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TSQ Series II

TSQ Altis, TSQ Quantis, and TSQ Fortis

Hardware Manual

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DOCUMENTATION SURVEY

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Software version: (Thermo) Foundation 3.1 SP4 and later, Xcalibur 4.1 SP1 and later, Tune 3.1 and later
Note: You can access this hardware manual from the TSQ II Series version 3.2 instrument control software.

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This device was tested by TÜV Rheinland and complies with the following EMC standards: EN 61326-1 and subordinate EMC standards 47 CFR 15, Subpart B, Class A: 2015
RoHS II Directive 2011/65/EU

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Preface

The *TSQ Altis, Quantis, and Fortis Hardware Manual* describes how to set up and calibrate the Thermo Scientific™ TSQ Altis™, TSQ Quantis™, and TSQ Fortis™ triple quadrupole mass spectrometry systems. It also describes the modes of operation, hardware components, and how to maintain the instrument.

Suggesting Changes to the Documentation or to the Help

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

Accessing Documentation

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

Viewing the Product Manuals

- (Windows 7) From the Microsoft™ Windows™ taskbar, choose **Start > All Programs > Thermo Instruments > *model x.x***, and then open the applicable PDF file.
- (Windows 10) From the Windows taskbar, choose **Start > All Apps > Thermo Instruments > *model x.x***, and then open the applicable PDF file.

Viewing the Help

Do the following as applicable:

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

Viewing User Documentation from the Thermo Fisher Scientific Website

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

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

Special Notices, Symbols, and Cautions

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

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

Notice, symbol, or label	Meaning
IMPORTANT	Highlights information necessary to prevent damage to software, loss of data, or invalid test results; or might contain information that is critical for optimal performance of the product.
Note	Highlights information of general interest.
Tip	Highlights helpful information that can make a task easier.

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

Notice, symbol, or label	Meaning
	**Caution:** Read the cautionary information associated with this task.
	**Chemical hazard:** Observe safe laboratory practices and procedures when handling chemicals. Only work with volatile chemicals under a fume or exhaust hood. Wear gloves and other protective equipment, as appropriate, when handling toxic, carcinogenic, mutagenic, corrosive, or irritant chemicals. Use approved containers and proper procedures to dispose of waste oil and when handling wetted parts of the instrument.
	**Hot surface:** Before touching the API source assembly, allow heated components to cool.
	**Risk of electric shock:** This instrument uses voltages that can cause electric shock and/or personal injury. Before servicing, shut down the instrument and disconnect it from line power. While operating the instrument, keep covers on.
	**Risk of eye injury:** Eye injury can occur from splattered chemicals, airborne particles, or sharp objects. Wear safety glasses when handling chemicals or servicing the instrument.
	**Sharp object:** Avoid handling the tip of the syringe needle.

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1

Introduction

The TSQ Altis, TSQ Quantis, and TSQ Fortis MSs are triple quadrupole atmospheric pressure ionization (API) mass spectrometers.

Note The Glossary defines some of the terms used in this manual.

- Mass Spectrometry Models
- MS Mass-To-Charge Ratio Ranges

Mass Spectrometry Models

This manual describes the operation of these mass spectrometers:

- TSQ Altis MS
- TSQ Quantis MS
- TSQ Fortis MS

TSQ Altis MS

The TSQ Altis MS can address your most stringent analytical challenges for targeted quantitation workflows. The improved Active Ion Management (AIM™) technology, segmented quadrupoles, advanced electron multipliers, and enhanced ion transmission tubes, help you to achieve unprecedented experimental sensitivity for all molecular species in complex matrices without sacrificing robustness.

TSQ Quantis MS

The TSQ Quantis MS answers critical analytical challenges during targeted quantitation workflows.

TSQ Fortis MS

The TSQ Fortis MS ensures superior productivity in the quantitation of hundreds of compounds of all types—in any matrix, by any user.

