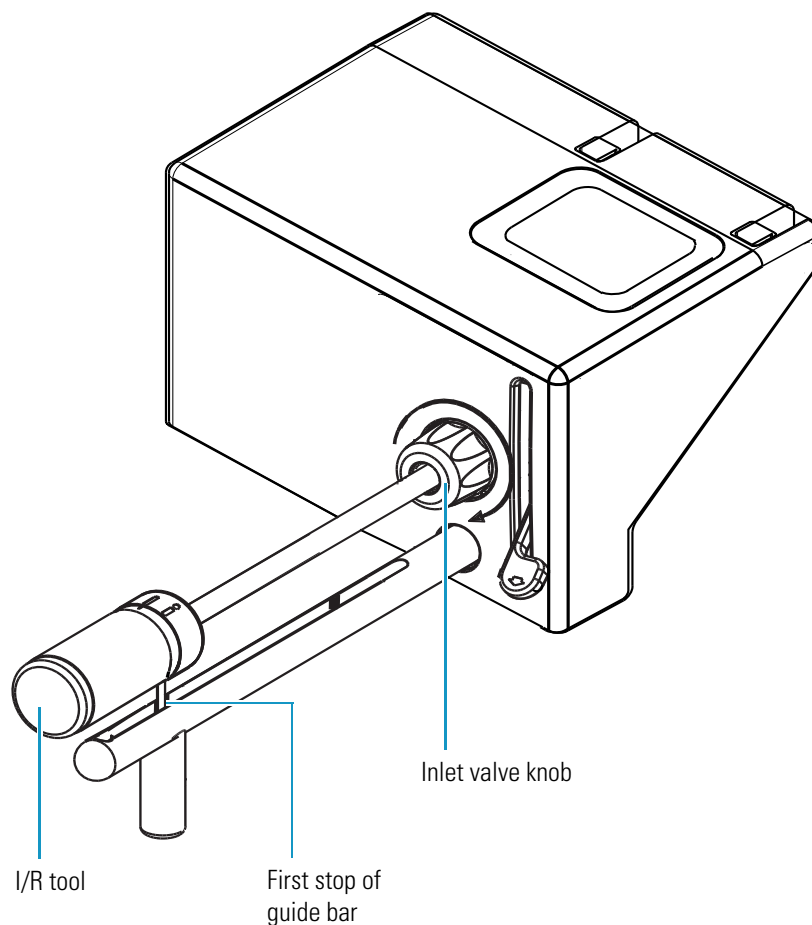
3. Choose **Start > All Programs > Thermo Instruments > TSQ > TSQ Tune** to open the EZ Tune window.
4. Click the **Probe** button, , in the EZ Tune toolbar. The Insert Probe message appears (Figure 43).

**Figure 43.** Insert Probe message



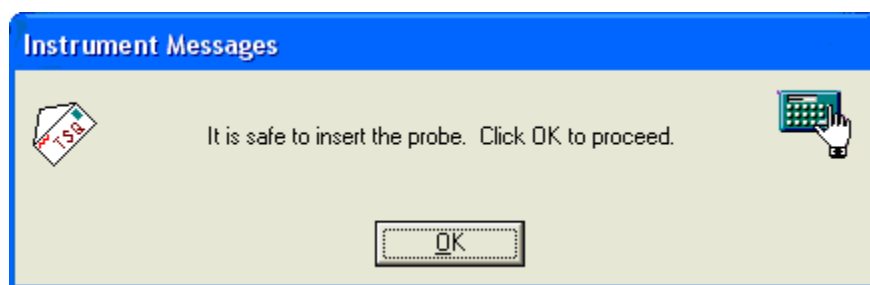
5. Insert the I/R tool into the inlet valve:
  - a. Insert the guide ball into the guide ball hole.
  - b. Slide the I/R tool forward into the inlet valve until the guide ball is at the guide bar's first stop (see Figure 44).
  - c. Tighten the inlet valve knob clockwise to ensure a leak-tight seal.

**Figure 44.** I/R tool at the first stop on guide bar and the inlet valve knob tightened



6. Click **OK**. The forepump evacuates the inlet valve. Wait until you can safely insert the probe (Figure 45), and then click **OK**.

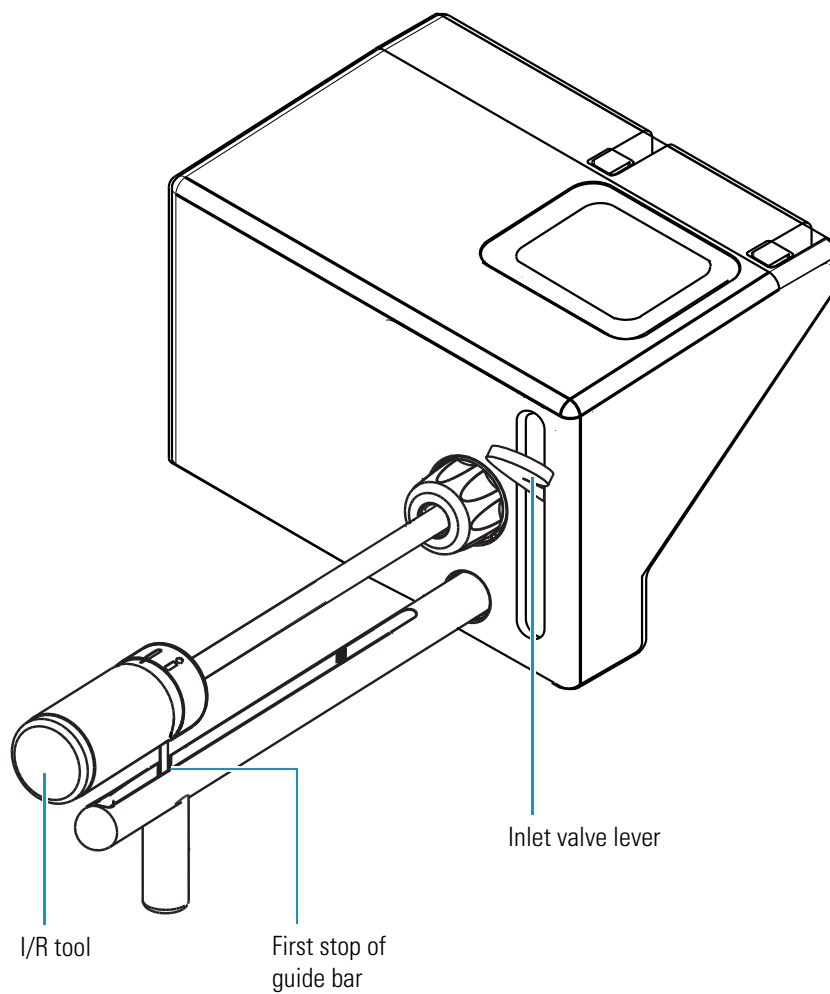
**Figure 45.** Safe to insert the probe message



7. Once evacuation is complete, pull the inlet valve lever up (Figure 46).



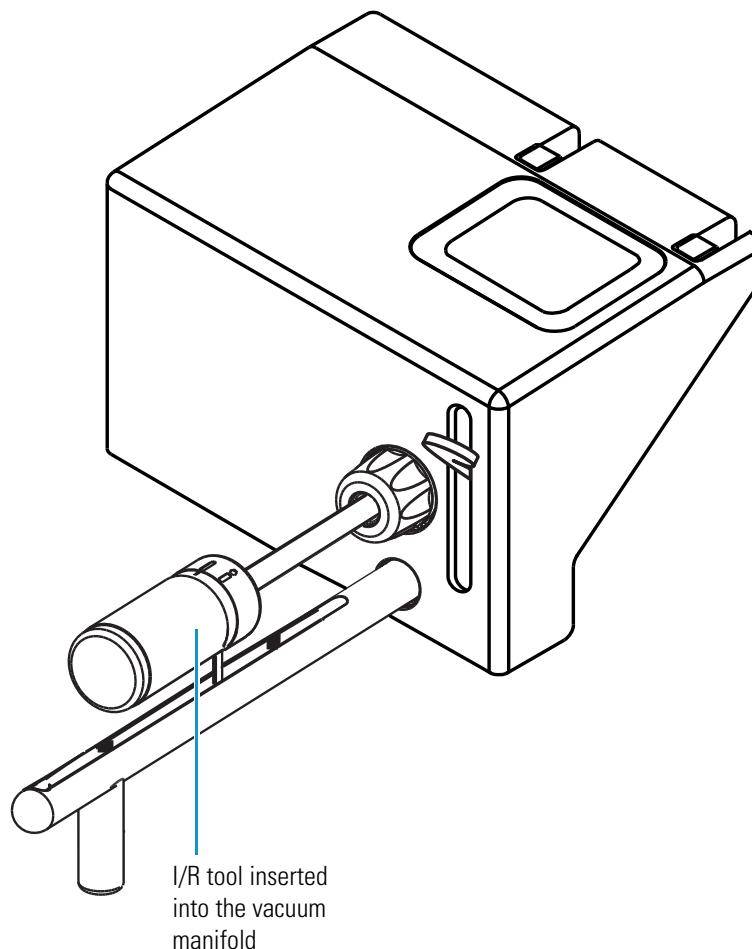
**Figure 46.** I/R tool at first stop and inlet valve lever up




The inlet valve is now open.

8. Remove the ion volume:
  - a. Slide the I/R tool into the vacuum manifold until the tip of the I/R tool is fully inserted into the ion volume holder. See [Figure 47](#). The head of the arrow on the I/R tool, when viewed through the window of the ion source manifold, should not be visible.

**Figure 47.** I/R tool inserted into the inlet valve



- b. Turn the I/R tool handle counterclockwise to put the I/R tool into lock position, . Listen for a click, which indicates that the handle is fully engaged in the lock position and is holding the ion volume.



**CAUTION** Do not withdraw the I/R tool beyond the point where the guide ball reaches the first stop in the guide bar. Close the inlet valve first. Otherwise, the system vents to the atmosphere.

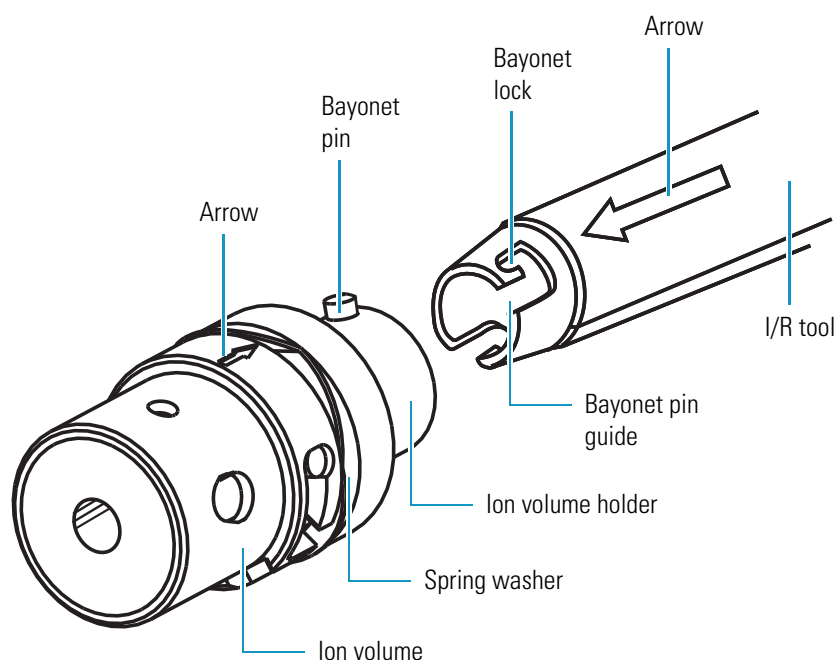
- c. Withdraw the I/R tool (with the ion volume attached) until the guide ball reaches the first stop (see [Figure 46](#) on [page 77](#)).
- d. Pull the lever down to close the inlet valve.
- e. Loosen the inlet valve knob by turning it counterclockwise to release the seal.
- f. Continue withdrawing the I/R tool completely from the inlet valve by sliding the I/R tool through the guide ball track in the guide bar.



**WARNING Burn Hazard.** Because the ion volume might be too hot to touch, let it cool to room temperature before handling it.

9. Remove the ion volume from the I/R tool (see [Figure 48](#)):
  - a. Wearing clean gloves, press the ion volume forward into the tip of the I/R tool and rotate it to disconnect the bayonet pins from the pin guides.
  - b. Pull the ion volume out of the I/R tool.

**Figure 48.** Ion volume, ion volume holder, and I/R tool



10. To clean the ion volume, use the instructions in [“Cleaning Stainless Steel Parts”](#) on [page 98](#). If you are cleaning a CI ion volume, be sure to clean out the small electron entrance hole. Aluminum oxide can get trapped in this hole, which can adversely affect sensitivity. Use a dental pick or old syringe needle to clean the hole.

## Installing the Ion Volume

Install an ion volume after cleaning or when you change ionization modes.



❖ **To install the ion volume**

**Note** Wear clean, lint- and powder- free gloves when you handle a clean ion volume.


1. Place the clean ion volume on the I/R tool with the arrows aligned. See [Figure 48](#).



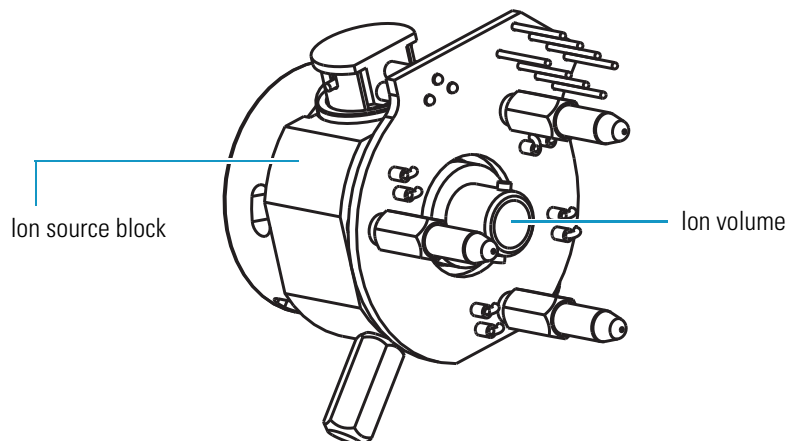
**CAUTION** To avoid damage to the ion source, make sure to align the arrows on the I/R tool and ion volume.

2. Turn the I/R tool handle to the lock position, .
3. Install the guide bar:
  - a. With the guide ball track facing left, insert the guide bar into the entry housing (see [Figure 41](#) on [page 74](#)).
  - b. Push the guide bar in as far as it will go, and then rotate it 90° clockwise to lock the guide bar into the entry housing.
4. Prepare the inlet valve for insertion:
  - a. Make sure the inlet valve is closed. [Figure 42](#) shows the inlet valve lever, closed in the down position.
  - b. Loosen the inlet valve knob counterclockwise and remove the inlet valve plug. The inlet valve plug prevents air from entering the vacuum manifold in case the inlet valve is inadvertently opened.
5. Choose **Start > Programs > Thermo Instruments > TSQ > TSQ Tune** to open the EZ Tune window.
6. Click the **Probe** button, , in the EZ Tune toolbar. The Insert Probe message appears. See [Figure 43](#).
7. Inset the I/R tool into the inlet valve:
  - a. Insert the guide ball into the guide ball hole.
  - b. Slide the I/R tool forward into the inlet valve until the guide ball is at the guide bar's first stop. See [Figure 44](#) on [page 76](#).
  - c. Tighten the inlet valve knob clockwise to ensure a leak-tight seal.
8. Click **OK**. The forepump evacuates the inlet valve. Wait until you can safely insert the probe ([Figure 45](#) on [page 76](#)); then click **OK**.
9. Once evacuation is complete, pull the inlet valve lever up to open the inlet valve.

10. Install the ion volume:

- a. Slide the I/R tool and ion volume assembly into the vacuum manifold until the ion volume assembly is fully inserted and seated into the ion source block. Listen for a click, which indicates that the ion volume has connected with the ion source block.
- b. Turn the I/R tool handle to the unlock position, , to release the ion volume from the I/R tool.

**Figure 49.** Ion volume seated in the ion source block



11. Verify that the ion volume is fully seated in the ion source block:

- Withdraw the I/R tool away from the ion volume about 2.5 cm (1 in.), and turn the I/R tool handle to the lock position.
- Slide the I/R tool back into the vacuum manifold until the end of the I/R tool just touches the ion volume.
- Test that the I/R tool does not go into the inlet valve completely, which indicates that the ion volume is seated properly.

12. Remove the I/R tool:



**CAUTION** Do not withdraw the I/R tool beyond the point where the guide ball reaches the first stop in the guide bar. Close the inlet valve first. Otherwise, the system vents to the atmosphere.

- a. Withdraw the I/R tool until the guide ball reaches the first stop (see [Figure 46](#) on [page 77](#)).
- b. Close the inlet valve by pulling the inlet valve lever down (see [Figure 44](#) on [page 76](#)).
- c. Loosen the inlet valve knob by turning it counterclockwise.
- d. Continue withdrawing the I/R tool completely from the inlet valve by sliding the I/R tool through the guide ball track in the guide bar.

## 5 Changing Ionization Modes

### Installing the Ion Volume

13. Remove the guide bar by rotating it 90° counterclockwise and sliding it out of the entry housing.
14. Replace the inlet valve plug. Orient the plug to indicate whether an EI or CI ion volume is installed.
15. Tighten the inlet valve knob clockwise to create a leak-tight seal.
16. (Optional) To prevent the inlet valve from being opened accidentally, pull free and remove the inlet valve lever.

# Maintenance

This chapter describes routine maintenance procedures that you must perform to ensure optimum performance of the TSQ Quantum XLS Series mass spectrometer. Optimum performance of the mass spectrometer depends on the maintenance of all parts of the instrument. **You are responsible for properly maintaining your instrument through regular performance of these maintenance procedures.**

Table 6 lists routine and infrequent mass spectrometer maintenance procedures. For instructions on maintaining the GC or autosampler, refer to the manuals that come with the GC or autosampler.

## Contents

- [Cleaning Ion Source Components](#)
- [Replacing the Filament of the Ion Source](#)
- [Completely Disassembling and Reassembling the Ion Source](#)
- [Maintaining the Forepump](#)
- [Adding Calibration Compound](#)
- [Replacing the Ball Valve Seal](#)
- [Removing and Installing a GC Capillary Column](#)

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

**Table 6.** Maintenance procedures (Sheet 1 of 2)

Mass spectrometer component	Procedure	Frequency	Reference
Ion source	Cleaning the ion volume	As needed <sup>a</sup>	<a href="#">Page 87</a>
Ion source	Cleaning the lenses	As needed <sup>a</sup>	<a href="#">Page 87</a>

**Table 6.** Maintenance procedures (Sheet 2 of 2)

Mass spectrometer component	Procedure	Frequency	Reference
Ion source	Cleaning the entire ion source	As needed <sup>a</sup>	<a href="#">Page 96</a>
Ion source	Replacing the filament	If the filament fails	<a href="#">Page 93</a>
Inlet valve	Replacing the ball valve seal	If there is an air leak in the inlet valve	<a href="#">Page 105</a>
Calibration compound	Adding calibration compound	If EZ Tune error message indicates low intensity of calibration gas ions	<a href="#">Page 102</a>
Gas chromatograph	Replacing the capillary column	If chromatographic separation is bad or if a different stationary phase is needed for the application	<a href="#">Page 107</a>
Q0 ion optics	Cleaning the Q0 quadrupole and L11 and L12 lenses <sup>b</sup>	As needed <sup>a</sup>	
Mass analyzer	Cleaning the Q1, Q2, and Q3 quadrupoles and lenses <sup>b</sup>	As needed <sup>a</sup>	
Forepump	Purging the forepump pump oil	If pump oil is cloudy	Manufacturer's documentation
Forepump	Adding pump oil	If pump oil level is low	Manufacturer's documentation
Forepump	Changing the pump oil	Every 4 months or if pump oil is cloudy and discolored	Manufacturer's documentation
Ion detection system	Replacing the electron multiplier assembly <sup>b</sup>	If noise in spectrum is excessive or proper electron multiplier gain cannot be achieved	
Electronic modules	Replacing an electronic module <sup>b</sup>	If electronic module fails	
PCBs	Replacing a PCB <sup>b</sup>	If PCB fails	

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

<sup>b</sup> A Thermo Fisher Scientific Field Service Engineer must perform this maintenance procedure.