MS Mass-To-Charge Ratio Ranges

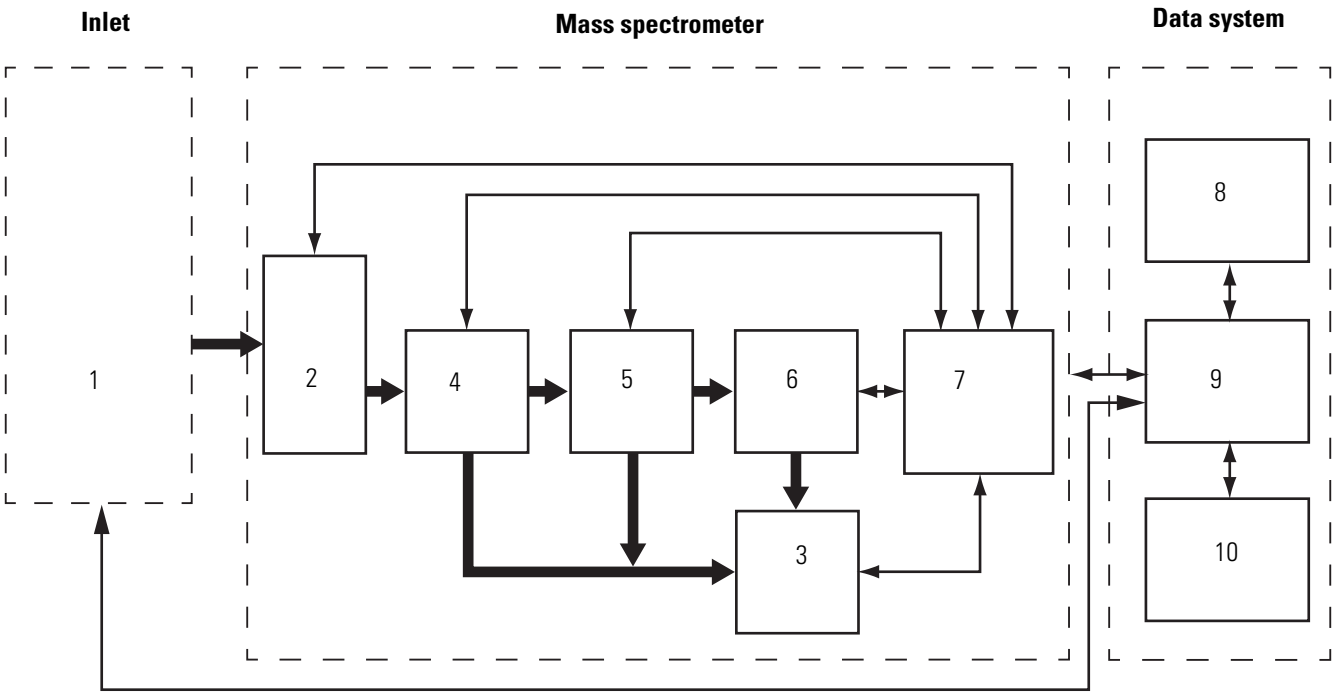
The TSQ Altis, TSQ Quantis, and TSQ Fortis MSs detect different ranges of mass-to-charge ratios.

Instrument	*m/z* Range in amu
TSQ Altis	5–2000
TSQ Quantis	5–3000
TSQ Fortis	5–3000