## Cleaning Ion Source Components

An important part of maintaining your TSQ Quantum XLS Series mass spectrometer is making sure that the ion source components are clean. Follow the cleaning procedures in this section to clean stainless steel and non-stainless steel parts.

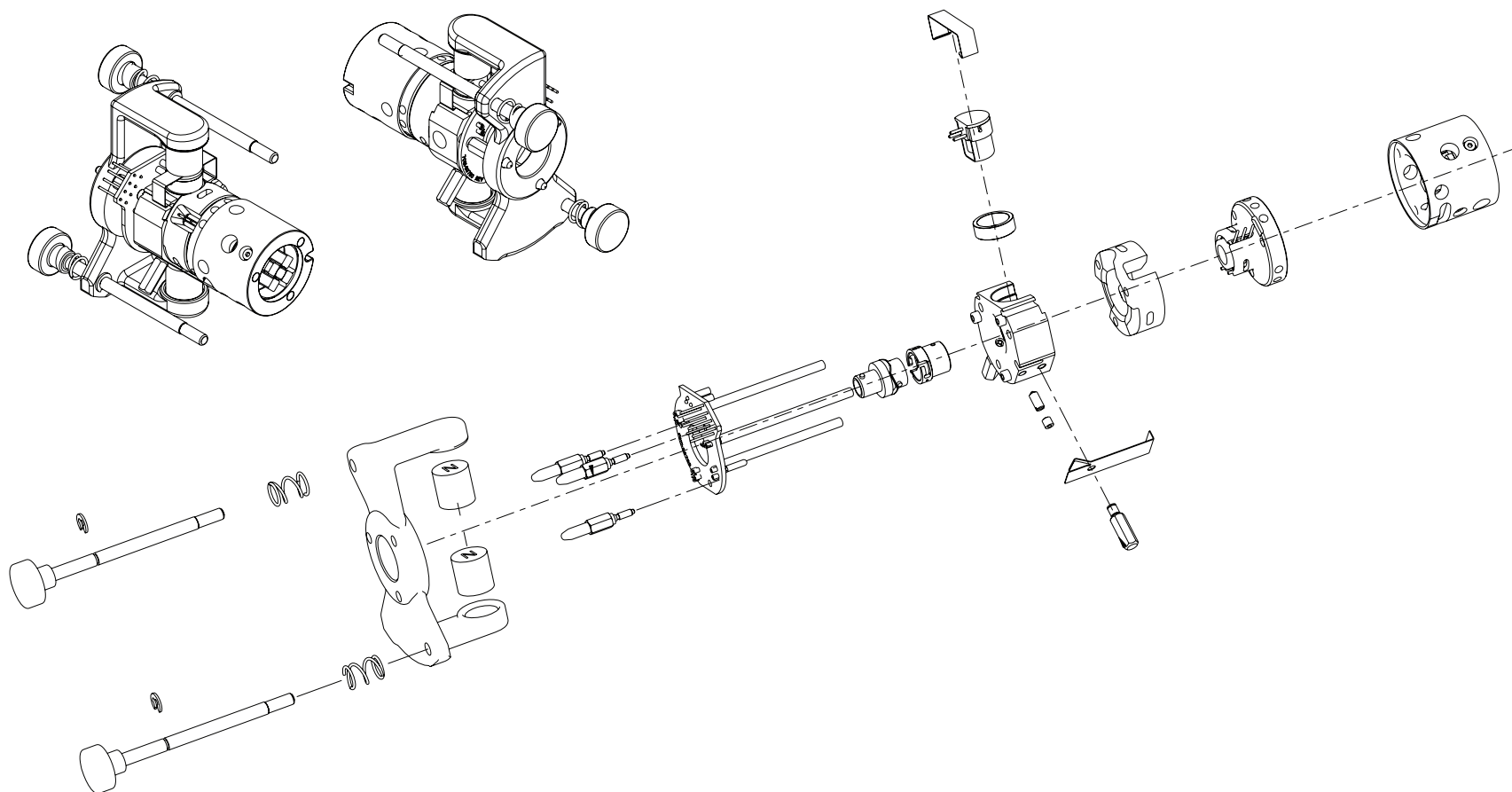
When your mass spectrometer is clean and in good working order, perform benchmark tests and record the results. When the tested performance of your system decreases significantly from your benchmark test results, clean the ion volume. If this does not restore performance, clean the lenses.

How often you clean the ion source depends on the types and amounts of samples and solvents you introduce into the system. In general, the closer a component is to the sample introduction point, the more rapidly the component becomes dirty. The ion volume becomes dirty faster than other parts. If you just want to change or clean the ion volumes, you do not need to shut down the system.

You can remove and disassemble most parts by hand. Make sure you have all the tools needed before starting each procedure.

[Figure 50](#) shows exploded and assembled views of the ion source assembly.

**Figure 50.** Ion source assembly, assembled and exploded views



## Cleaning Ion Volumes

You do not need to vent the mass spectrometer to atmosphere to clean the ion volume.

### ❖ To clean the ion volume

1. Remove the ion volume. See [“Removing the Ion Volume”](#) on page 73.



**WARNING Burn Hazard.** The ion volume might be hot. Allow the ion volume to cool to room temperature before touching it.

2. Clean the ion volume. See [“Cleaning Stainless Steel Parts”](#) on page 98. If you are cleaning a CI ion volume, be sure to clean out the small electron entrance hole. Aluminum oxide can get trapped in this hole, which can adversely affect sensitivity. Use a dental pick or old syringe needle to clean the hole.
3. Reinstall the ion volume. See [“Installing the Ion Volume”](#) on page 80.

## Cleaning the Lenses of the Ion Source

If cleaning the ion volume does not restore system performance, clean the ion source lenses.

### ❖ To clean the ion source lenses

1. Shut down and vent the system. See [“Shutting Down the System Completely”](#) on page 51.



**WARNING Shock Hazard.** Unplug the TSQ Quantum XLS Series system before proceeding.



**WARNING Burn Hazard.** The ion source might be hot. Allow the ion source to cool to room temperature before touching it.

2. Remove the ion source. See [“Removing the Ion Source”](#) on page 88.
3. Remove the ion source lens assemblies from the ion source and disassemble it. See [“Removing the L1, L2, L3 Lens Assembly and the Heated Q0 Quadrupole Assembly”](#) on page 90.
4. Clean the lenses and the spacers. See [“Cleaning Stainless Steel Parts”](#) on page 98 and [“Cleaning Non-Stainless Steel or Hybrid Parts”](#) on page 100, respectively.
5. Reassemble L1, L2, L3 lens assembly and install it and the heated Q0 quadrupole onto the ion source. See [“Reassembling the L1, L2, L3 Lens Assembly”](#) on page 92.

6. Reinstall the ion source into the mass spectrometer and reinsert the capillary column into the ion source. See [“Reinstalling the Ion Source”](#) on [page 92](#).
7. Restart the system. See [“Starting Up the System after a Complete Shutdown”](#) on [page 53](#).

## Removing the Ion Source

Remove the ion source to clean the lenses or replace the filament.



### Tools needed

- Gloves, cleanroom grade (P/N 23827-0008 and 23827-0009)
- Lint-free cloth



### Frequency

As needed to perform ion source maintenance

### ❖ To remove the ion source

1. Shut down and vent the mass spectrometer. See [“Shutting Down the System Completely”](#) on [page 51](#).



**WARNING Shock Hazard.** Unplug the mass spectrometer before proceeding.



**CAUTION** Do not remove the ion source without first pulling back the GC capillary column, or else the capillary column might break.

2. Pull back the capillary column:
  - a. Lower the oven, injector, and transfer line temperatures to 30 °C and allow them to cool before continuing.

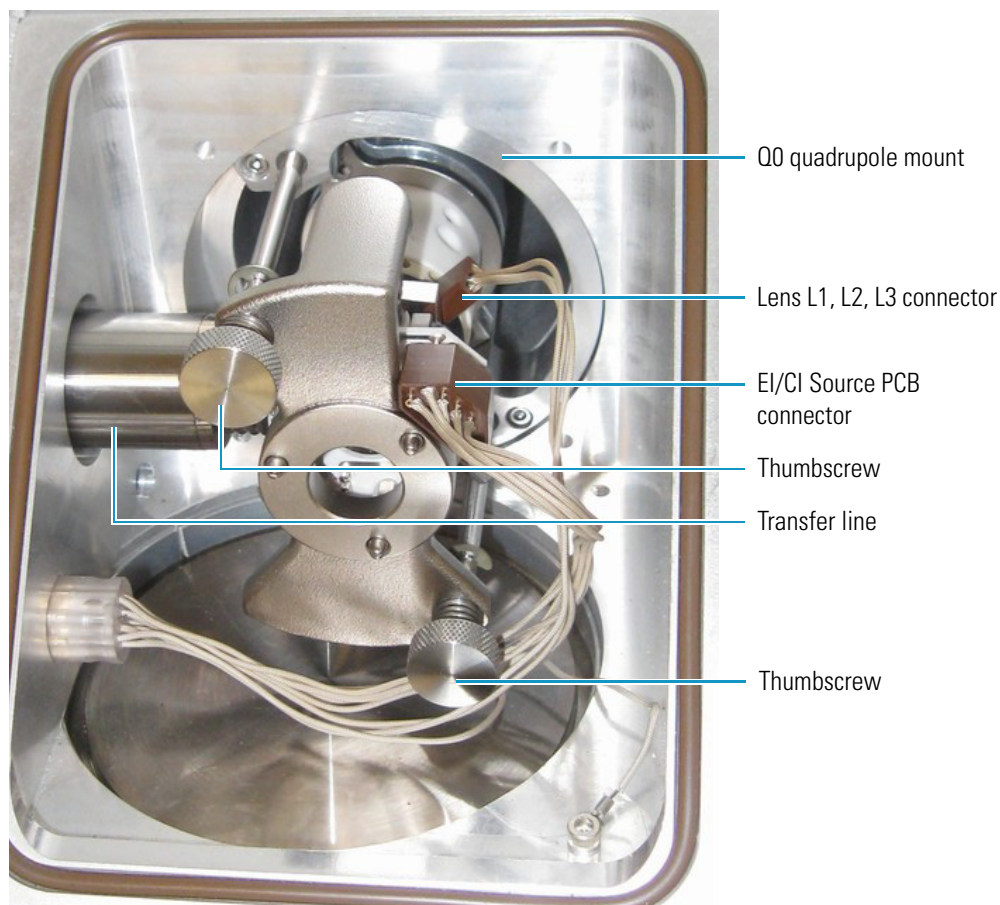


**WARNING Burn Hazard.** The GC oven, injector, and transfer line are hot. Allow them to cool to room temperature before touching them.

- b. Once the oven, injector, and transfer line are cool, turn off the gas chromatograph.
  - c. Loosen the transfer line nut. See [Figure 61](#) on [page 108](#).
  - d. Pull back the column. (You can first mark the column's position with white correction fluid or something similar.)
3. Prepare a clean work area by covering the area with lint-free cloth.
4. Undo the two latches that secure the lid of the ion source vacuum manifold, and open the lid.

5. Disconnect the connectors from the lead pins at the EI/CI Source PCB, and L1, L2, L3 lens assembly. See [Figure 51](#).

**Figure 51.** TSQ Quantum XLS Series ion source, installed



**WARNING Burn Hazard.** The ion source might be hot. Allow the ion source to cool to room temperature before touching it.

**Note** Wear clean, lint- and powder-free gloves when you handle the ion source.

6. While holding the ion source assembly, loosen the two thumbscrews that secure the ion source assembly to the Q0 quadrupole mount.
7. Pull the ion source assembly away from the Q0 quadrupole mount and slightly to the right to clear the transfer line bellows.
8. Slide the ion source off the magnet yoke.
9. Place the ion source and magnet yoke on a clean, lint-free cloth.
10. Close the lid of the ion source vacuum manifold.

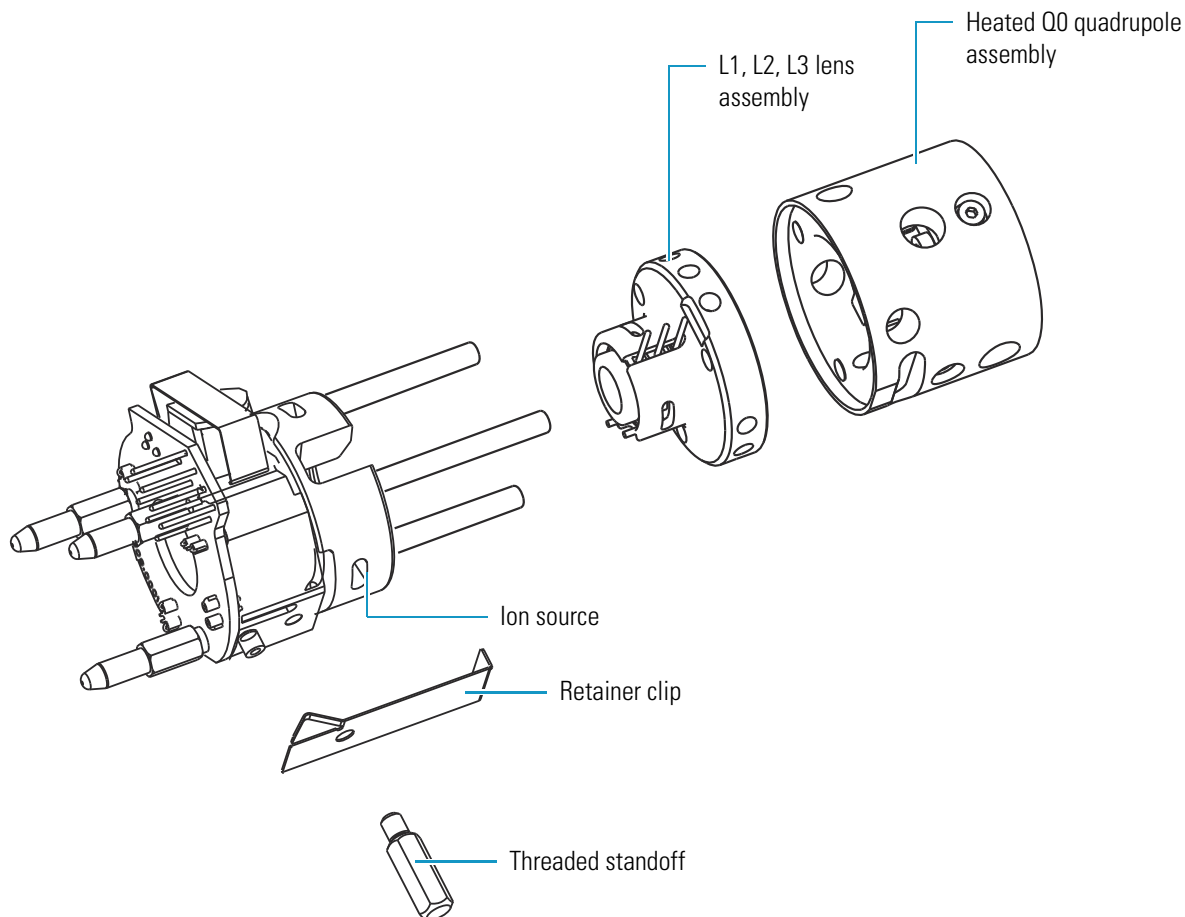
## Removing the L1, L2, L3 Lens Assembly and the Heated Q0 Quadrupole Assembly

The ion source includes the L1, L2, L3 lens assembly and the heated Q0 quadrupole assembly. You must remove and disassemble the L1, L2, L3 lens assembly to clean the lenses. A retainer clip fastens the L1, L2, L3 lens assembly and the heated Q0 quadrupole assembly to the ion source block.

### To remove the ion source lens assemblies

1. Wearing clean, lint- and powder- free gloves, unscrew the threaded hexagonal standoff and remove the retainer clip that secures the lens assembly to the ion source block. See [Figure 52](#).
2. Remove the heated Q0 quadrupole assembly and the L1, L2, L3 lens assembly from the heater cartridges of the ion source. Place them on a clean surface.

**Figure 52.** L1, L2, L3 lens assembly and heated Q0 quadrupole assembly removed from the ion source

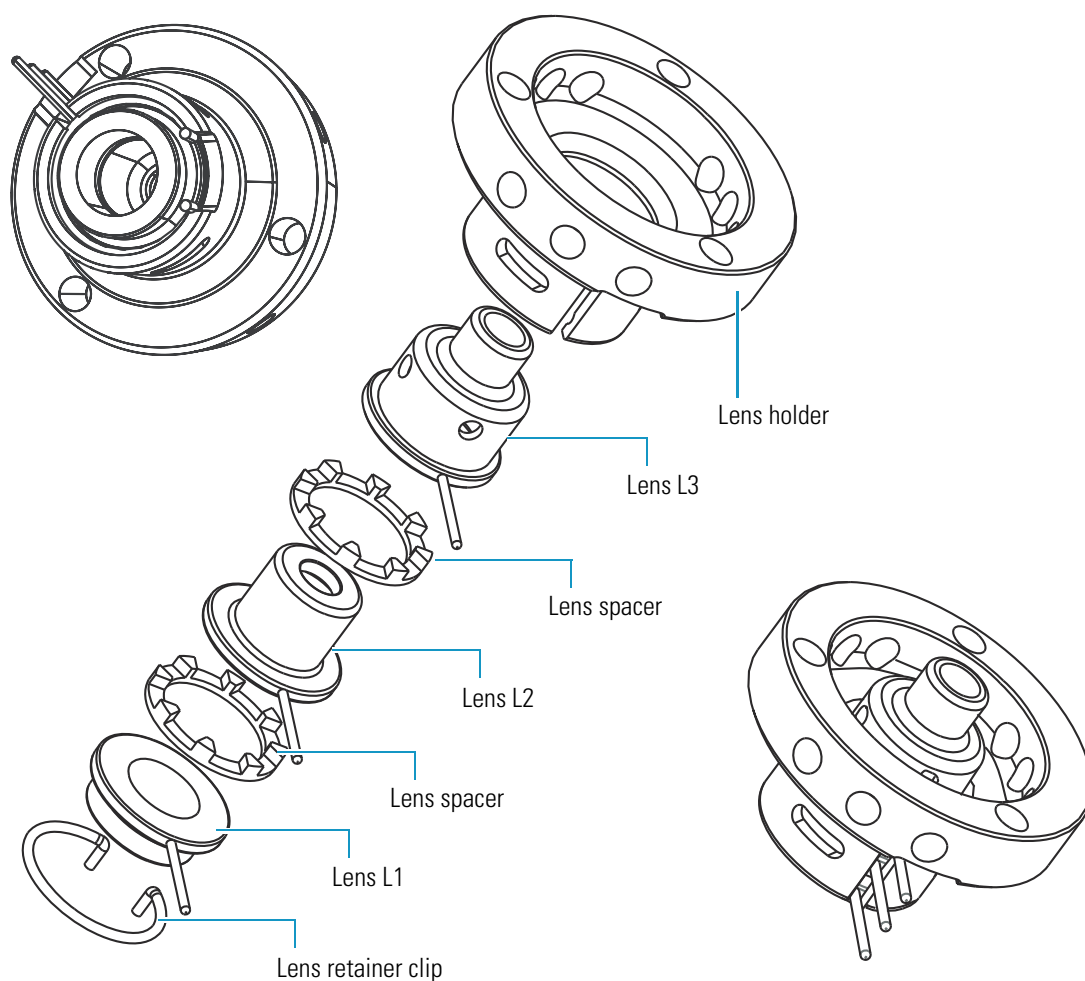


## Disassembling the L1, L2, L3 Lens Assembly

### ❖ To disassemble the L1, L2, L3 lens assembly

1. Remove the lens retainer clip by pinching the ends with your fingers or a pair of tweezers. See [Figure 53](#).
2. Remove the lenses and spacers from the lens holder.
3. Place the components on a clean surface.

**Figure 53.** L1, L2, L3 lens assembly, assembled and exploded views



**Note** To clean the ion source lenses, follow the procedure in “[Cleaning Stainless Steel Parts](#)” on [page 98](#). To clean the remaining parts, follow the procedure in “[Cleaning Non-Stainless Steel or Hybrid Parts](#)” on [page 100](#).