Principles of Operation

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

MS System Hardware Components

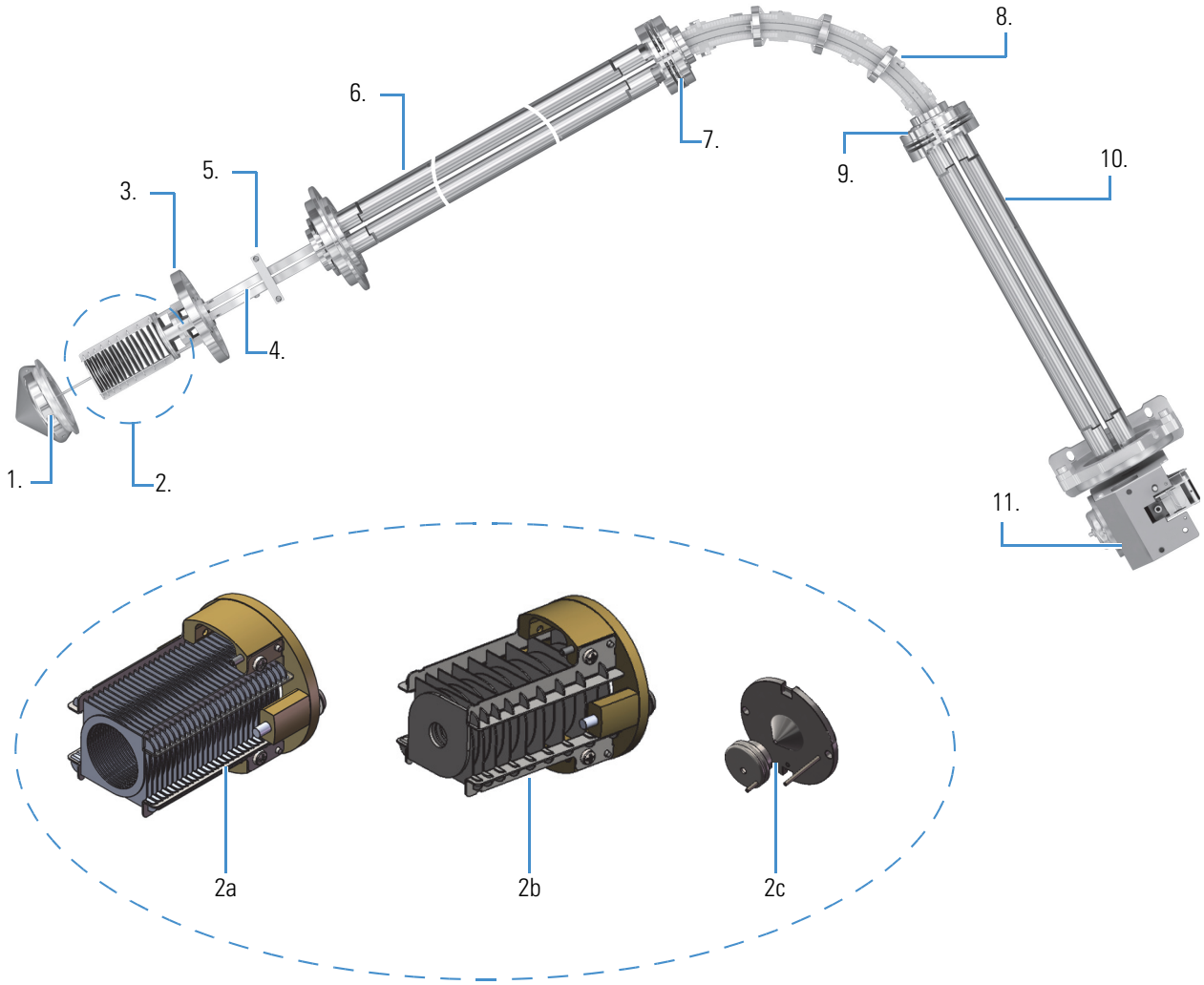


No.	Description	Function
Inlet Region		
1.	Inlet: autosampler (optional), LC pump (optional), Syringe pump, divert/inject valve	The sample enters the MS from the inlet.
Mass Spectrometer		
2.	API source: H-ESI, APCI, or APPI	Generates ions.
3.	Vacuum system	Creates a vacuum for regions 4, 5, 6, and 7.
4.	Ion optics	In the ion optics and mass analyzer, the scan functions manipulate the ions.
5.	Mass analyzer	
6.	Ion detection systems	As the ions strike the dynode detector, they release a cascade of electrons. These electrons generate a voltage signal.
7.	Instrument control electronic assemblies	Control the MS components.
Data System		
8.	Monitor	The data system processes the voltage signal and displays it as a graph that can be printed.
9.	Computer	
10.	Printer (optional)	

Ion Optics and Mass Analyzer

The ion optics assemblies and the mass analyzer assemblies control the path of the ions from the ion source to the detector.

Figure 1. Ion optics and mass analyzer assemblies



No.	Item	Description
1	Sweep cone	The ions pass through the sweep cone into the vacuum system.
2	RF lens and exit lens	In the RF lens, which is a series of stainless-steel electrodes, the MS applies an RF voltage to the electrodes. As the RF amplitude increases, ions of progressively higher mass-to-charge ratios (*m/z*) pass through to the exit lens. The exit lens acts as a vacuum baffle before the ion beam enters the next region of the optics, which is at lower pressure.
2a	RF lens (TSQ Altis MS)	Electrodynamic Ion Funnel (EDIF)

No.	Item	Description
2b	RF lens (TSQ Quantis MS)	Stacked ring ion guide (SRIG)
2c	MSIG (TSQ Fortis MS)	Tube lens and skimmer
3	MP00 multipole and lens L0	The MP00 RF lens generates an electric field that guides the ions along the axis of the lens. At Lens L0, the MS applies a positive electrical potential for positive ions and a negative one for negative ions to be detected.
4	MP0 Ion Optics	The Multipole MP0 generates an electric field that guides the ions along the axis of the multipole rods (Figure 14). Because the rods are curved, the charged ions follow the curve.
5	Ion beam guide with neutrals blocker	The neutral species in the ion beam strike the neutrals blocker and are removed from the ion beam.
6	Quadrupole 1	The ions pass to quadrupole 1 (Q1), which can act as a mass filter or as an ion transmission device. Mass filter: The MS applies RF and DC voltages and only the selected mass goes through. The paths of the other ions become unstable and hit the rods. Ion transmission device: The MS applies RF voltage and all ions go through.
7	Lenses EL21, EL22, EL23	Lenses EL21, EL22, and EL23 shield Q1 from the RF voltage that is applied to Q2 and focus the ion beam. These lenses also help to keep the collision gas out of Q1.
8	Quadrupole 2	The ion beam enters quadrupole 2, (Q2). Q2 can act as an ion transmission device or as a collision cell. • Ion transmission device: The MS applies RF voltage and all ions go through. • Collision cell: Adding pressurized argon gas and an offset voltage fragments the ions.
9	Lenses EL31, EL32, EL33	The ions go through lenses EL31, EL32, and EL33. These lenses help to contain the argon gas in Q2 and focus the beam of the fragments.
10	Quadrupole 3	The fragments enter quadrupole 3, (Q3). Q3 can act as a mass filter or as an ion transmission device like Q1.
11	Dual-mode, discrete-dynode detector	Ions and electrons strike the electron multiplier and release a cascade of electrons. The detector converts the current of the electrons to a voltage that the data system records.

Vacuum System

The TSQ Altis, TSQ Quantis, and TSQ Fortis MSs require either one or two external forepumps, depending on the model. The forepumps create the vacuum necessary for the turbomolecular pump to operate.

Vacuum Pumps

Forepump: Creates the vacuum necessary to properly operate the turbomolecular pump. It also evacuates the ion transfer tube region of the vacuum manifold.

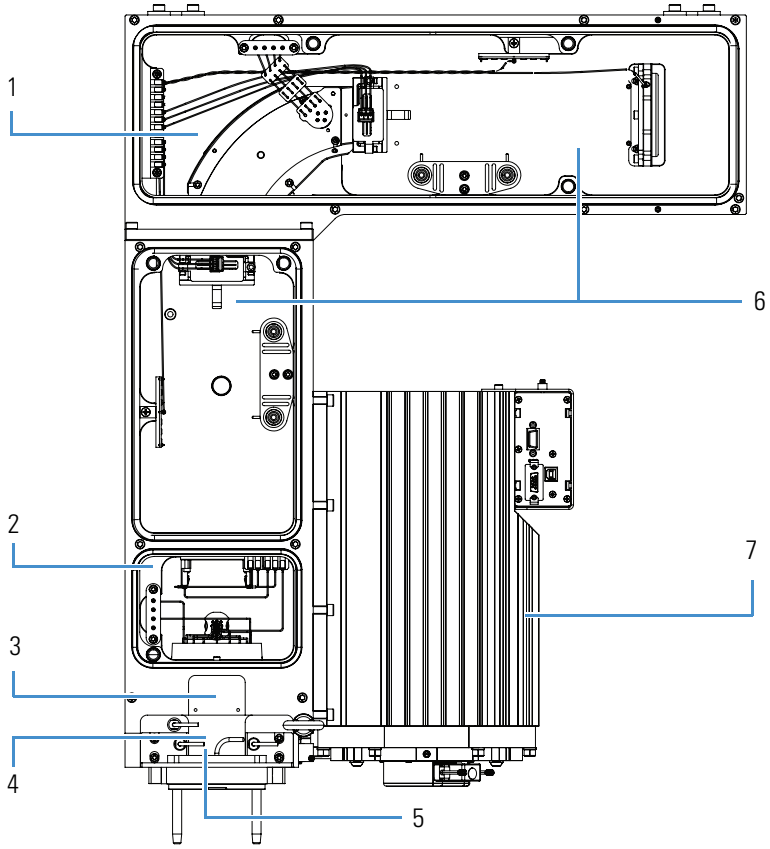
- The TSQ Fortis MS and the TSQ Quantis MS each need one external foreline pump.
- The TSQ Altis MS needs two external forepumps.

Turbomolecular pump: Controls the vacuum for the vacuum regions. It also sends status information, such as temperature or rotational speed, to the data system computer.