## Reassembling the L1, L2, L3 Lens Assembly

Ensure that the lenses are clean and dry before you reassemble the lens assembly.

### ❖ To reassemble the L1, L2, L3 lens assembly

1. Wearing clean, lint- and powder- free gloves, reinstall the lenses and spacers in the lens holder in the order and orientation shown in [Figure 53](#) on [page 91](#), starting with lens L3.
2. Reinstall the lens clip by pinching the ends with your fingers or a pair of tweezers and seating it in the lens holder.
3. Insert the lens alignment tool (in the TSQ Quantum XLS Accessory Kit) into the lens assembly and align the lenses.

## Reinstalling the Ion Source Lens Assemblies

### ❖ To reinstall the ion source lens assemblies onto the ion source

1. Wearing clean, lint- and powder- free gloves, insert the three heater cartridges of the ion source through their corresponding holes in the L1, L2, L3 lens assembly. See [Figure 52](#) on [page 90](#).
2. Insert the three heater cartridges of the ion source through their corresponding holes in the heated Q0 quadrupole assembly. Verify the correct orientation of the guide pin hole and the retainer clip groove on the heated Q0 quadrupole assembly.
3. Use the retainer clip and threaded standoff to secure the lens assemblies to the ion source.

**IMPORTANT** For accurate temperature readings of the heater block, fully screw the threaded standoff into the ion source to ensure contact between the temperature sensor and the heater block.

## Reinstalling the Ion Source

For the location of the ion source components, see [Figure 50](#) on [page 86](#).

### ❖ To reinstall the ion source into the vacuum manifold

1. Wearing clean, lint- and powder- free gloves, place the ion source onto the magnet yoke.
2. Position the ion source in the vacuum manifold and ensure the following:
  - The transfer line is seated in the sample inlet aperture in the ion source.
  - The guide pin on the Q0 quadrupole mount inserts into the guide pin groove on the heated Q0 lens assembly.
  - The two thumbscrews are aligned with the screw holes in the Q0 quadrupole mount.
3. Secure the ion source to the Q0 quadrupole mount by alternately tightening each thumbscrew one-half turn at a time. Make sure there is no play in the ion source.



4. Align and reconnect the 8-pin connector to the lead pins on the EI/CI Source PCB.
5. Align the 3-pin connector so that the side with the beveled edge is closest to the L3 lead pin and the side with the rounded corners is closest to the L1 lead pin.
6. Reconnect the 3-pin connector to the lead pins on the L1, L2, and L3 lenses.
7. Reinsert the capillary column into the ion source:
  - a. Using the I/R tool, remove the ion volume. See [“Removing the Ion Volume”](#) on [page 73](#).
  - b. Push the capillary column in until you can see it in the ion source.
  - c. Pull the column back just far enough that you cannot see it.
  - d. Tighten the transfer line nut and transfer line union.
  - e. Using the I/R tool, install the ion volume. See [“Installing the Ion Volume”](#) on [page 80](#).
8. Close and secure the cover to the ion source vacuum manifold.

## Replacing the Filament of the Ion Source

The number of ions produced in the ion source is approximately proportional to the filament emission current. If ion production is lacking, you might have to replace the filament. If the measured emission current is substantially less than the value that the emission current is set to, or if the measured emission current decreases over time, then the filament has failed or is failing and requires replacement.



### Tools needed

- Filament (P/N 120320-0030)
- Gloves, cleanroom grade (P/N 23827-0008 and 23827-0009)
- Lint-free cloth



### Frequency

If filament fails

For the location of the ion source components, see [Figure 50](#) on [page 86](#) and [Figure 54](#) on [page 94](#).

### ❖ To replace the filament of the ion source

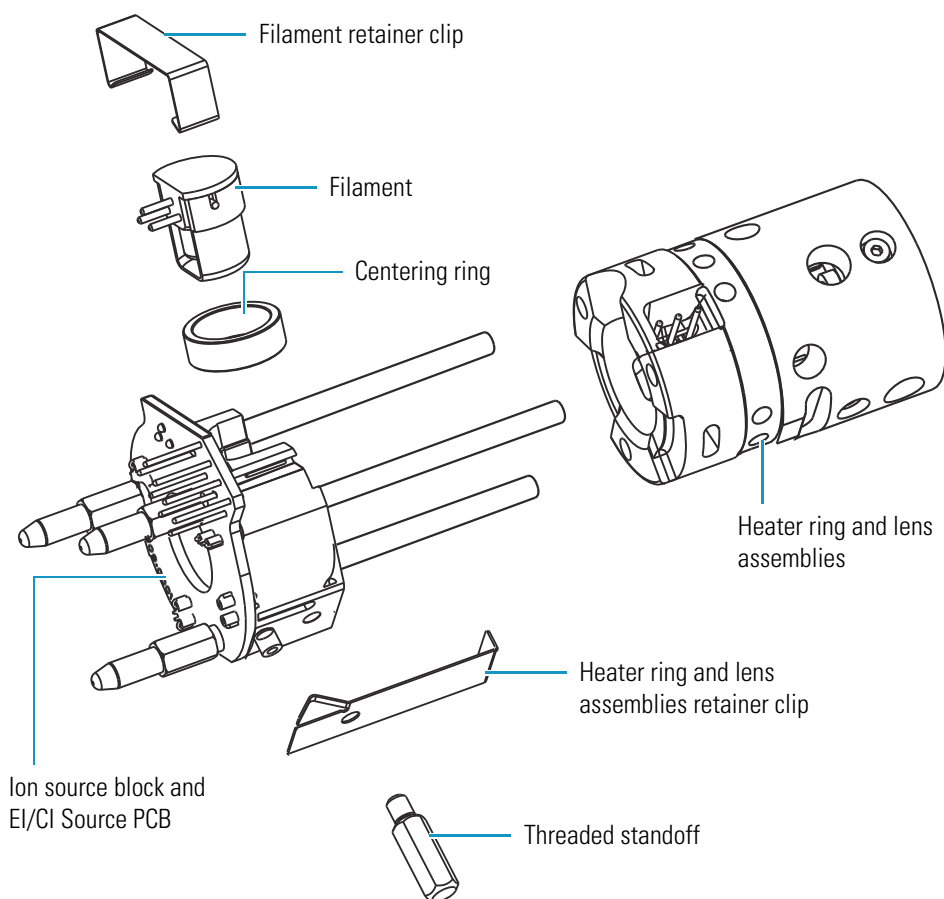
1. Prepare a clean work area by covering the area with lint-free cloth.
2. Shut down and vent the mass spectrometer. See [“Shutting Down the System Completely”](#) on [page 51](#).



**WARNING Shock Hazard.** Unplug the mass spectrometer before proceeding.

3. Remove the ion source. See [“Removing the Ion Source”](#) on [page 88](#).
4. Wearing clean, lint- and powder-free gloves, remove the ion source from the magnet yoke.

**Figure 54.** Disassembling the source to replace the filament



5. Unscrew the threaded standoff and remove the retainer clip that secures the heater ring and lens assemblies to the ion source block. See [Figure 54](#).
6. Pull the heater ring and lens assemblies off of the cartridge heaters on the ion source block. Place them on a clean surface.
7. Remove the retainer clip that secures the filament and centering ring to the ion source block.
8. Remove the filament and centering ring from the ion source block.

**Tip** Now is a good time to clean the ion source block and lenses. To do so, use the procedure described in [“Cleaning Stainless Steel Parts”](#) on [page 98](#).

Inspect and install a new filament (P/N 120320-0030, in the TSQ Quantum XLS Accessory Kit):

- a. Verify that the filament wire is centered in the electron lens hole.
  - b. Insert the filament into the centering ring.
  - c. Align the filament leads with the EI/CI Source PCB connectors and gently press the leads into the connectors. Normally, there is a small gap of about 0.4 mm (0.016 in.) between the filament and the connectors. The gap allows the ceramic centering ring to properly position and align the electron lens hole with the ion volume.
  - d. Secure the filament and centering ring with the retainer clip.
9. Press the heater ring and lens assemblies onto the cartridge heaters on the ion source block.
  10. Use the retainer clip and threaded standoff to secure the lens assemblies to the ion source. See [Figure 54](#) on [page 94](#).

**IMPORTANT** For accurate temperature readings of the heater block, fully screw the threaded standoff into the ion source to ensure contact between the temperature sensor and the heater block.

11. Reinstall the ion source onto the magnet yoke.
12. Reinstall the ion source into the vacuum manifold and reinsert the capillary column into the ion source. See [“Reinstalling the Ion Source”](#) on [page 92](#).

Restart the system. See [“Starting Up the System after a Complete Shutdown”](#) on [page 53](#).

## Completely Disassembling and Reassembling the Ion Source

Disassemble the ion source completely to clean the ion source block or to replace the EI/CI Source PCB.



### Tools Needed

- Gloves, cleanroom grade (P/N 23827-0008 and 23827-0009)
- Lint-free cloth



### Frequency

As needed

## Complete Disassembly and Reassembly of the Ion Source

See [Figure 55](#) for the location of the ion source components.

### ❖ To disassemble the ion source completely

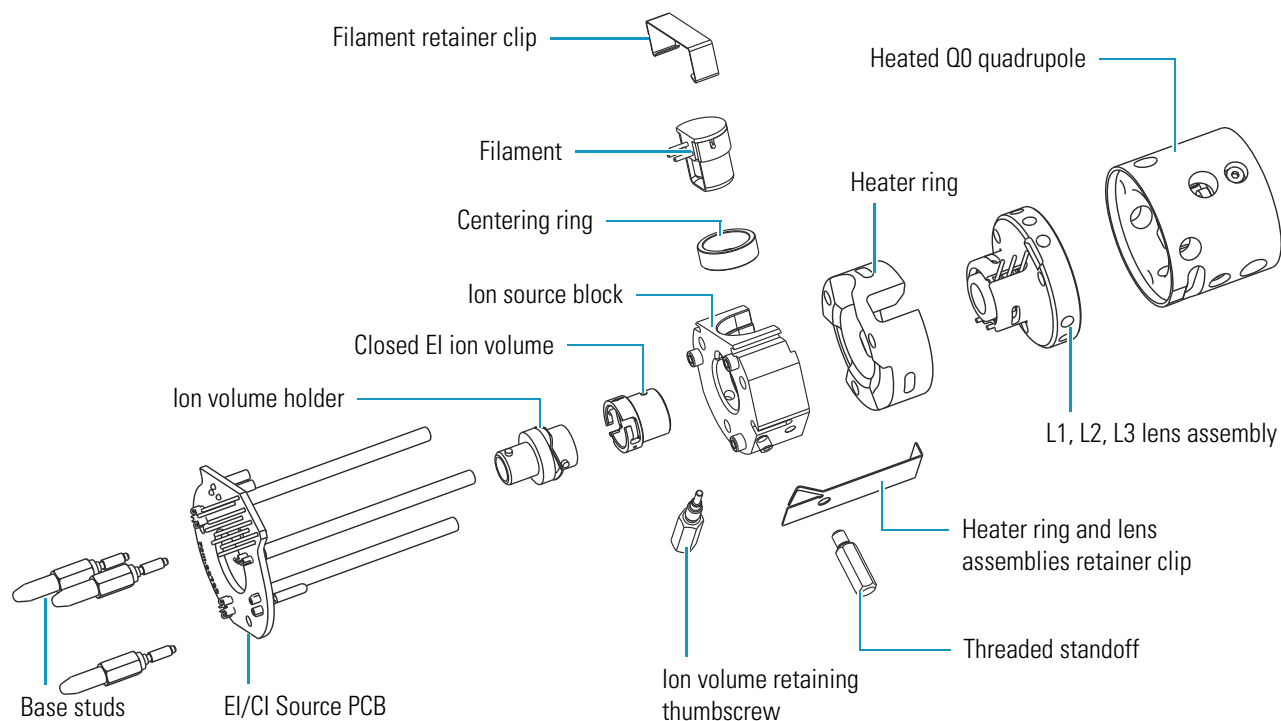
1. Prepare a clean work area by covering the area with lint-free cloth.
2. Shut down and vent the TSQ Quantum XLS Series system. See [“Shutting Down the System Completely”](#) on [page 51](#).



**WARNING Shock Hazard.** Unplug the mass spectrometer before proceeding.

3. Wearing clean, lint- and powder- free gloves, remove the ion source. See [“Removing the Ion Source”](#) on [page 88](#).
4. Remove the ion source from the magnet yoke.

**Figure 55.** TSQ Quantum XLS Series ion source, disassembled



5. Unscrew the threaded hexagonal standoff and remove the retainer clip that secures the heater ring and lens assemblies to the ion source block.
6. Pull the heated Q0 quadrupole assembly and the L1, L2, L3 lens assembly off the ion source.

7. Pull the heater ring off the ion source.
8. Unscrew and remove the three base studs.



**CAUTION** To prevent damage, do not pull the EI/CI Source PCB out of the ion source block.

9. Remove the EI/CI Source PCB:
  - a. Place the ion source on a clean surface with the cartridge heaters down and the EI/CI Source PCB up.
  - b. Press down on the ion source block to separate it from the EI/CI Source PCB.
10. Remove the retainer clip that secures the filament and centering ring to the ion source block.
11. Remove the filament and centering ring from the ion source block.
12. Clean the ion source block and lenses. See [“Cleaning Stainless Steel Parts” on page 98](#). Clean non-stainless steel parts as described in [“Cleaning Non-Stainless Steel or Hybrid Parts” on page 100](#).

❖ **To reassemble the ion source**

1. Reinstall the EI/CI Source PCB:
    - a. Align and insert the cartridge heaters and temperature sensor on the EI/CI Source PCB with the corresponding holes in the ion source block.
- IMPORTANT** Ensure that the temperature sensor is seated snugly.
- b. Reinstall the three base studs.
  2. Reinstall the filament and centering ring:
    - a. Insert the filament into the centering ring.
    - b. Align the filament leads with the EI/CI Source PCB connectors and gently press the leads into the connectors. Normally, there is a small gap of about 0.4 mm (0.016 in.) between the filament and the connectors. The gap allows the ceramic centering ring to properly position and align the electron lens hole with the ion volume.
    - c. Secure the filament and centering ring with the retainer clip.
  3. Press the heater ring and lens assemblies onto the ion source block.
  4. Use the retainer clip and threaded standoff to secure the heater ring lens assembly to the ion source. See [Figure 55 on page 96](#).

**IMPORTANT** For accurate temperature readings of the heater block, fully screw the threaded standoff into the ion source to ensure contact between the temperature sensor and the heater block.

5. Reinstall the ion source into the vacuum manifold and reinsert the capillary column into the ion source. See [“Reinstalling the Ion Source”](#) on page 92.
6. Restart the system. See [“Starting Up the System after a Complete Shutdown”](#) on page 53.

## Cleaning Stainless Steel Parts



### Tools needed

- Acetone, reagent grade (or other suitable polar solvent)
- Aluminum oxide abrasive, number 600 (P/N 32000-60340)
- Applicators, cotton-tipped (P/N 00301-01-00015)
- Beaker, 450 mL
- Clean, dry gas
- Deionized water
- Detergent (Alconox™, Micro, or equivalent)
- Dremel™ rotary tool or equivalent (recommended)
- Foil, aluminum
- Forceps (P/N 76360-0400)
- Gloves, cleanroom grade (P/N 23827-0008 and 23827-0009)
- Glycerol, reagent grade
- Lint-free cloth
- Protective eyewear
- Tap water
- Toothbrush, soft
- Ultrasonic cleaner



### Frequency

As needed to clean these stainless steel parts:

- Ion volumes
- Ion source block
- Ion source lenses



**WARNING Material and Eye Hazard.** Wear impermeable laboratory gloves and eye protection when performing cleaning procedures.

❖ **To clean stainless-steel parts**

1. Remove contamination from all the surfaces you are cleaning:
  - a. Use a slurry of number 600 aluminum oxide in glycerol and a cleaning brush or cotton-tipped applicator. Contamination appears as dark or discolored areas, but often is not visible. The heaviest contamination is usually found around the apertures, such as the electron entrance hole on an ion volume.
  - b. Clean each part thoroughly, even if no contamination is visible.
  - c. To clean the inside corners, use the wooden end of an applicator cut at an angle.
  - d. Use a Dremel tool with the polishing swab at its lowest speed. This increases cleaning efficiency as well as decrease the time required to clean the items.



**WARNING** To prevent personal injury, be sure to keep the Dremel tool away from possible hazards, such as standing water or flammable solvents.

2. Rinse the parts with clean water. Use a clean applicator or toothbrush to remove the aluminum oxide slurry. Do not let the slurry dry on the metal; dried aluminum oxide is difficult to remove.
3. Sonicate the parts in a warm detergent solution:
  - a. Using forceps, place the parts in a beaker containing warm detergent solution.
  - b. Place the beaker and contents in an ultrasonic bath for five minutes.
  - c. Rinse the parts with tap water to remove the detergent.
4. Sonicate the parts in deionized water:
  - a. Using forceps, place the parts in a beaker containing deionized water.
  - b. Place the beaker and contents in an ultrasonic bath for five minutes.
  - c. If the water is cloudy after sonicating, pour off the water, add fresh water, and place the beaker and its contents in an ultrasonic bath again for five minutes. Repeat until the water is clear.
5. Sonicate the parts in acetone:
  - a. Using forceps, place the parts in a beaker containing acetone.
  - b. Using forceps, transfer the parts to a beaker containing fresh acetone.
  - c. Place the beaker and contents in an ultrasonic bath again for five minutes.
6. Blow-dry the parts immediately. Use clean, dry gas to blow the acetone off the parts.
7. Using forceps, place the parts in a beaker, cover the beaker with aluminum foil, and put the beaker in the oven.
8. Dry the parts in an oven set at 100 °C for 30 minutes.

9. Allow the parts to cool before putting them back together.

## Cleaning Non-Stainless Steel or Hybrid Parts



### Tools needed

- Acetone, reagent grade (or other suitable polar solvent)
- Aluminum oxide abrasive, number 600 (P/N 32000-60340)
- Applicators, cotton-tipped (P/N 00301-01-00015)
- Beaker, 450 mL
- Clean, dry gas
- Deionized water
- Detergent (Alconox, Micro, or equivalent)
- Dremel rotary tool or equivalent (recommended)
- Forceps (P/N 76360-0400)
- Gloves, cleanroom grade (P/N 23827-0008 and 23827-0009)
- Glycerol, reagent grade
- Lint-free cloth
- Protective eyewear
- Tap water
- Toothbrush, soft



### Frequency

As needed to clean non-stainless steel parts (such as aluminum, ceramic, or gold plated), or to clean hybrid parts that are partially made of stainless steel:

- Lens holder and spacers
- Filament spacer
- Heater ring



**WARNING Material and Eye Hazard.** Wear impermeable laboratory gloves and eye protection when performing cleaning procedures.

### ❖ To clean non-stainless steel or hybrid parts

1. Remove contamination from stainless steel surfaces. You only need to clean a surface that comes in contact with the ion beam.
  - a. Use a slurry of number 600 aluminum oxide in glycerol and a cleaning brush or cotton-tipped applicator.

**Note** Contamination appears as dark or discolored areas, but often is not visible.

- b. Clean each part thoroughly, even if no contamination is visible.
    - c. To clean the inside corners, use the wooden end of an applicator cut at an angle.
    - d. Use a Dremel tool with the polishing swab at its lowest speed. This will increase cleaning efficiency as well as decrease the time required to clean the items.





**WARNING** To prevent personal injury, be sure to keep the tool away from possible hazards, such as standing water or flammable solvents.

- e. Rinse the parts with clean water. Use a clean applicator or toothbrush to remove the aluminum oxide slurry. Do not let the slurry dry on the metal; dried aluminum oxide is difficult to remove.
2. Scrub all of the parts with a warm detergent solution:
    - a. Scrub the parts with a toothbrush or clean applicator. Do not soak or sonicate the parts in detergent.
    - b. Using forceps, rinse the parts thoroughly with tap water to remove the detergent.



**CAUTION** Do not leave aluminum parts, such as the heater ring, in the detergent. Basic solutions, like detergent, discolor aluminum.

3. Rinse the parts in deionized water.

Using forceps, dip the parts in a beaker of deionized water. Change the water if it becomes cloudy. Do not soak or sonicate the parts.

4. Rinse the parts with acetone. Using forceps, dip the parts in a beaker of acetone. Change the acetone if it becomes cloudy. Do not soak or sonicate the parts.
5. Blow-dry the parts immediately. Use clean, dry gas to blow the acetone off the parts.