Vacuum Manifold

Figure 2 shows the vacuum manifold (1–6) with the top cover plates removed next to the turbomolecular pump (7). The vacuum manifold is a thick-walled, aluminum chamber that encloses the API source interface, ion optics, mass analyzer, and ion detection system assemblies. It has multiple removable top cover plates, various electrical feedthroughs, and gas inlets.

Figure 2. Placement of the turbomolecular pump next to the vacuum manifold



No.	Description	No.	Description
1.	Collision cell chamber	2.	MP0 ion optics chamber
3.	MP00 ion optics chamber	4.	RF lens and ion transfer tube chamber
5.	API source interface	6.	Mass analyzer chambers
7.	Turbomolecular pump		

Table 1 lists the five vacuum regions, the pumps that evacuate them, and the chamber pressures. The block diagram in Figure 3 shows the vacuum regions.

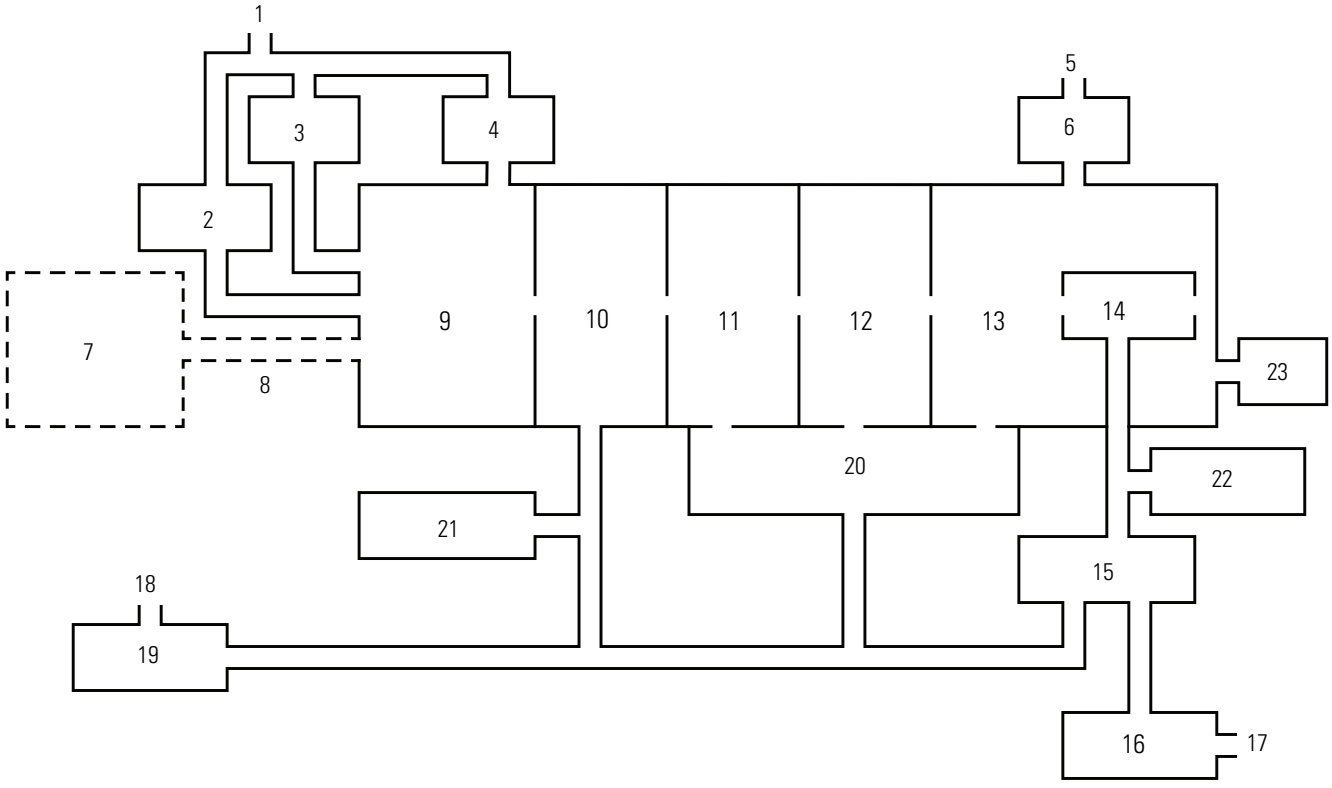
Table 1. Vacuum regions, evacuation devices, and typical pressures