## Maintaining the Forepump

Inspecting, adding, purging, and changing the forepump oil are all that is required to maintain the forepump.

Forepump oil is a translucent, light amber color, which you must check often. During normal operation, oil must always be visible in the oil level sight glass between the MIN and MAX marks. If the oil level is below the MIN mark, add oil. If the oil is cloudy or discolored, purge the oil to decontaminate dissolved solvents. If the pump oil is still discolored, change it. Plan to change the pump oil every 3000 hours (about four months) of operation. Refer to the manufacturer's documentation for procedures for purging, adding, and changing the forepump oil.



**CAUTION** If you use ammonia as a chemical ionization reagent gas, change the oil every month. Ammonia is highly basic and quickly damages seals in the forepump. Purging the oil with the Gas Ballast Control helps remove dissolved ammonia from the oil.

## Adding Calibration Compound



### Tools needed

- Calibration compound (P/N 50010-02500)
- Syringe (P/N 36502019)



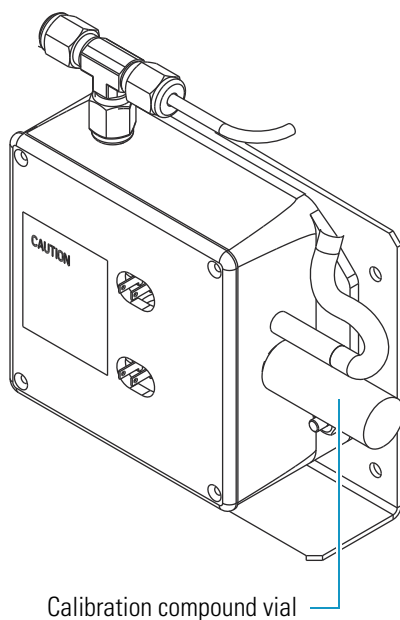
### Frequency

Yearly or as needed

The calibration compound is a liquid whose mass spectrum of ions is used to tune and calibrate the TSQ Quantum XLS Series mass spectrometers. The mass spectrometers use FC-43 as their calibration compound. Although you cannot *visually* determine when to add a calibration compound, Xcalibur Automatic Tune produces the error message: “the intensity of calibration gas ions is too low.” You must add calibration compound; however, many factors other than a decrease in the calibration compound can cause a shortage of calibration gas ions. As a rule, add calibration compound once a year.

The calibration compound resides in a cylindrical vial (see [Figure 56](#)).

**Figure 56.** Calibration gas flow modules, showing the calibration compound vial



### ❖ To add calibration compound

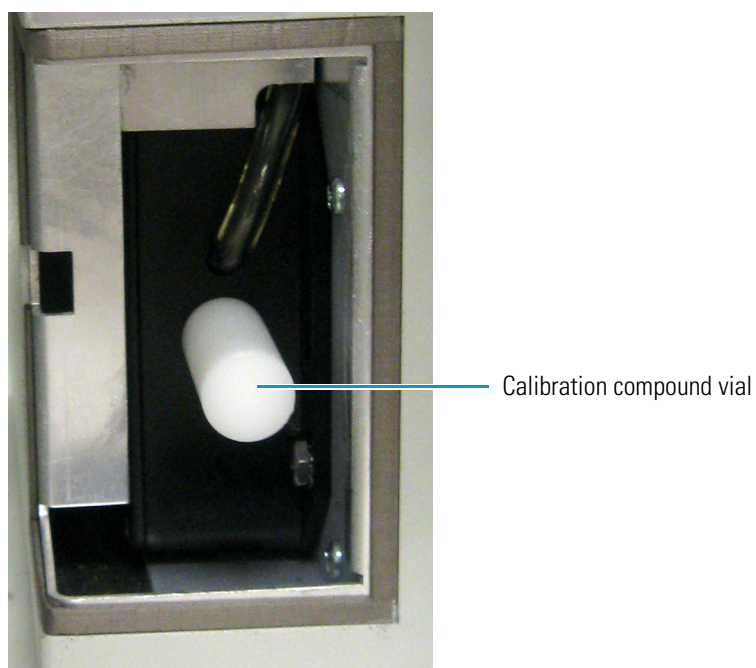
1. In EZ Tune, place the instrument in standby.
2. Remove the cover to the calibration compound vial compartment. See [Figure 57](#).

**Figure 57.** Location of the calibration compound vial compartment



3. Twist the calibration compound vial counterclockwise and remove it from the calibration gas flow module. See [Figure 58](#). Set the vial on the work table.

**Figure 58.** Calibration compound vial





**CAUTION** Having more than 0.1 mL of the calibration compound can contaminate the calibration gas flow module. Be sure that less than 0.1 mL of the calibration compound is in the vial. Be sure that liquid does not get into the flow module when you reattach the vial.

4. Add the calibration compound.
  - a. Draw up no more than 0.1 mL of calibration compound into a clean syringe.
  - b. Insert the syringe in the calibration compound vial.
  - c. Inject no more than 0.1 mL of calibration compound into the white frit. The frit absorbs the calibration compound, so if the calibration compound is pooled (calibrant covers the top of the frit), then you have too much in the vial. Immediately pour out the excess calibrant according to local environmental regulations.
5. Remove the syringe from the calibration compound vial.
6. Reinstall the calibration compound vial to the calibration gas flow module. Turn the vial clockwise to tighten it.
7. Reinstall the cover to the calibration compound vial compartment.

## Replacing the Ball Valve Seal



### Tools needed

- Ball valve seal kit (P/N 119265-0003)



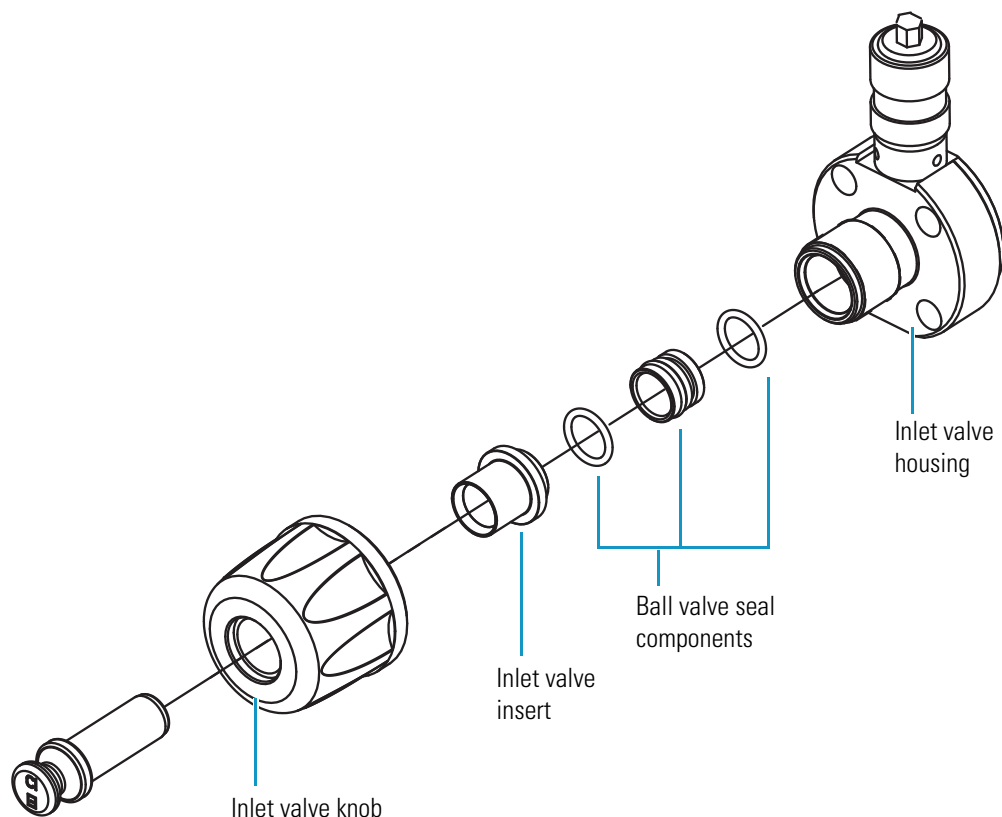
### Frequency

If the ball valve seal leaks air after you insert the direct insertion probe or I/R tool into the inlet valve and tighten the inlet valve knob

The ball valve seal in the inlet valve can become worn over time. Replace the ball valve seal if it leaks air after you insert the direct insertion probe or I/R tool and tighten the inlet valve knob. The ball valve seal kit (P/N 119265-0003) is included in the Accessory Kit.

The ball valve seal consists of a Teflon™ spool and two O-rings. See [Figure 59](#).

**Figure 59.** Components of the ball valve seal and inlet valve

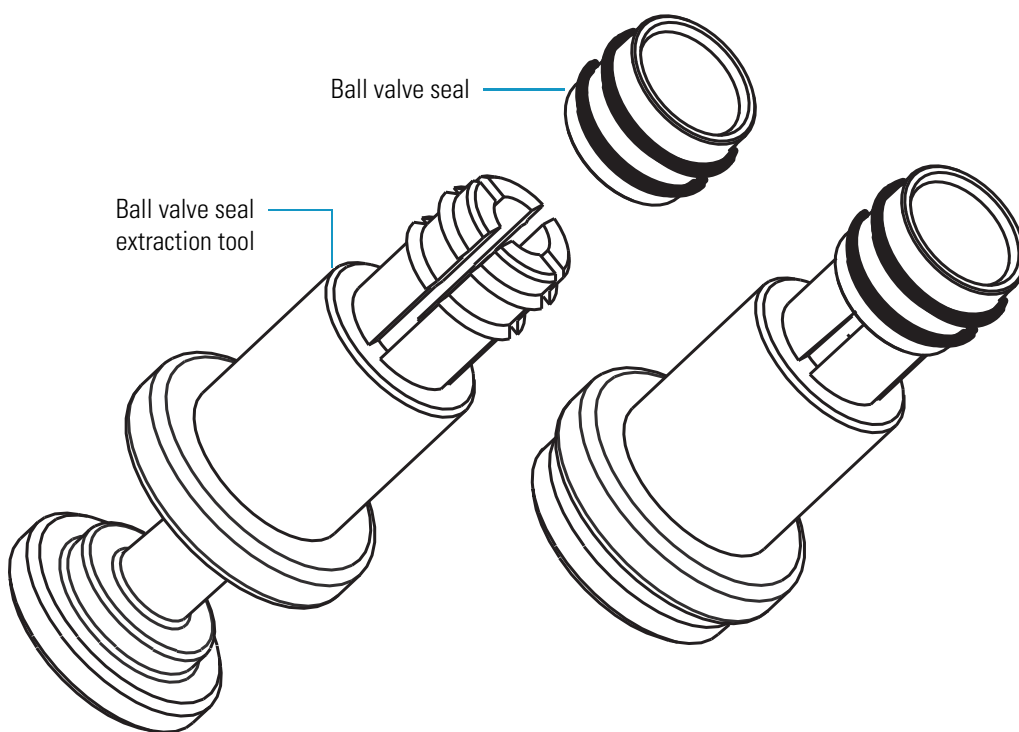


You use the ball valve seal extraction tool (part of the Ball Valve Seal Kit, P/N 119265-0003) to remove the ball valve seal. See [Figure 60](#).

❖ **To remove the ball valve seal**

1. Loosen the inlet valve knob counterclockwise until you can remove it.
2. Remove the inlet valve knob, plug, and insert.
3. Insert the not-engaged ball valve seal extraction tool into the inlet valve housing.
4. Engage the ball valve seal by pushing the plunger of the ball valve seal extraction tool forward.
5. Remove the seal and tool.
6. Pull the plunger back to disengage the seal.

**Figure 60.** Ball valve seal extraction tool and ball valve seal, not engaged (left) and engaged (right)



❖ **To install the ball valve seal**

1. Obtain the Ball Valve Seal Kit (P/N 119265-0003) from the Accessory Kit.
2. Assemble the ball valve seal by installing the two O-rings onto the Teflon spool.
3. Insert the ball valve seal into the ball valve manifold with your finger.
4. Install the inlet valve knob and insert.
5. Install the inlet valve plug and tighten the inlet valve knob clockwise.

## Removing and Installing a GC Capillary Column

Replace the GC capillary column if the chromatographic separation is bad or if it does not have the appropriate stationary phase for your application.



### Tools needed

- Gloves, cleanroom grade (P/N 23827-0008 and 23827-0009)
- Wrench, open-ended, 5/16 in.
- Wrench, open-ended, 7/16 in.
- Wrench, open-ended, 6 mm



### Frequency

As needed for maintenance or column replacement

## Removing a GC Capillary Column

### ❖ To remove a GC capillary column

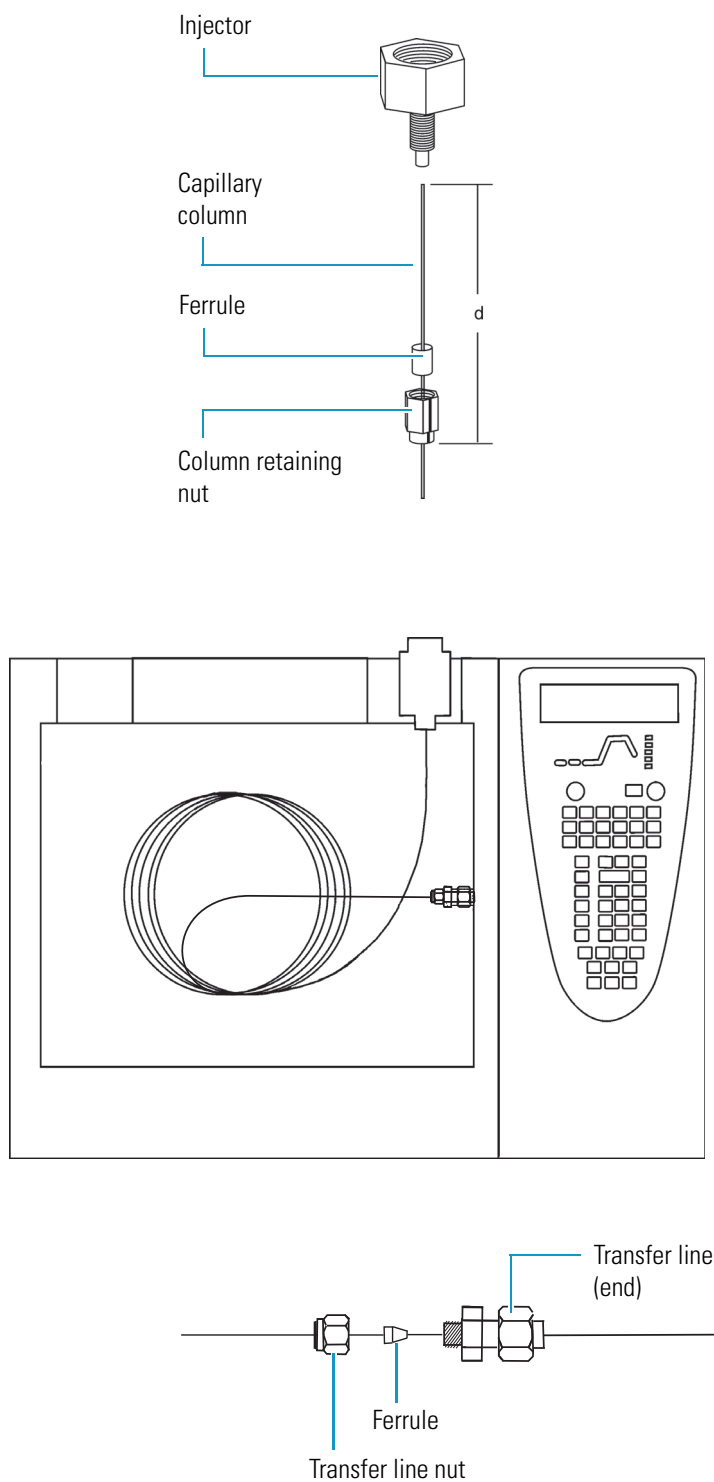
1. Shut down the mass spectrometer and the gas chromatograph:
  - a. Shut down and vent the mass spectrometer. See [“Shutting Down the System Completely”](#) on [page 51](#).
  - b. Lower the oven, injector, and transfer line temperatures to 30 °C and allow them to cool before continuing.



**WARNING Burn Hazard.** The oven, injector, and transfer line are hot. Allow them to cool to room temperature before touching them.

- c. Once the oven, injector, and transfer line are cool, turn off the gas chromatograph.
2. Remove the column from the transfer line. See [Figure 61](#).
    - a. Unscrew the transfer line nut.
    - b. Remove the column from the transfer line.

**Figure 61.** GC injector and transfer line unions



3. Remove the column from the injector. For instructions, refer to the Columns chapter of the *TRACE GC Ultra Operating Manual*.



## Installing a GC Capillary Column



### Tools needed

- Capillary column
- Gloves, cleanroom grade (P/N 23827-0008 and 23827-0009)
- Injector ferrule, for 0.25 mm column (P/N 290 134 88)
- Leak detector, hand-held electronic (GL Sciences, Inc., model LD-228, or equivalent)
- Lint-free tissue
- Magnifying glass
- Methanol or other suitable solvent
- Scoring wafer (or sapphire scribe) to cut capillary column
- Transfer line ferrule, 0.4 mm ID (P/N A0101-18100)
- Wrench, open-ended, 5/16 in.
- Wrench, two, open-ended, 7/16 in.
- Wrench, open-ended, 6 mm



### Frequency

As needed

For additional GC column installation information, refer to the *TRACE GC Ultra Operating Manual* and the *TRACE GC Ultra Maintenance and Troubleshooting Manual*.

### ❖ To install a GC capillary column



**WARNING Burn Hazard.** The injector, oven, and transfer line might be hot. Allow them to cool to room temperature before touching them.

**Note** Wear clean, lint- and powder-free gloves when you handle the column and injector ferrule.

1. Connect the column to the injector. For instructions, refer to the Columns chapter of the *TRACE GC Ultra Operating Manual*. For the column depth length for your injector, refer to the *TRACE GC Ultra Quick Reference* card.
2. Set up the gas chromatograph:
  - a. Turn on the gas chromatograph.
  - b. Set the oven and injector temperatures to 30 °C.
  - c. Set the injector flow to 1.0 mL/min.
  - d. Turn off vacuum compensation (under the Right or Left Carrier menu).
  - e. Dip the column outlet in a small vial of methanol. Bubbles indicate there is flow through the column.

- f. Allow the column to purge for at least 10 minutes.
3. Perform a manual column leak check. For instructions, refer to the Ensuring Tightness chapter of the *TRACE GC Ultra Maintenance and Troubleshooting Manual*.
4. Perform a column evaluation. For instructions, refer to the Columns chapter of the *TRACE GC Ultra Operating Manual*. For expected K factors for various column diameters, column lengths, and carrier gases refer to the *K-Factor Quick Reference* card.

**Note** The K factor is a measure of the resistance of the column. A K factor that is too low might indicate a leak in the system, while a K factor that is too high might indicate a blockage.

5. Perform an automatic column leak check:
  - a. Run an automatic leak check. Refer to the Columns chapter of the *TRACE GC Ultra Operating Manual* for instructions.
  - b. If the report indicates a leak, look for leaks and use the leak detector to fix leaks at all the fittings in the GC.
  - c. Repeat column evaluation and leak check procedures until no leaks can be found.



**CAUTION** Do not raise the oven temperature until you are sure the system is leak-free. At temperatures above 100 °C, oxygen exposure will destroy the column.

6. Condition the capillary column according to the manufacturer's instructions. You must condition new columns before inserting them in the mass spectrometer.



**CAUTION** Do not insert the column into the transfer line during the conditioning. The material released from the column during the conditioning (column bleed) will contaminate the ion source, which you must then clean.



**CAUTION** Never exceed the column manufacturer's maximum operating temperature.

7. Connect the column to the transfer line:
  - a. Shut down and vent the mass spectrometer. See [“Shutting Down the System Completely”](#) on [page 51](#).
  - b. Lower the GC oven temperature to 30 °C and allow it to cool before continuing.



**WARNING** Burn Hazard. The GC oven and transfer line might be hot. Allow them to cool to room temperature before touching them. Do not touch the injector when it is hot.

- c. Wearing clean, lint- and powder-free gloves, unwind about one turn of the capillary column (shown in [Figure 61](#) on [page 108](#)) from the column outlet end.
- d. Wipe about 450 mm (18 in.) of the column with a tissue soaked in methanol.

**Note** Sliding a septum on the column before the transfer line nut helps you measure the proper distance between the nut and the end of the column. Ensure that the column extends approximately 1 to 2 mm past the end of the transfer line.

- e. Insert the column through the transfer line nut and ferrule. Wipe the column again with a tissue soaked in methanol.
- f. Score and break the end of the column with a scoring wafer. With the magnifying glass, check for an even, flat cut. Repeat if necessary.
- g. Insert the column into the transfer line:
  - i. Open the lid of the ion source vacuum chamber so that you can get a better view of the column.
  - ii. Using the I/R tool, remove the ion volume. See [“Removing the Ion Volume”](#) on [page 73](#).
  - iii. Insert the column into the transfer line and tighten the transfer line nut by hand.
  - iv. Push the column in until you can see it through the inlet valve.
  - v. Pull the column back just far enough so that you cannot see it.
  - vi. Tighten the transfer line nut and transfer line union.
  - vii. Using the I/R tool, replace the ion volume. See [“Installing the Ion Volume”](#) on [page 80](#).
- 8. Condition the transfer line ferrule. Graphite/Vespel™ ferrules like the transfer line ferrule require conditioning to ensure a leak-tight seal.
  - a. Raise the oven temperature to the maximum temperature for operating the column (normally 300 °C).
  - b. Wait 10 minutes.
  - c. Lower the oven temperature to 30 °C and allow it to cool before continuing.



**WARNING Burn Hazard.** The oven might be hot. Allow it to cool to room temperature before opening it. Do not touch the injector, which will still be hot.

- d. Retighten the transfer line nut and the transfer line union.
- 9. Set up the gas chromatograph:
  - a. Make sure the column does not have any sharp bends and that it does not touch any metal objects or walls inside the oven.

## 6 Maintenance

### Removing and Installing a GC Capillary Column

- b. Raise the oven temperature to the initial temperature that you will use (normally 40 °C).
- c. Turn on the vacuum compensation (under the Right or Left Carrier menu).

## Diagnostics and Troubleshooting

The TSQ Quantum XLS Series system diagnostics can test many components of the TSQ Quantum XLS Series mass spectrometers. If there is a problem in the instrument electronics, the diagnostics can often locate it. Replacing a faulty PCB or assembly will usually correct the problem. After replacing a PCB or assembly, your Thermo Fisher Scientific field service engineer will run diagnostic tests again to verify that the instrument is functioning properly.

### Contents

- [Diagnostics](#)
- [Troubleshooting](#)
- [Replacing Fuses](#)
- [Replacing PCBs and Power Supplies](#)

## Diagnostics

The TSQ Quantum XLS Series system diagnostics test the major electronic circuits within the instrument and indicate whether the circuits pass or fail the tests. If the instrument electronics do have a problem, the system diagnostics can often pinpoint the location.

Because the system diagnostics only diagnose problems that are electrical in nature (for example, they do not diagnose poor sensitivity due to misaligned or dirty components or to improper tuning), whoever runs the diagnostics must be familiar with system operation and basic hardware theory as well as the details of the diagnostics.

**IMPORTANT** Typically, only a Thermo Fisher Scientific field service engineer runs diagnostic tests because certain tests can overwrite system parameters.

Before calling a Thermo Fisher Scientific field service engineer to run diagnostics, consider the following:

- Did the system fail when you were running samples?
- Did problems occur after you performed maintenance on the instrument, data system, or peripherals?

- Did you change the configuration of the system, cables, or peripherals just before the problem occurred?

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

If the answer is yes to either of the last two questions above, the problem is probably mechanical, not electrical. Reconfirm that alignment, configurations, and cable connections are correct before you call the Thermo Fisher Scientific field service engineer. Keep careful notes documenting the nature of the problem and the corrective steps you have taken. If you are not successful in correcting the problem, you can e-mail this information to your service engineer. Field Services can then do a preliminary evaluation of the problem before the field service engineer arrives at your site.

## Troubleshooting

The following topics discuss possible TSQ Quantum XLS Series system problems and solutions.

### Communication Issues

Communication issues likely involve links between the data system and the mass spectrometer, gas chromatograph, or autosampler. This section does not address communication issues with other devices.

Communication issues can occur during the following:

- Data transfer between the mass spectrometer and the data system
- Mass spectrometer, gas chromatograph, and autosampler current status readbacks
- Instrument control, method downloading, and uploading
- Start, stop, pause, and initialize functions
- Error messages

### How does the MS communication work?

The flow of digital information in the TSQ Quantum XLS Series systems is bidirectional; the data system downloads analytical methods to the instrument and activates functions to start, stop, shut down, start up, and initialize. The TSQ Quantum XLS Series systems report their readiness state, current tasks, various voltages, heated zones, and pressure readings. They also deliver a steady stream of mass spectral data during acquisition.

## Why does the MS have communication issues?

Some communication issues are due to mechanical faults—for instance, a cable might be unplugged, or a device might be turned off. In other cases, the instrument method could be incorrect for TSQ Quantum XLS Series system operations. Less common communication issues are due to defective electronic hardware components.

## How do I detect communication issues?

You might detect communication issues from an error message delivered by the data system, or you might notice the failure of the data system to perform some expected task.

**Issue:** Data system is unable to initiate communication with the mass spectrometer.

### Possible causes/solutions

- The software is not configured correctly. Select and configure the mass spectrometer from the Instrument Configuration window.
- The Ethernet cable is unplugged. Verify that the Ethernet cable is connected to the Ethernet port on the mass spectrometer. See [Figure 14](#) on [page 25](#).
- The Ethernet card in the PC is not configured or is faulty. Check the configuration or replace the Ethernet card if necessary.
- The electronics service switch of the mass spectrometer is in the Service Mode position. Return the electronics service switch to the Operating position.
- An incorrect Ethernet cable is used for the mass spectrometer. Use the supplied 10 Base-T Category 5 crossover cable (P/N 76396-0052, in the TSQ Quantum XLS Accessory Kit).

**Note** You can extend the length of the Ethernet cable by plugging a standard Category 5 cable in series with the supplied crossover cable.

**Issue:** Computer intermittently loses communication with the mass spectrometer.

### Possible cause/solution

- The Ethernet cable is loose or damaged. Inspect the cable and replace it if necessary.

**Issue:** Unable to download methods to the mass spectrometer.

### Possible cause/solution

- The software is not properly configured. Verify the correct settings in Instrument Configuration.

**Issue:** Acquisition does not begin as expected.

**Possible causes/solutions**

- The start mode is not properly configured. Verify that the instrument is configured properly. Refer to the Xcalibur Help for more information.
- The mass spectrometer Instrument Setup file has incorrect settings. Check the start time in the Instrument Setup file.
- The forepressure is too high due to the solvent peak. Reduce injection volume or extend the filament/multiplier delay time until after solvent peak.
- The remote start cable to the GC is disconnected. Connect the remote start cable.
- The GC did not start. Verify GC instrument method and configuration. Verify the connection between the autosampler and GC.
- The autosampler did not start. Verify autosampler instrument method and configuration. Verify that the sample is present.
- The heated zone stipend is not attained. See [“Heated Zone Issues”](#) on [page 120](#).

**Issue:** Acquisition terminates unexpectedly.

**Possible causes/solutions**

- The end run time in the TSQ Quantum XLS Series instrument method is incorrect. Check the instrument method for the GC and the MS.
- The data system is out of disk space. Check disk space; back up and remove files.

**Issue:** Unable to initialize the gas chromatograph.

**Possible causes/solutions**

- The GC is not turned on. Turn on the GC.
- The GC is not configured properly in the Xcalibur data system. Check Instrument Configuration.
- The cable between COM1 and GC is disconnected. Verify connection.
- COM1 is not configured properly. Verify COM port configuration.

**Issue:** Unable to download methods to the gas chromatograph.

**Possible causes/solutions**

- There is a discrepancy between the instrument method and configuration. Verify consistency between method and instrument configuration.
- COM1 is not configured properly. Verify COM port configuration.



**Issue:** Unable to initialize the autosampler.

**Possible causes/solutions**

- The autosampler is not turned on. Turn on autosampler.
- The autosampler is not configured properly in the Xcalibur data system. Check Instrument Configuration.
- The cable between the GC and autosampler is disconnected. Verify connection.
- The autosampler instrument configuration is not set to the correct port. Verify connection and configuration.

**Issue:** Unable to download methods to the autosampler.

**Possible cause/solution**

- There is a discrepancy between instrument method and configuration. Verify consistency between instrument method and instrument configuration.

## Contamination Issues

Chemical noise is always present in any mass spectrometer. As a result, the high sensitivity of the mass spectrometer can cause new users to confuse background with a contamination problem. Additionally, the spectra shown in Xcalibur Tune and Real-Time Display are auto-normalized, which can make the background level appear high.

Some chemical noise does occur, such as septum bleed after a series of injections, vial sample bleed (which occurs if more than one injection is made from a sample vial), and siloxane peaks that appear in the chromatogram at regular intervals from focusing at the head of the column or in the injector.

Other possible contamination sources include hydrocarbon contamination of the carrier gas, pump oil, or instrument cleaning solvents.

Always wear clean, lint- and powder- free gloves when handling ion source and mass analyzer components, and ensure that the carrier gas filter, carrier gas lines, and gas regulators are free of contamination and leaks.

**Issue:** Excessive chemical background due to a column bleed ( $m/z$  429, 355, 281).

**Possible causes/solutions**

- The capillary column has not been properly conditioned. Condition the capillary column.
- The capillary column is damaged as a result of exposure to oxygen. Find the source of the oxygen in the carrier gas or air leak. Recondition or replace the capillary column.

**Issue:** Excessive injection port septum bleed (Typical  $m/z$  207, 429, 355, 281).

**Possible causes/solutions**

- The septum is worn out or damaged. Replace the septum.
- Small pieces of septum are in the injection port liner. Replace the injection port liner; condition the capillary column.

**Issue:** Phthalate background ( $m/z$  149, 167, 279).

**Possible causes/solutions**

- Phthalate contamination has occurred due to sample handling or solvent contamination.
- Packaging materials could be the source of phthalates.
- Isolate source of phthalates such as vial lids or plastic solvent containers and remedy.

**Issue:** Excessive hydrocarbon contamination (Typical ions are  $m/z$  43, 57, 71, 85, 99).

**Possible causes/solutions**

- Carrier gas tubing is contaminated.
- Isolate source of hydrocarbon contamination and remedy.
- Replace carrier gas tubing.
- Change carrier gas filters.

**Issue:** Chemical background due to rhenium oxide ( $m/z$  185/187, 201/203, 217/219, 233/235, 250/252).

**Possible causes/solutions**

- These series of rhenium oxide ions come from oxidation of the rhenium filament wire due to introducing air into the ion source while the filament is on.
- Check for air leaks and remedy. For more information, see [“High Vacuum Issues”](#) on [page 121](#).

**Issue:** Spectra are observed due to the following solvents:

**Solvent spectra**

Acetone ( $m/z$  43, 58, 59)

Hexane ( $m/z$  41, 43, 56, 57, 58, 85, 86)

Methanol ( $m/z$  31)

Methylene chloride ( $m/z$  84, 83)

Toluene ( $m/z$  91, 92)

Trichloroethane ( $m/z$  151, 153)

Xylene ( $m/z$  105, 106)

**Possible causes/solutions**

- There is residual solvent from a cleaning procedure or laboratory background contamination. When you finish performing a cleaning procedure, allow cleaned components to dry thoroughly. Warm parts in the GC oven to drive off residual solvent.
- The observed compounds have been introduced through sample injection. The ultimate source is either a sample solvent or the autosampler rinsing solvent. Optimize GC method to separate solvent peak from the area of interest in the chromatogram.

## Filament and Lens Control Issues

The lifetime of a filament depends on its exposure to oxygen and solvent vapors. The filament assembly protects the filament and increases its lifetime for many months.

Xcalibur diagnostics test the filament for continuity and current regulation. Testing the filament for continuity before each acquisition ensures that an open filament condition will stop an autosampler sequence and generate an error message.

Diagnostics test the lenses of the TSQ Quantum XLS Series mass spectrometers. A flat line, which represents voltage readback versus the predicted voltage ramp, indicates a lens or other control fault. Contamination causes lens performance to deteriorate over time; the amount of time depends on what type of sample and ionization mode you use.



**CAUTION** Handle the lenses with care, and do not use harsh cleaning techniques. Damaged lenses cause short circuits, which in turn can cause damage to the lens drivers.

**Issue:** Diagnostics indicate that the filament is open.

**Possible cause/solution**

- The filament is open. Vent the system and remove the filament. Normal resistance is 1.0  $\Omega$ . Replace if open.

**Issue:** Unstable emission current.

**Possible cause/solution**

- The filament is near the end of its life span. Replace the filament.

**Issue:** Short filament lifetime.

**Possible causes/solutions**

- There is an air leak contributing to short filament lifetime. Check for leaks; repair if any are found. For more information, see [“High Vacuum Issues”](#) on [page 121](#).
- The filament is on during the solvent peak. Increase acquisition delay time until the solvent peak has passed.
- High emission current is being used. Use lower emission current to extend lifetime.

**Issue:** Diagnostics indicate a flat lens response.

**Possible causes/solutions**

- The power supply to the lens has a fault. Contact Thermo Fisher Scientific Technical Support.
- There is a fault with the lens drivers. Contact Thermo Fisher Scientific Technical Support.

## Heated Zone Issues

The ion source and transfer line are heated zones. The mass spectrometer controls the ion source heater and the Aux1 heated zone of the TRACE GC Ultra controls the transfer line heater.

A heated zone problem is often the result of downloading an instrument method to the instrument that has a different setpoint than the current setting, causing a delay while the heated zone heats or cools.

Component failures are less common but can occur. These are usually related to open circuits in heater cartridges or faulty temperature sensors.

This manual does not discuss heated zones in the gas chromatograph.

**Issue:** Excessive chromatographic peak tailing.

**Possible causes/solutions**

- The ion source, transfer line, or both are not hot enough. Increase the transfer line temperature so that it is at least as hot as the highest GC oven temperature. Then, try increasing the ion source temperature.
- The sample analyte is adsorbing in the GC injector. Clean and deactivate the injection liner. You can also try liners made of different materials.
- The GC oven is not ramped to a high enough temperature. Extend upper oven temperature.
- The GC column must be replaced or does not have the appropriate stationary phase for your application. Change the GC column. See [“Removing and Installing a GC Capillary Column”](#) on [page 107](#).
- The GC column does not extend far enough past the end of the transfer line tip. If the end of the column is inside the tip, an excessive amount of GC effluent will contact the inside wall of the tip. Follow the procedure described in [“Installing a GC Capillary Column”](#) on [page 109](#).

**Issue:** Source heater will not heat.

**Possible causes/solutions**

- No contact between the ion source temperature sensor and the heater block. For accurate temperature readings of the heater block, fully screw the threaded standoff into the ion source to ensure contact between the temperature sensor and the heater block. See [“Reassembling the L1, L2, L3 Lens Assembly” on page 92.](#)
- One or more heater cartridges on the EI/CI Source PCB is defective. Replace the EI/CI Source PCB. See [“Completely Disassembling and Reassembling the Ion Source” on page 95.](#)
- The ion source temperature sensor (RTD) is defective. Replace the EI/CI Source PCB. See [“Completely Disassembling and Reassembling the Ion Source” on page 95.](#)

**Issue:** Source heater overheats.

**Possible cause/solution**

- The ion source temperature sensor (RTD) is defective. Replace the EI/CI Source PCB if necessary. See [“Completely Disassembling and Reassembling the Ion Source” on page 95.](#)

**Issue:** Transfer line will not heat.

**Possible causes/solutions**

- Aux1 zone of the GC is not configured for MS Transfer Line. Configure Aux1 zone of the GC and set transfer line temperature in the GC Method Editor.
- Transfer line heater elements are defective. Replace the transfer line.
- The transfer line temperature sensor (RTD) is defective. Replace the transfer line.

**Issue:** Transfer line overheats.

**Possible cause/solution**

- The transfer line temperature sensor is defective. Replace the transfer line.

## High Vacuum Issues

High vacuum problems can become obvious in two ways:

- An intermittent vacuum condition (the vacuum pressure in the vacuum manifold fluctuates intermittently) can cause chromatographic signals to drop out; or if the pressures exceed the maximum allowed pressures set in the Xcalibur data system (see [Table 3 on page 55](#)), then the TSQ Quantum XLS Series system turns off.
- If the vacuum is consistent enough that it does not exceed the maximum allowed pressure and avoids automatic shutdown of the Xcalibur system, non-reproducible false chromatographic peaks can be generated in the chromatogram.

Typical forepressure readbacks are 30 to 40 mTorr (in EI mode), and typical manifold pressure (ion gauge readback) is  $2 \times 10^{-5}$  Torr with argon collision gas on, and  $2 \times 10^{-6}$  Torr with Ar collision gas off.

**Note** The mass spectrometer performs a leak check during the automatic tuning and calibration procedure and during the maintenance tune procedure. The mass spectrometer returns a pass or fail report.

The most reliable way to find vacuum leaks is to spray a gas around the vacuum manifold and look for the characteristic ions in full-scan EI mode. Argon produces  $m/z$  40. Or, you can use compressed electronic dusting spray containing an HFC. For example, Falcon™ Dust-Off™ and MicroCare™ Micro-Blast™ contain tetrafluoroethane, which produces ions at  $m/z$  69 and 83.

**Issue:** Forepump will not turn on.

**Possible causes/solutions**

- The forepump is off. Check the forepump switch.
- The vacuum service switch is in the Off position. Place the vacuum service switch in the operating position.
- The forepump power cable from the mass spectrometer is not connected. Connect the power cable.
- The forepump is faulty. Replace the forepump.

**Issue:** Forepump powers on, but will not pump down.

**Possible causes/solutions**

- The oil level in the forepump is insufficient. Check oil level; add oil if necessary.
- The foreline is leaking. Check the clamps and connectors. Replace the foreline hose if a hole is found.
- The vacuum manifold is leaking.
- The forepump is faulty. Replace the forepump.

**Issue:** Turbo pump shuts off during operation.

**Possible cause/solution**

- The foreline pressure is too high. Check for leaks in the foreline.

**Issue:** Unexpected full ventilation occurs.

**Possible causes/solutions**

- A gross leak is present. Check for leaks.
- The system was vented through the inlet valve. Close and plug the inlet valve.
- The GC column broke at the transfer line. Replace the GC column. See [“Removing and Installing a GC Capillary Column”](#) on page 107.
- The foreline was cut. Replace the foreline hose.

**Issue:** Vacuum is faulty.

**Possible Solutions**

- A gross leak is present. Check for leaks.
- The pressure in the analyzer region of the vacuum manifold, as measured by the ion gauge, must be below the pressures listed in [Table 3](#) on [page 55](#).

## Linearity Issues

Linearity issues occur when a plot of intensity versus concentration of a known compound is not linear. Poor instrument operating conditions can cause linearity problems. In addition, certain compounds do not give a desired linear response due to chromatographic activity.

A well-maintained instrument provides good linear response over a wide range of concentrations for most compounds. Like all instruments, however, the TSQ Quantum XLS Series mass spectrometers have a saturation point.

Perform routine injector and column maintenance to minimize linearity problems. Usually, a hardware fault that affects linearity shows different issues than those that might be attributed to linearity.

**Issue:** Calibration plots not sufficiently linear.

**Possible causes/solutions**

- High-end standards are too concentrated for the MS. Use the split injection technique to decrease the amount of sample, or lower emission current to reduce MS sensitivity.
- The ion volume and lenses are dirty. Clean ion volume and lenses as described in [“Cleaning Ion Source Components”](#) on [page 85](#).
- The electron multiplier setting is incorrect. Run the tune and calibration procedure as described in [“Running Auto Tune and Calibration”](#) on [page 64](#).
- The injection port liner or capillary column is dirty. Change the injection port liner and trim the capillary column.
- The capillary column stationary phase is too thin for high concentration samples. Use a higher capacity capillary column with a thicker stationary phase, or use a split injection technique.
- The capillary column is bad. Replace the capillary column. See [“Removing and Installing a GC Capillary Column”](#) on [page 107](#).