Region	Components	Evacuated by	Pressure		
			TSQ Altis	TSQ Quantis	TSQ Fortis
1	API source	N/A	Atmosphere	Atmosphere	Atmosphere
2	RF lens	Forepump or forepumps	3–4 Torr	1–2 Torr	1–2 Torr
3	MP00 ion optics	Triple-inlet turbomolecular pump (first inlet [molecular drag])	150 mTorr	120 mTorr	120 mTorr
4	MP0 ion optics	Triple-inlet turbomolecular pump (second inlet [interstage])	2 mTorr	1 mTorr	1 mTorr
5	Mass analyzer	Triple-inlet turbomolecular pump (third inlet [high vacuum])	3–7 $\times 10^{-6}$	2–4 $\times 10^{-6}$	9 $\times 10^{-7}$

Vacuum System Block Diagram

The vacuum system evacuates the region around the API source interface, ion optics, mass analyzer, and ion detection system.

Figure 3. Functional block diagram of the TSQ Altis MS vacuum system



No.	Description	No.	Description
1.	Nitrogen gas port	2	Aux gas valve
3.	Sheath gas valve	4.	Sweep gas valve
5.	Filtered air	6.	Vent valve
7.	Ion source	8.	Sample tube
9.	Atmospheric pressure region	10.	Ion transfer tube and RF lens region
11.	MP00 ion optics region	12.	MP0 ion optics region
13.	Mass analyzer region	14.	Collision cell
15.	Collision gas divert valve	16.	Collision gas valve
17.	Argon gas port	18.	Exhaust
19.	Forepump	20.	Triple-inlet turbomolecular pump
21.	Convection vacuum gauge	22.	Convection vacuum gauge
23.	Ion gauge		

Vacuum Gauges

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

- Convection pressure gauge—Measures pressure down to a fraction of a milliTorr (mT). The instrument uses two convection gauges:
  - Source pressure gauge—Measures the pressure in the RF lens and API ion transfer tube region in the vacuum manifold and the foreline, which connects the triple-inlet turbomolecular pump and the forepump or forepumps.
  - Collision gas pressure gauge—Measures the pressure in the collision cell.
- Ionization gauge—Measures the pressure in the analyzer region of the vacuum manifold. The ionization gauge produces energetic electrons that cause molecular ionization. A collector attracts positive ions formed in the ionization gauge, and the collector current is related to the pressure in the vacuum manifold. The ionization gauge is also involved in vacuum protection.

Internal Gas Supply

The inlet gas hardware controls the flow of gases into the MS.

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

  Argon gas enters the left side of the MS through a 1/8 in. port. The valves for the collision gas control the flow of argon gas into and out of the Q2 collision cell. When activated, a solenoid valve shuts off the argon gas flow to the cell.

- Nitrogen Gas Valves—The data system controls the valves that regulate the nitrogen pressure. You can set the gas flow rates in the Ion Source pane of the Tune application.

  Dry nitrogen gas enters the left side of the MS through a 1/4 in. port. The valves for the sheath, auxiliary, and sweep gases control the flow of dry nitrogen gas into the API source (Figure 4).