## Power Supply Issues

Xcalibur diagnostics detect most power supply issues. Power supply problems often involve a blown fuse, faulty electronic components, or something as simple as a disconnected cable. Have a Thermo Fisher Scientific field service engineer replace a blown fuse.

**Issue:** Mass spectrometer will not power on.

**Possible causes/solutions**

- The power cord is disconnected. Verify that the power cord is plugged in.
- Voltage is not coming from the electrical outlet. Verify that the electrical outlet is operational.
- The Power Module is faulty. Contact Thermo Fisher Scientific Technical Support.

**Issue:** Mass spectrometer powers on but trips the circuit breaker.

**Possible causes/solutions**

- The Power Module is faulty. Contact Thermo Fisher Scientific Technical Support.
- The forepump causes the circuit breaker to trip. Check forepump; replace it if necessary.

## Sensitivity Issues

If you observe a drop in instrument sensitivity, determine if the sensitivity drop was sudden or if it occurred gradually. A sudden loss of sensitivity can be the result of sudden component failure or an unnoticed change in the analytical method. Simple errors such as a plugged autosampler syringe or too low sample level in the sample vial can give the appearance of instrument failure.

Gradual drops in sensitivity are usually the result of ion volume or lens contamination, and are easily remedied by cleaning the ion volume or lenses.

The electron multiplier influences sensitivity and has a limited lifetime. Eventually you must replace the electron multiplier.

Improper GC maintenance is another cause of diminished sensitivity. It is important to establish a routine maintenance program for the GC. For more information on establishing a maintenance program, refer to the *TRACE GC Maintenance Manual*.



**Issue:** The chromatogram has a low total ion current signal.

**Possible causes/solutions**

- The GC temperature ramp does not continue to a high enough temperature to elute high boiling point compounds. Multiple injections cause these compounds to accumulate in a column, reducing sensitivity. Extend upper temperature or the time at upper temperature in the GC oven ramp.
- The instrument is out of tune, or the tune file is incorrect. Select the correct tune file for the method or run automatic tune as described in [“Running Auto Tune and Calibration”](#) on [page 64](#).
- The ion volume is contaminated. Clean the ion volume.
- The ion volume is incorrectly positioned. Position the ion volume properly.
- The magnets above and below the ion source are installed incorrectly. Position both magnets so that the south pole is on top. Electrons will not focus into the ion volume if one magnet is upside down.
- Dust has collected in the electron multiplier or on the conversion dynode. Contact Thermo Fisher Scientific Technical Support.
- The emission current is set too low. Check the setting listed for the emission current.
- The ground connection between the Electrometer PCB and anode feedthrough is faulty. Contact Thermo Fisher Scientific Technical Support.
- There is a problem with the filament or lens control. See [“Filament and Lens Control Issues”](#) on [page 119](#) for more information.
- The EI/CI Source PCB is faulty, which allows emission current to leak to ground. Contact Thermo Fisher Scientific Technical Support.
- Reagent gas is leaking into the analyzer and suppressing EI signal. Check for presence of CI reagent ions in the spectrum. Replace CI Gas Flow Module if necessary.

**Issue:** Poor compound sensitivity.

**Possible causes/solutions**

- The syringe, injection port liner, and column depth in the injector are incorrectly matched. For the correct combination, refer to the *TRACE GC Ultra Operators Manual*.
- Sample delivery is insufficient due to a plugged syringe needle. Clean or replace the syringe.
- The injection port liner is contaminated. Clean or replace the injection port liner.
- Graphite or septa particles contaminate the injection port. Clean the injection port.
- The injector or septum is leaking. Replace septum and perform leak check on the GC.
- The capillary column is at the end of its life span. Replace the capillary column.
- Method development problems are present. Contact Thermo Fisher Scientific Technical Support.

**Issue:** Sensitivity is unstable or shows decrease with repeated injections.

**Possible causes/solutions**

- The GC temperature ramp does not continue to a high enough temperature to elute high boiling point compounds. Multiple injections cause these compounds to accumulate in a column, reducing sensitivity. Extend the upper temperature or the time at upper temperature in the GC oven ramp.
- The ion volume or lenses are contaminated. Clean the ion volume and lenses as described in [“Cleaning Ion Source Components”](#) on [page 85](#).
- The ion source temperature is too low and causes the ion source to contaminate too quickly. Clean ion volume and lenses as described in [“Cleaning Ion Source Components”](#) on [page 85](#) and then raise ion source temperature.
- There is a problem with the filament emission current control. See [“Filament and Lens Control Issues”](#) on [page 119](#) for more information.
- The electron multiplier is faulty. Contact Thermo Fisher Scientific Technical Support.
- The injection port liner or capillary column is contaminated. Replace the injection port liner and trim the capillary column.

**Issue:** Poor sensitivity in CI mode.

**Possible causes/solutions**

- An EI ion volume is installed. Install a CI ion volume as described in [“Changing Ionization Modes”](#) on [page 73](#).
- The small hole in the CI ion volume is plugged. Use a dental pick or old syringe needle to clear it.
- The filament is not aligned. Remove the ion volume and check if the ion burn is centered around the small electron entrance hole. Be sure the filament is properly inserted into the connector. Carefully bend the filament wire to better align it with the ion volume.
- The ion volume is not inserted properly. While running the instrument, you can push on the ion volume with the I/R tool. Be sure to monitor the pressure to ensure that you get a good seal around the I/R tool. Otherwise, you might damage the filament. An increase in signal calibration gas as you push on the ion volume usually indicates that the filament is not aligned properly.

## Stability Issues

Stability helps provide consistent instrument precision and the reproducibility of accurate results. Good operating conditions for the mass spectrometer, gas chromatograph, and autosampler contribute to instrument stability.

Sample preparation, spiking errors, sample injection errors, and lack of routine maintenance on the instruments can cause false stability issues.

When hardware faults affect instrument stability, investigate simple solutions first, such as cleaning the ion volume and lenses, or checking for air leaks. Usually, a hardware fault that affects stability shows different issues than those which might be attributed to stability.

**Issue:** The signal response is unstable or drops out unexpectedly.

**Possible causes/solutions**

- There is a problem with the filament or lens control. See [“Filament and Lens Control Issues”](#) on [page 119](#) for more information.
- There is an air leak. Run the maintenance tune or the Xcalibur auto tune and calibration procedure, which performs a leak check and returns a pass or fail message. If necessary, check for leaks. See [“High Vacuum Issues”](#) on [page 121](#) for more information.
- There is a high vacuum problem. See [“High Vacuum Issues”](#) on [page 121](#) for more information.
- There is a contamination problem. See [“Contamination Issues”](#) on [page 117](#) for more information.
- Dust has collected in the electron multiplier or on the conversion dynode. Contact Thermo Fisher Scientific Technical Support.

## Tuning Issues

You can suspect a tuning problem when Xcalibur auto tune and calibration fails. The auto tune and calibration procedure performs several functions, and issues or error messages indicate different problems. Diagnostics can usually uncover a tuning problem.

**Issue:** "Cannot find Calibration Gas" error message received.

**Possible causes/solutions**

- There is a mechanical problem with the ion source or lenses. Verify that an EI ion volume is installed. Verify correct orientation and cleanliness of ion volume. Verify cleanliness and correct operation of lenses.
- Tune file settings are out of usable range. Restore default tune settings and calibration settings. Run Auto Tune and Calibration. See ["Tuning and Calibrating"](#) on [page 61](#).
- The calibration gas vial is empty. Add 100 µL (max) of calibration compound to calibration gas vial. See ["Adding Calibration Compound"](#) on [page 102](#).

**Issue:** The electron multiplier gain calibration fails.

**Possible causes/solutions**

- The electron multiplier has not been given sufficient time to outgas since venting. Allow more time to pump out.
- The GC column flow is too high. Lower it to 1 mL/min.
- The multiplier is near the end of its lifetime. Multipliers typically last about 2 to 3 years before they are too noisy for the gain to be set accurately. Contact Thermo Fisher Scientific Technical Support.
- The multiplier power supply is faulty. Contact Thermo Fisher Scientific Technical Support.
- The filament is the source of too much background noise. See ["Filament and Lens Control Issues"](#) on [page 119](#) for more information.
- Chemical background in the manifold is elevated. Remedy leaks or sources of water contamination in carrier gas. See ["High Vacuum Issues"](#) on [page 121](#) for more information.
- The difference between the electron energy and the setpoint is greater than 5 V. Contact Thermo Fisher Scientific Technical Support for assistance.

**Issue:** Poor high mass response.

**Possible causes/solutions**

- Poor high  $m/z$  ion intensity because the ion source temperature is too high. Reduce the ion source temperature to reduce the amount of thermal decomposition and fragmentation of your analyte.
- Poor high  $m/z$  ion intensity because of bad ion source lens settings. Run the tune and calibration procedure. See “[Tuning and Calibrating](#)” on [page 61](#).
- Helium pressure in the ion source is too high or low. Set flow to 1.0 mL/min for most applications.
- There is a vacuum leak. Find and repair any leaks. Be sure to check the transfer line fitting in the GC oven. See “[High Vacuum Issues](#)” on [page 121](#) for more information.
- An excess amount of low  $m/z$  ions, such as hydrocarbons or column bleed. Remedy the source of these low  $m/z$  ions.
- The ion volume or lenses are contaminated. Clean the ion volume or lenses. See “[Cleaning Ion Source Components](#)” on [page 85](#).
- $m/z$  131 is not base peak because the multiplier gain is too low. The multiplier gain calibration may set the multiplier voltage too low for a noisy multiplier. Electron multipliers older than 2 to 3 years are often noisy. Contact Thermo Fisher Scientific Technical Support.
- There is poor high  $m/z$  intensity and poor resolution of low  $m/z$  ions because the conversion dynode is faulty. Contact Thermo Fisher Scientific Technical Support.
- The injection rf is not calibrated. Run the tune and calibration procedure as described in “[Tuning and Calibrating](#)” on [page 61](#).
- There is a problem with the filament or lens control. See “[Filament and Lens Control Issues](#)” on [page 119](#) for more information.
- Reagent gas is leaking into the analyzer and suppressing the EI signal. Check for the presence of CI reagent ions in the spectrum. Replace the CI Reagent Gas Flow Module if necessary.

**Issue:** Weak signal.

**Possible causes/solutions**

- The ion volume or ion source lenses are dirty. Clean the contaminated components as described in [“Cleaning Ion Source Components”](#) on page 85.
- The multiplier is set too low. Run multiplier gain calibration in the tune and calibration procedure as described in [“Tuning and Calibrating”](#) on page 61. An electron multiplier older than 2–3 years may be too noisy for the multiplier gain calibration to accurately set the voltage. You might need to replace the electron multiplier. Contact Thermo Fisher Scientific Technical Support.
- The wrong type of ion volume is installed. EI and CI require different ion volumes. They may not be used interchangeably. Change the ion volume as described in [“Changing Ionization Modes”](#) on page 73.
- The ion volume is absent or incorrectly positioned. Verify that the ion volume is positioned correctly.
- There is a filament or lens control problem. See [“Filament and Lens Control Issues”](#) on page 119 for more information.
- The electron multiplier is faulty. Contact Thermo Fisher Scientific Technical Support.

## Replacing Fuses



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

## Replacing PCBs and Power Supplies



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

## Using the Direct Sample Probe

With the direct sample probes (direct insertion probe and direct exposure probe) you can introduce compounds directly into the ion source without GC column separation. This chapter covers, step-by-step, a direct insertion probe (DIP) experiment using perfluorotetracosane ( $\text{CF}_3(\text{CF}_2)_{22}\text{CF}_3$ , molecular weight 1238.18, melting point 190 °C). You can perform a similar experiment using your compound.

### Contents

- [Creating an Instrument Method](#)
- [Creating a Sequence](#)
- [Preparing the Probe and Inlet Valve](#)
- [Preparing the Mass Spectrometer](#)
- [Running the Sequence](#)
- [Examining the Raw Data in Qual Browser](#)
- [Removing the Probe](#)

## Creating an Instrument Method

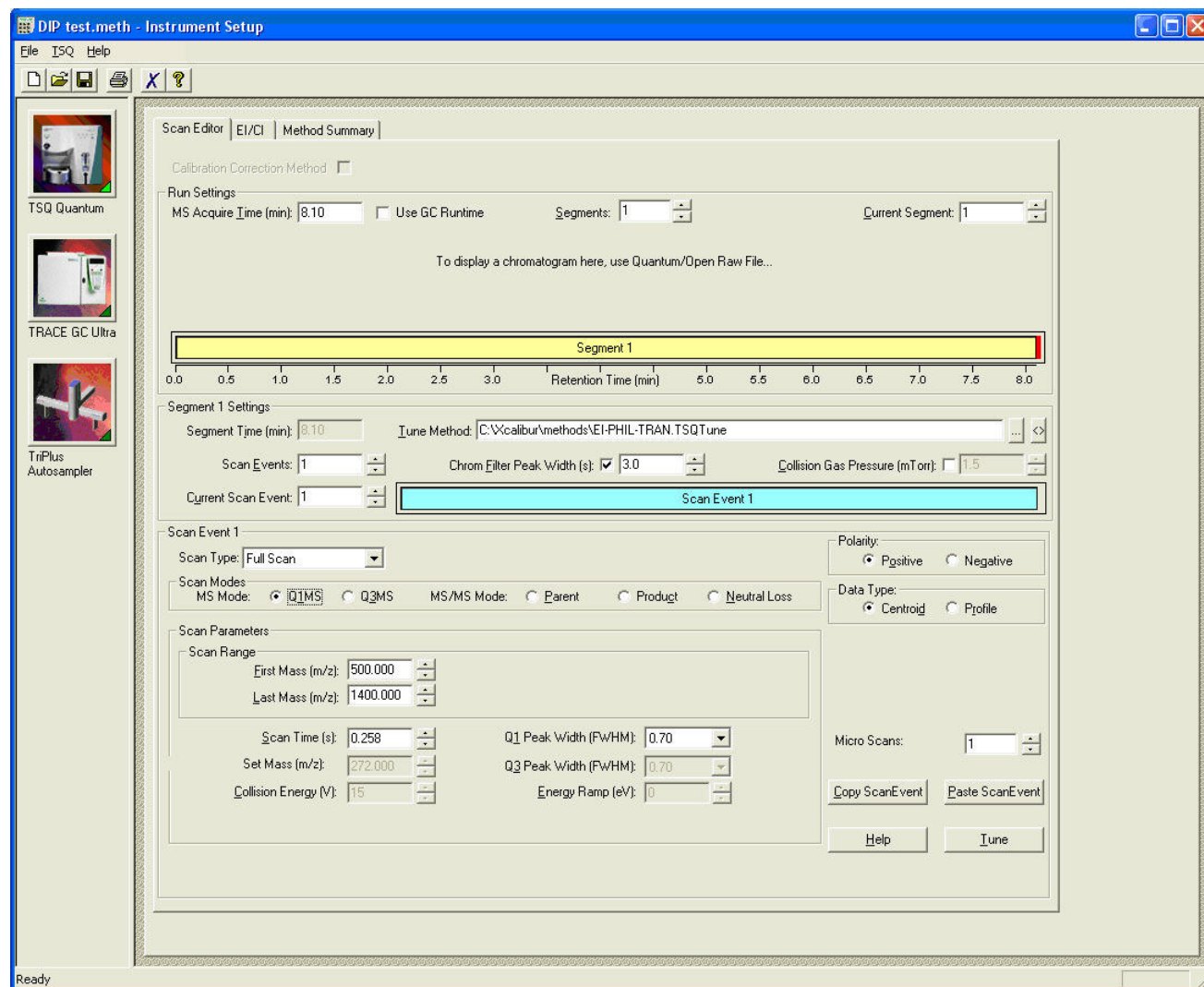
An instrument method contains the settings that the TSQ Quantum XLS Series mass spectrometer uses during an experiment. Use the Instrument Setup view to create the instrument method.

### ❖ To create an instrument method

1. On the Thermo Xcalibur Roadmap, click the **Instrument Setup** icon to open the Instrument Setup view.
2. Click the **TSQ** icon in the viewbar.
3. Choose **TSQ > Regular Method** to open the regular method Scan Editor page.
4. On the Scan Editor page, create a one segment, one scan event instrument method. In this example, the segment is 8 minutes long (see [Figure 62](#)).

- Specify the mass spectrometer settings: for this example, **Full-Scan** (Scan Type list), **Q1MS** (Scan Modes|MS Mode option), and **Positive** (Polarity area).

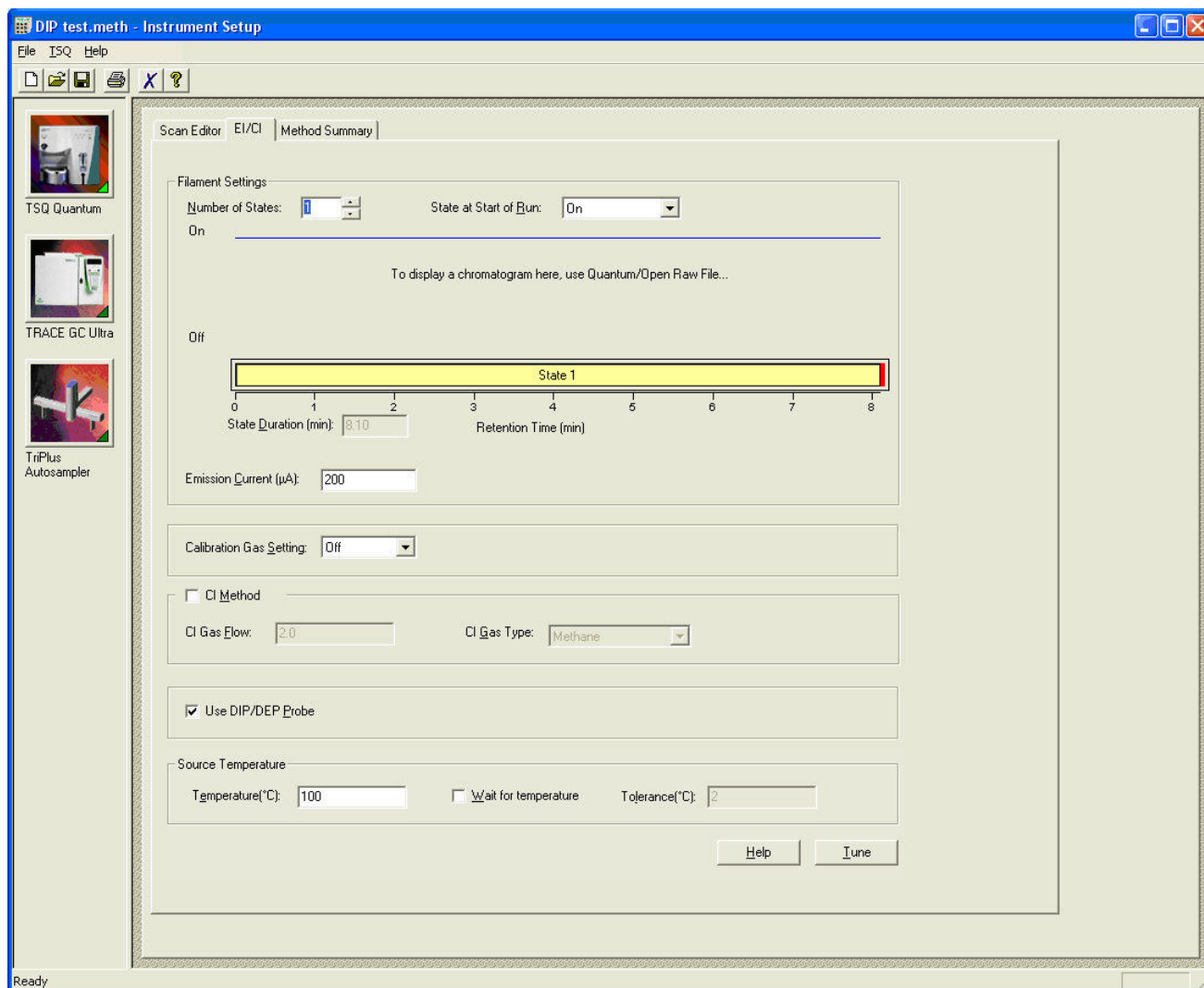
**Figure 62.** Scan Editor page of Instrument Setup




- Click the **EI/CI** tab to display the EI/CI page (see [Figure 63](#)).



**Figure 63.** EI/CI page of Instrument Setup



7. Enter or select the following settings:

- Number of States: **1**
- State at Start of Run: **On**
- Calibration Gas Setting: **Off**
- Use DIP/DEP Probe: 

This example is an EI experiment with a 200 µA emission current.

8. Save the instrument method.

- a. Choose **File > Save As** to open the Save As dialog box.
- b. Save the instrument method as a .meth file. In this example we name the instrument method **Dip test.meth**.

## Creating a Sequence

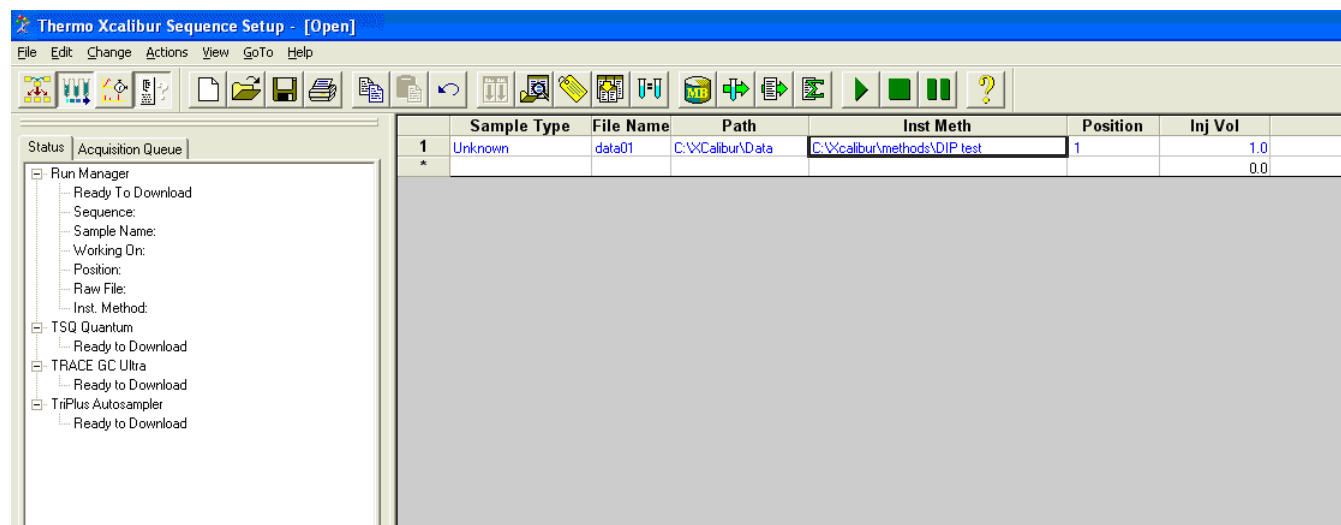
A sequence contains sample information—one sample per row. In this example the sequence has one sample.

**Note** If the sequence has more than one sample, the Xcalibur data system prompts you to reload the probe after each sample.

### ❖ To create a sequence

1. Click **Start > Programs > Thermo Xcalibur > Xcalibur** to open the Thermo Xcalibur Roadmap.
2. On the Thermo Xcalibur Roadmap, click the **Sequence Setup** icon to open the Sequence Setup view (see [Figure 64](#)).
3. Enter the name and path of the instrument method. In this example, it is **C:\Xcalibur\methods\DIP test**.
4. Enter a file name and path for the raw file that contains the acquired data. In this example, it is **C:\Xcalibur\Data\data01**.

**Figure 64.** Sequence Setup view, showing one sample in the sequence



## Preparing the Probe and Inlet Valve

### ❖ To prepare the probe and inlet valve

1. Connect the direct sample probe controller to the mass spectrometer by contact closure with the probe start cable (P/N 70111-63627, in the Accessory Kit).
2. Create a probe method on the controller. Refer to the probe manual. This example uses the following DIP settings:
  - Initial temperature: **50 °C**
  - Initial time: **5 s**
  - Ramp rate: **100 °C/min**
  - Final temperature: **200 °C**
  - Ramp hold time: **200 s**
3. Load sample on the probe.
4. Install the guide bar:
  - a. With the guide ball track facing left, insert the guide bar into the entry housing. See [Figure 17](#) on [page 28](#).
  - b. Push the guide bar in as far as it goes. Rotate it 90° clockwise to lock the guide bar in the entry housing.
5. Prepare the inlet valve:
  - a. Make sure the inlet valve is closed with the inlet valve lever down, as shown in [Figure 17](#) on [page 28](#).
  - b. Loosen the inlet valve knob counterclockwise, and remove the inlet valve plug.

## Preparing the Mass Spectrometer

### ❖ To prepare the mass spectrometer for the experiment

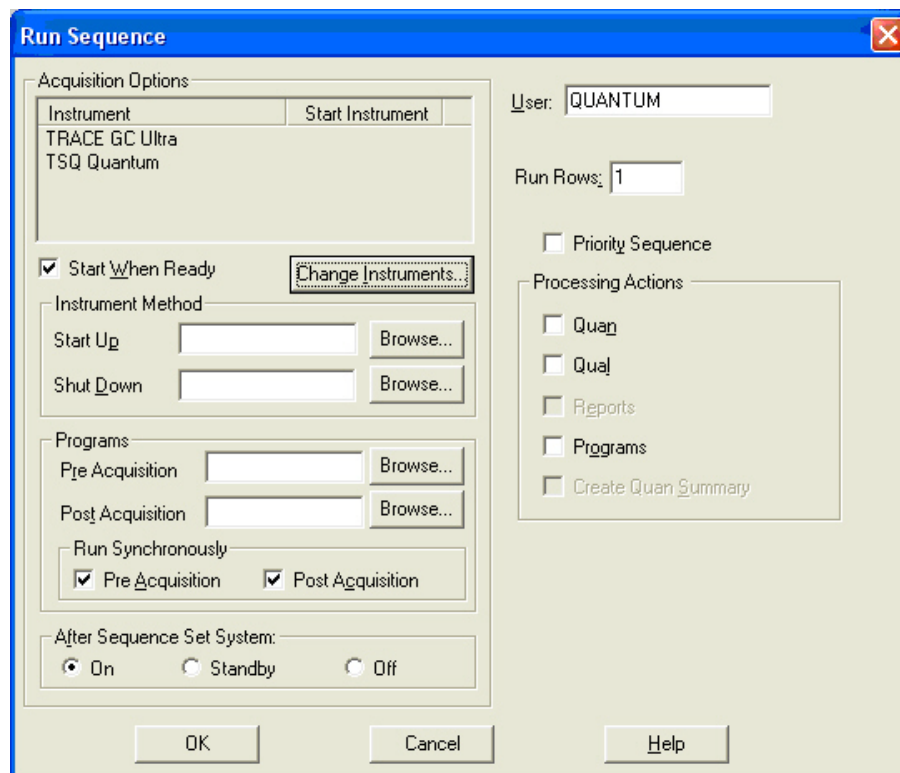
1. If the EZ Tune window is not already open, choose **Start > All Programs > Thermo Instruments > TSQ > TSQ Tune**.

**IMPORTANT** You must have the TSQ EZ Tune window open for the mass spectrometer to initiate the probe insertion sequence.

2. Ensure that the TSQ Quantum XLS Series mass spectrometer is the only instrument in use and that there are no start instruments.
  - a. On the Thermo Xcalibur Roadmap, click the **Sequence Setup** icon to open Sequence Setup, if it is not already open.

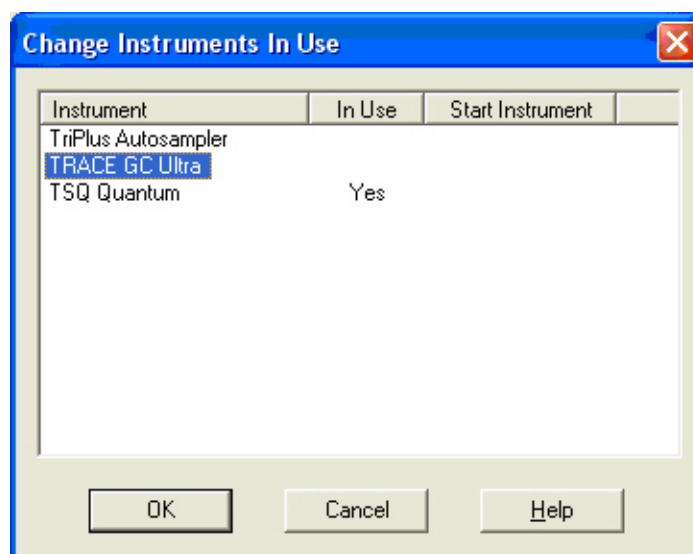
- b. In Sequence Setup, choose **Actions > Run Sequence**. The Run Sequence dialog box opens (see [Figure 65](#)).

**Figure 65.** Run Sequence dialog box, showing instruments in use



- c. Click **Change Instruments** to open the Change Instruments In Use dialog box (see [Figure 66](#)).

**Figure 66.** Change Instruments In Use dialog box, showing the TSQ Quantum mass spectrometer in use and no start instruments



- d. Click any **Yes** in the In Use column to clear all instruments other than the TSQ Quantum.
- e. Ensure that the TSQ Quantum has a Yes in the In Use column. Click the area if necessary.
- f. Click any **Yes** in the Start Instrument column to clear all start instruments.
- g. Click **OK** to save your settings and close the Change Instruments In Use dialog box.

## Running the Sequence

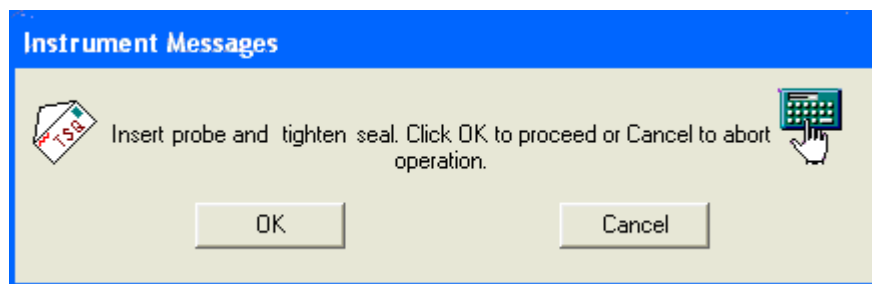
You acquire data by running the sequence. The Xcalibur data system saves the acquired data in a raw file.

**Note** You must have the TSQ EZ Tune or QuickQuan application running so that the Xcalibur application can display instrument methods.

### ❖ To run the sequence

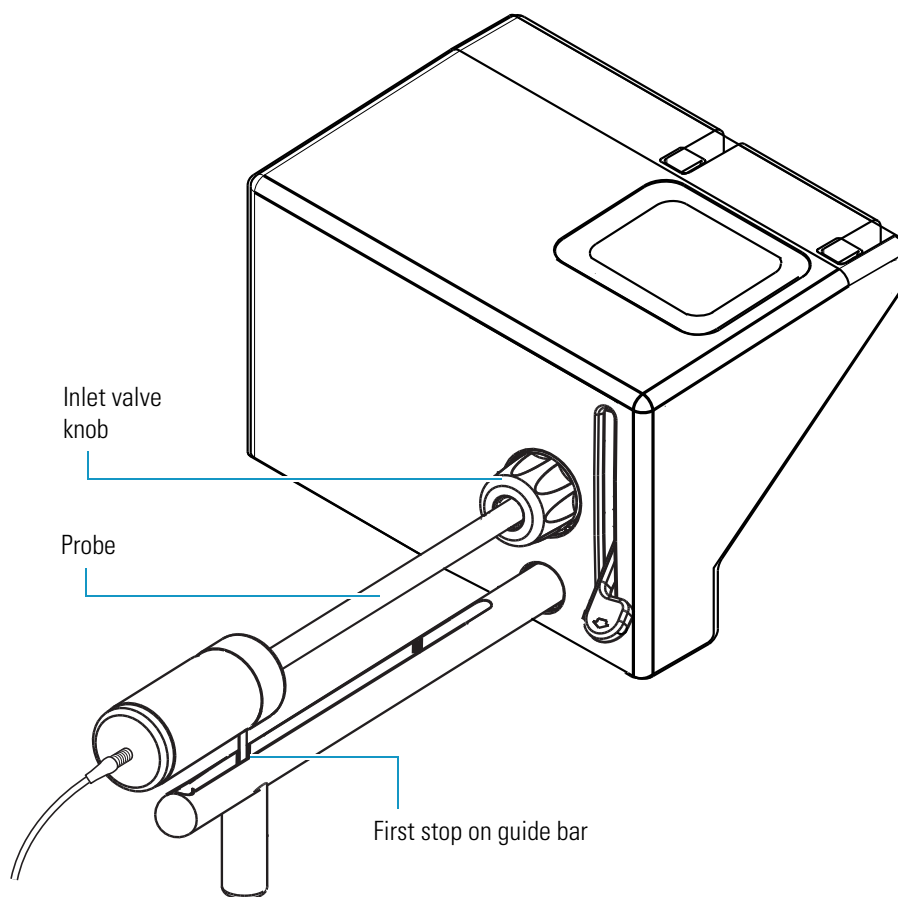
1. In the Run Sequence dialog box (see [Figure 65](#) on [page 136](#)), click **OK** to start the acquisition. The Xcalibur system displays a message to insert the probe ([Figure 67](#)).

**Figure 67.** Insert probe message



2. Inset the probe into the inlet valve:
  - a. Insert the guide ball on the DIP probe into the guide ball hole on the guide bar.
  - b. Slide the probe forward into the inlet valve until the guide ball is at the guide bar's first stop. See [Figure 68](#).
  - c. Tighten the inlet valve knob clockwise to ensure a leak-tight seal.

**Figure 68.** Probe at the first stop on guide bar



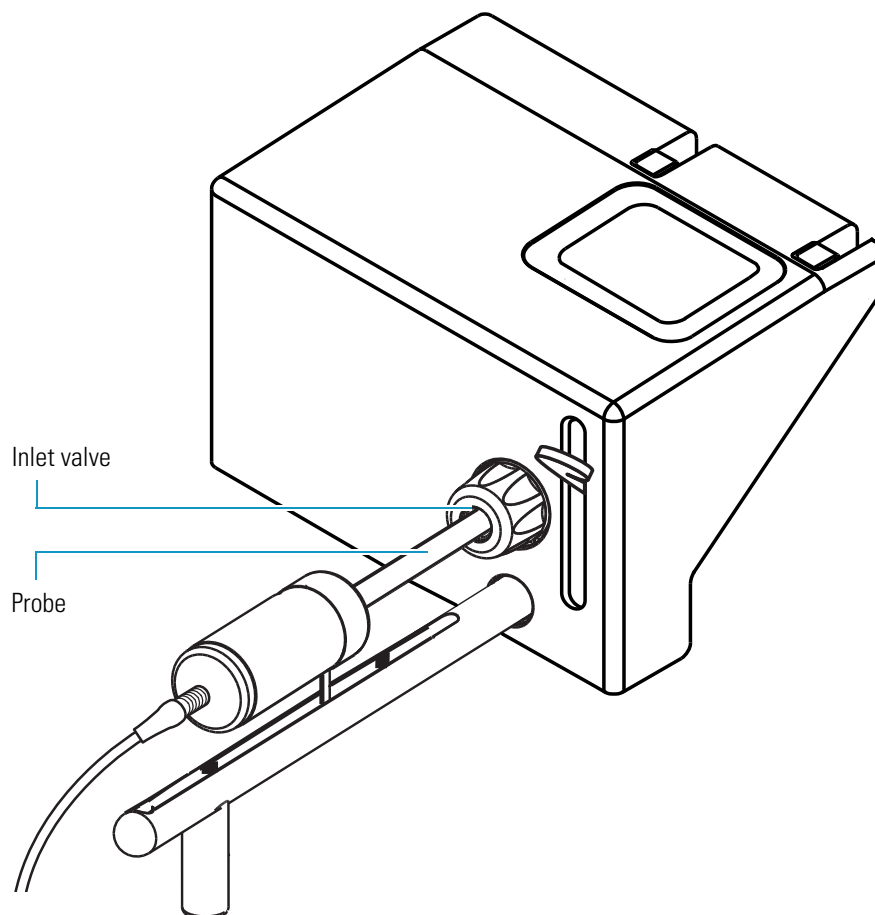
3. Click **OK**. The forepump evacuates the inlet valve.
4. When the Safe to Open the Valve message appears ([Figure 69](#)), click **OK**.

**Figure 69.** Safe to open the valve message



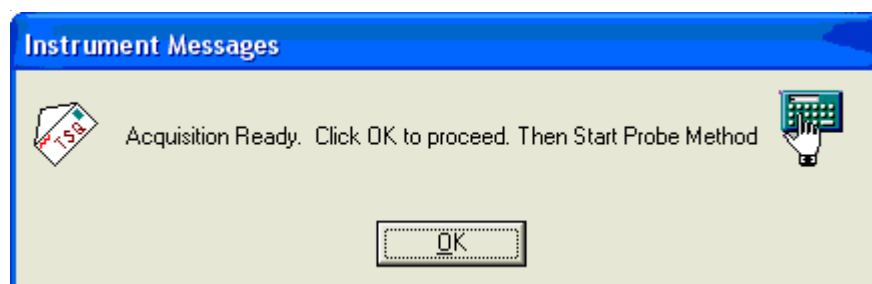
5. Pull the inlet valve lever up to open the inlet valve.
6. Slide the probe into the vacuum manifold until the tip of the probe is fully inserted into the ion volume holder. See [Figure 70](#).

**Figure 70.** Probe inserted into the inlet valve



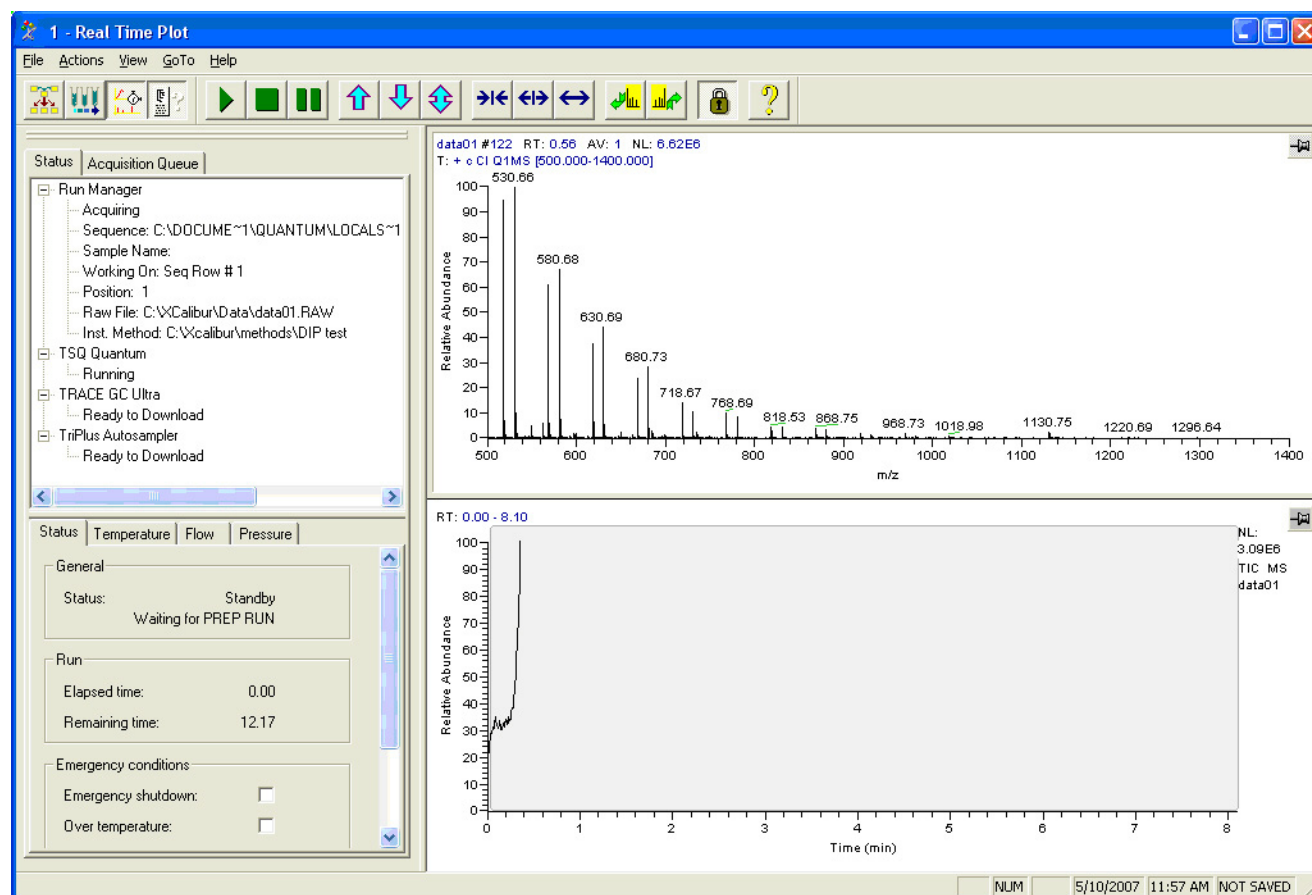
7. When you receive the Acquisition Ready message ([Figure 71](#)), click **OK**. The mass spectrometer is now waiting for contact closure.

**Figure 71.** Acquisition Ready message



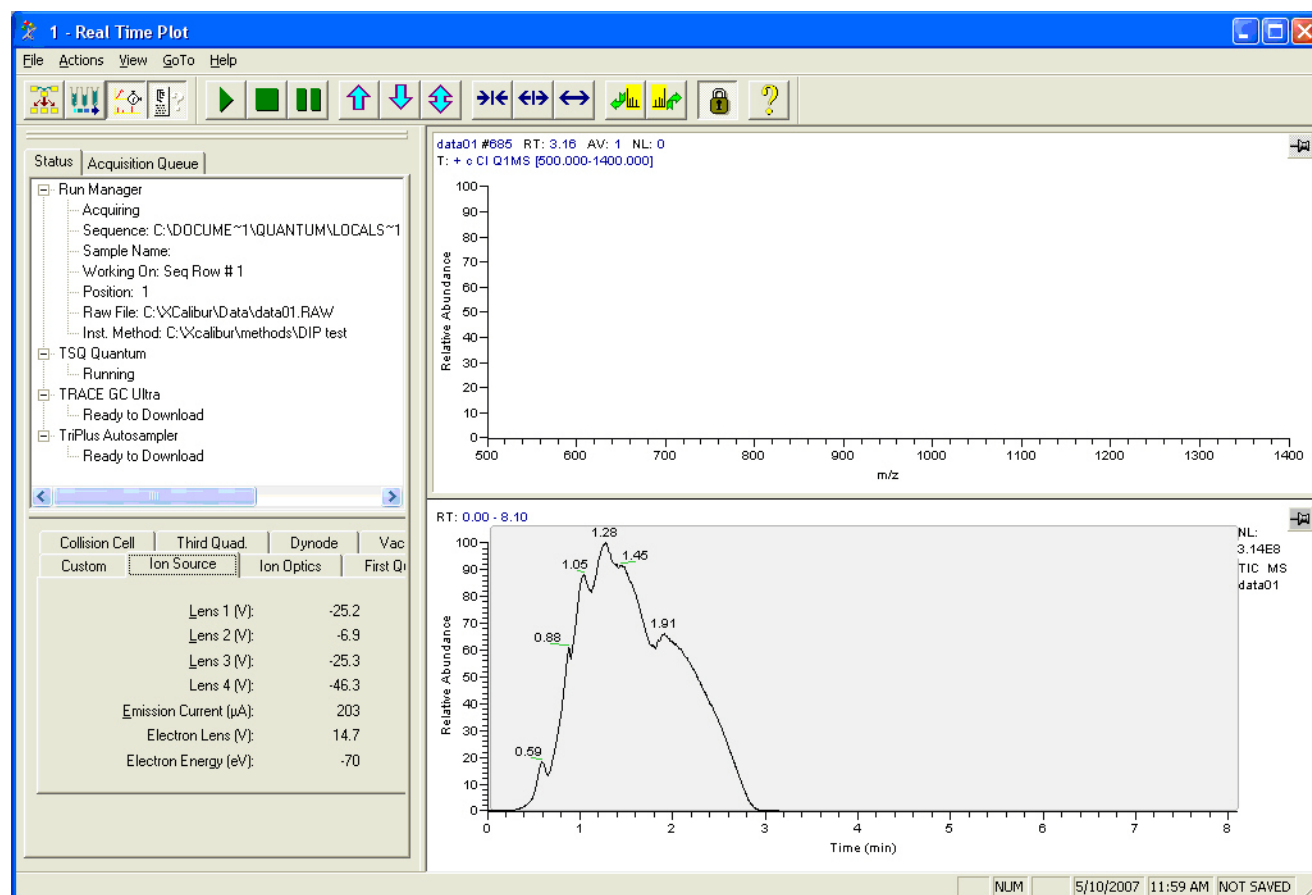
8. In Sequence Setup, choose **View > Real Time Plot View** to display the mass spectrum and chromatogram.
9. Start the probe method from the probe controller to initiate data acquisition. See [Figure 72](#), and [Figure 73](#) on [page 141](#).

**Figure 72.** Perfluorotetracosane mass spectrum at 0.56 minute retention time





**Figure 73.** Perfluorotetracosane chromatogram



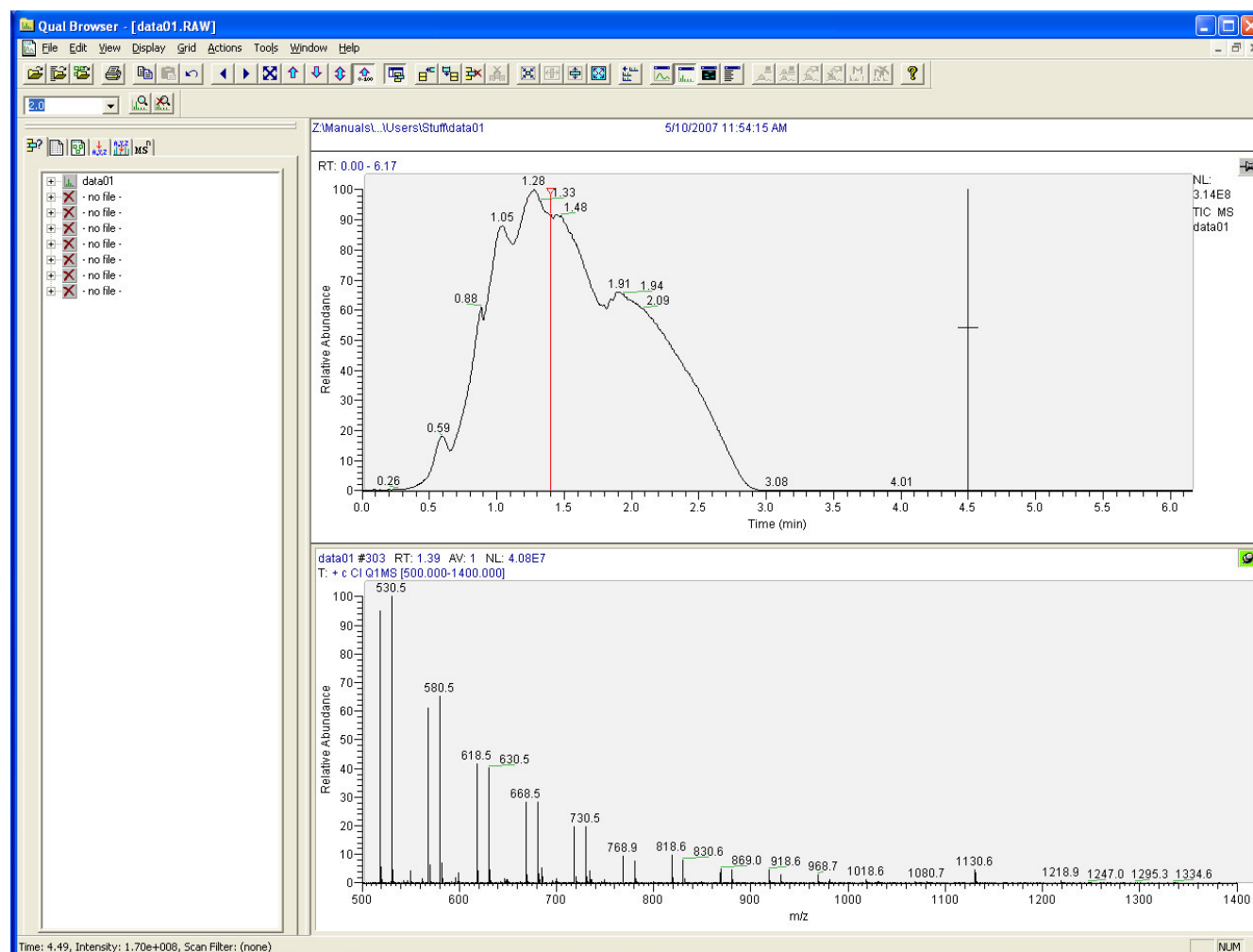
## Examining the Raw Data in Qual Browser

You can use Qual Browser to display the mass spectrum at various times in the chromatogram.

### ❖ To examine the raw data

1. On the Thermo Xcalibur Roadmap, click the **Qual Browser** icon to open the Qual Browser window.
2. Click on the chromatogram to display the mass spectrum at that retention time.  
See [Figure 74](#).

**Figure 74.** Raw file displayed in Qual Browser



## Removing the Probe

### ❖ To remove the probe



**CAUTION** Do not withdraw the probe beyond the point where the guide ball reaches the first stop in the guide bar. Close the inlet valve first. Otherwise, the system vents to the atmosphere.

1. Withdraw the probe until the guide ball on the probe reaches the first stop on the guide bar (see [Figure 68](#) on [page 138](#)).
2. Close the inlet valve by pushing the lever down.
3. Loosen the inlet valve knob by turning it counterclockwise.

4. Continue withdrawing the probe completely from the inlet valve by sliding it through the guide ball track in the guide bar.
5. Store the probe in its case.
6. Remove the guide bar by rotating it 90° counterclockwise and sliding it out of the entry housing.
7. Replace the inlet valve plug and tighten the inlet valve knob clockwise to form a seal. The inlet valve plug prevents air from entering the vacuum manifold in case the inlet valve is accidentally opened. You can also remove the inlet valve lever by pulling it free.



## Replaceable Parts and Consumables

This appendix contains TSQ Quantum XLS Series part numbers for replaceable parts and consumables. To ensure proper results in servicing the TSQ Quantum XLS Series mass spectrometer, order only the parts listed or their equivalent. Contact Thermo Fisher Scientific Austin and have your TSQ Quantum XLS Series mass spectrometer serial number ready.

These kits with replaceable parts and consumables are available for the TSQ Quantum XLS Series systems:

### Contents

- [EI/CI Ion Source Replaceable Parts](#)
- [Miscellaneous Replaceable Parts and Consumables](#)
- [Miscellaneous Replaceable Parts and Consumables](#)
- [Chemicals Kit](#)

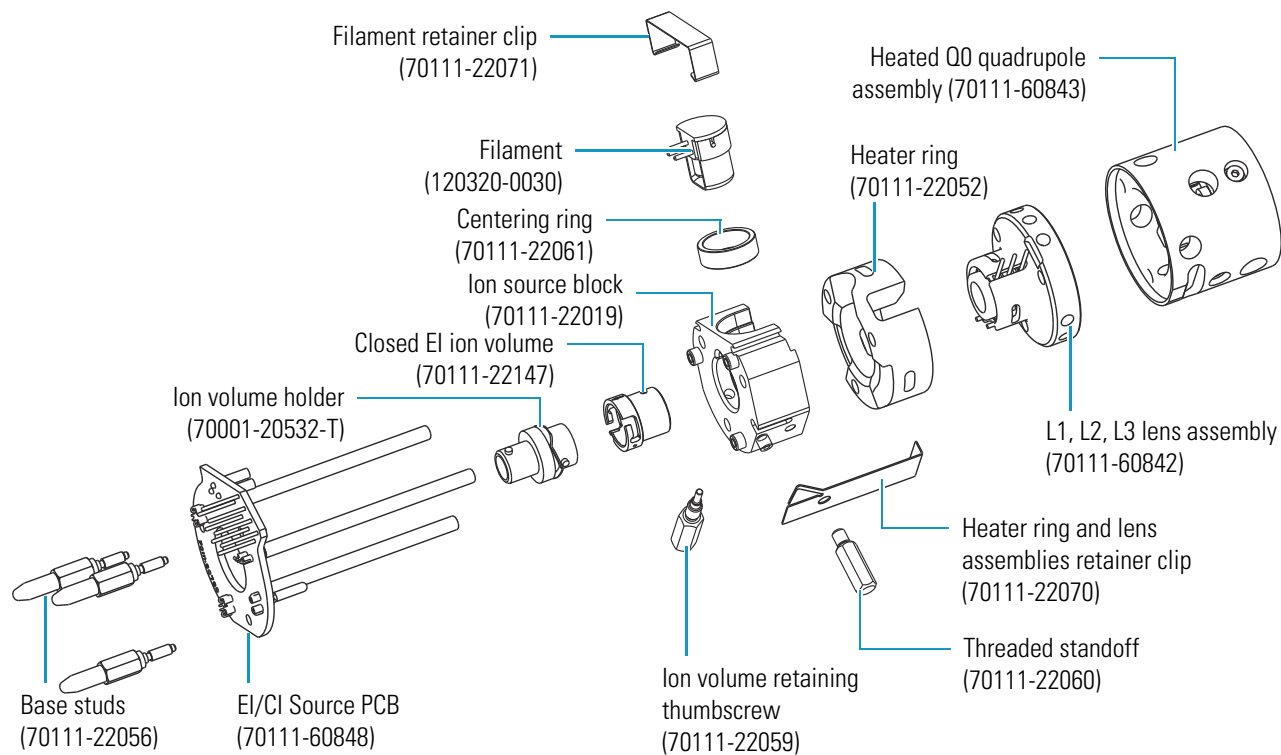
## EI/CI Ion Source Replaceable Parts

[Figure 75](#) and [Figure 76](#) show the replaceable parts of the EI/CI ion source of the TSQ Quantum XLS Series mass spectrometers.

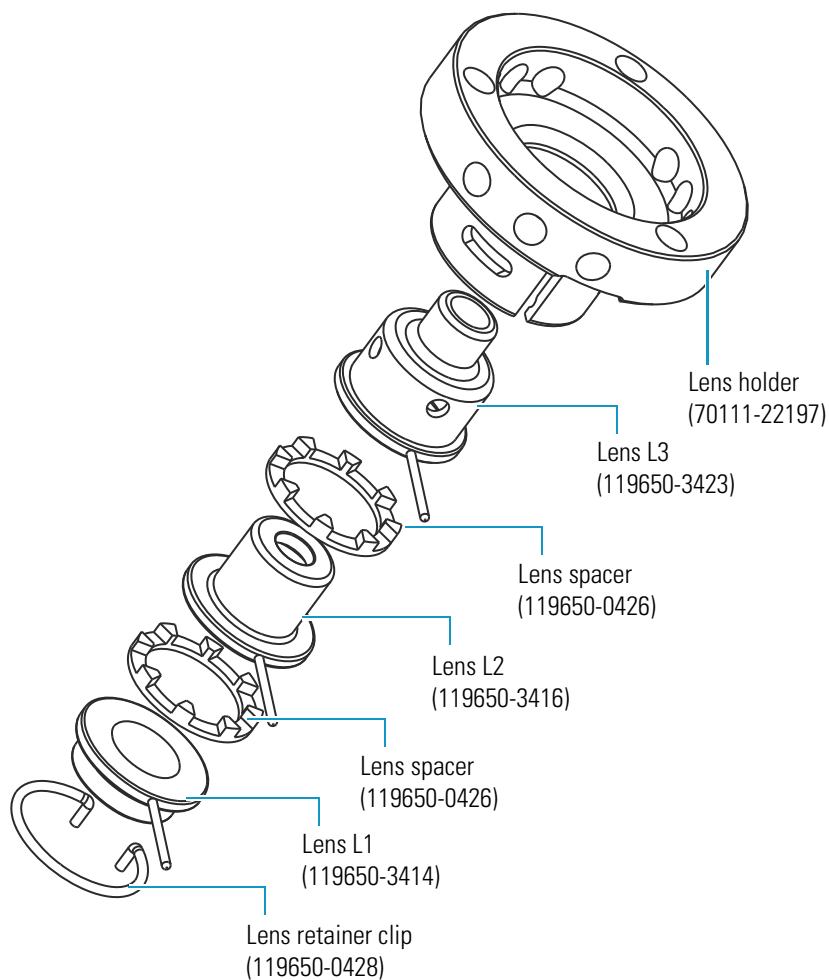
## B Replaceable Parts and Consumables

### El/CI Ion Source Replaceable Parts

**Figure 75.** Ion source (70111-60840)



**Figure 76.** L1, L2, L3 lens assembly (70111-60842)



## Miscellaneous Replaceable Parts and Consumables

**Table 7.** Miscellaneous replaceable parts (Sheet 1 of 2)

Description	Function	Part number
Calibration compound vial	Holds frit and FC-43 tuning and calibration compound.	120428-0002
Calibration compound frit	Holds FC-43 tuning and calibration compound.	120432-0001
Ion volume, closed EI, P type	Ni-Cr, for pesticides	70001-22202

**Table 7.** Miscellaneous replaceable parts (Sheet 2 of 2)

Description	Function	Part number
Ion volume holder, T type	Special alloy	70001-20532-T
GC capillary column, 15 m × 0.25 mm ID × 0.25 µm film thickness SQC install column	Replacement capillary column	76317-3015

## Accessory Kit

**Table 8.** Accessory Kit (P/N 70111-62077) (Sheet 1 of 2)

Description	Function	Part number
Fitting, ferrule, SWG, 1/8 in., brass, set		00101-08-00009
Fitting, connection, 1/4 to 1/8 in.		00101-01709
Fitting, connection, 1/4 to 1/8 in.		00101-01712
Fitting, ferrule, SWG, front, 3/8 in., brass		00101-11500
Ferrule, 0.4mm ID × 1/16 in.		00101-18100
Restek™ capillary-grade hydrocarbon trap	For removing hydrocarbons from the GC carrier gas	00106-99-00001
Restek high-capacity oxygen trap	For removing oxygen from the GC carrier gas	00106-99-00002
Cotton swabs	For applying cleaning paste to stainless steel parts	00301-01-00015
Tubing, 1/8 in., copper, precleaned	Gas lines	00301-22701
Ball valve seal kit (replacement)	For replacing the ball valve seal in the inlet valve	119265-0003
Lens alignment tool	For aligning ion source lenses 1, 2, and 3	120271-0001
Filament assembly	For replacing a failed filament in the ion source	120320-0030
Nitrile gloves medium	For handling clean parts that are under vacuum	23827-0008



**Table 8.** Accessory Kit (P/N 70111-62077) (Sheet 2 of 2)

Description	Function	Part number
Nitrile gloves large	For handling clean parts that are under vacuum	23827-0009
Syringe, 10 µL, 80 mm	For adding calibration compound	36502019
Tee union, 1/8 in.		00101-01-00012
Cable, start, probe	Contact closure cable between the direct sample probe and the mass spectrometer	70111-63627
Cable, start, GC	Contact closure cable between the GC and the mass spectrometer	70111-63626
Forceps, 10 in., stainless steel	For handling ion volumes and clean components	76360-0400
Cable, 10 base-T, crossover, 15 ft, shielded	Communication	76396-0052
Oil, vacuum pump, 1 L	Lubrication of forepump	00301-15101
Cable, RJ45, 7 ft.		00302-01838
Ethernet switch, 5 port	Communication	00825-01-00024
Software, QuanLab Forms 2.5.1 SP1	Chromatography analysis software	120395-0001
Software, GC Devices 2.1.0 for Xcalibur 2.1	GC devices control software	120399-0001

## Chemicals Kit

**Table 9.** Chemicals Kit (P/N 70111-62078)

Description	Function	Part number
Perfluorotributylamine (FC-43)	Tuning and calibration compound	50010-02500
Aluminum oxide	Cleaning stainless steel parts	32000-60340
Benzohexane	Performance testing	120150-TEST
Octafluoronaphthalene	Performance testing	120150-TEST



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