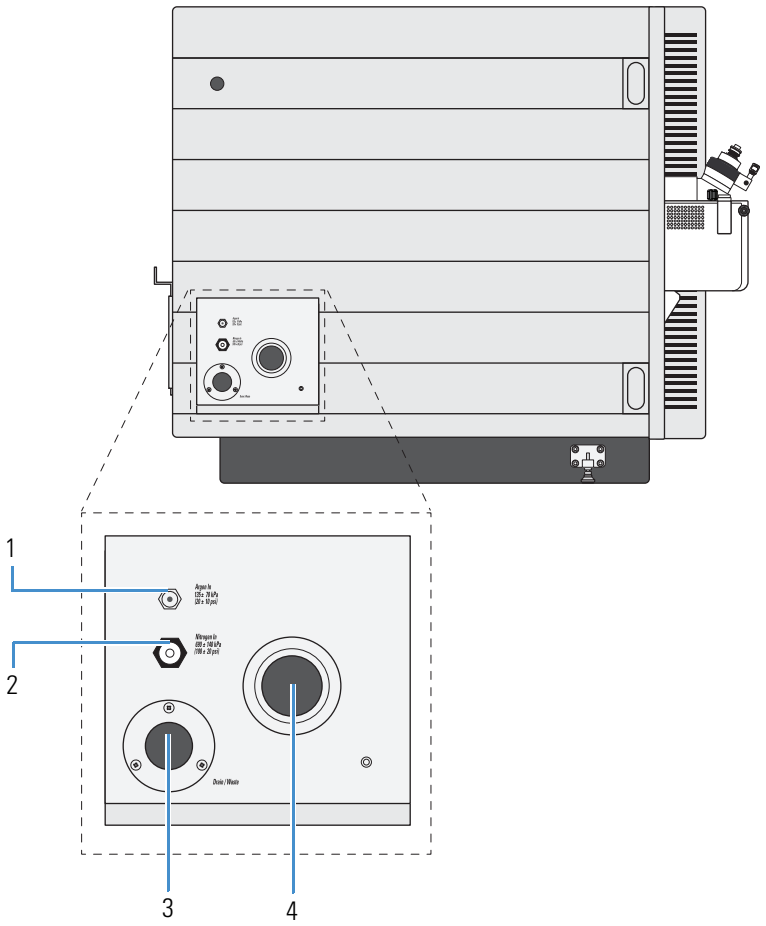
  – Sheath gas is the inner-coaxial nitrogen gas that helps nebulize the sample solution into a fine mist as the solution exits the API spray insert nozzle.

  – Auxiliary gas is the outer-coaxial nitrogen gas that helps the sheath gas to nebulize and evaporate the sample solution by focusing the vapor plume and lowering the humidity in the API source.

  – Sweep gas is the off-axis nitrogen gas that flows out from behind the optional ion sweep cone to aid in solvent declustering and adduct reduction. The optional ion sweep cone has an inlet for the sweep gas.

- Vent Valve—The solenoid-operated vent valve vents the vacuum manifold with filtered air. The vent valve is closed when the solenoid is energized. The vent opens when the MS no longer receives external power, as with a power failure or when you turn off the main power switch.

Figure 4. Gas inlets and vacuum (foreline) port (left side of the MS)



No.	Description	No.	Description
1.	Argon gas inlet	2.	Nitrogen gas inlet
3.	Drain/Waste Port	4.	Vacuum (foreline) port

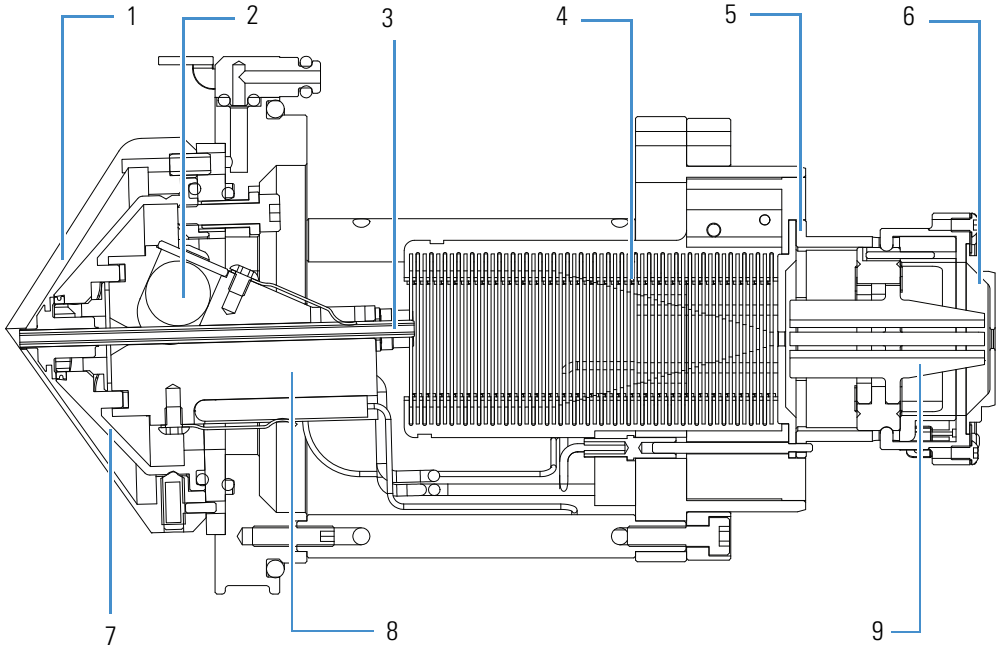
5

Atmospheric Source Interface

API Source Interface Overview

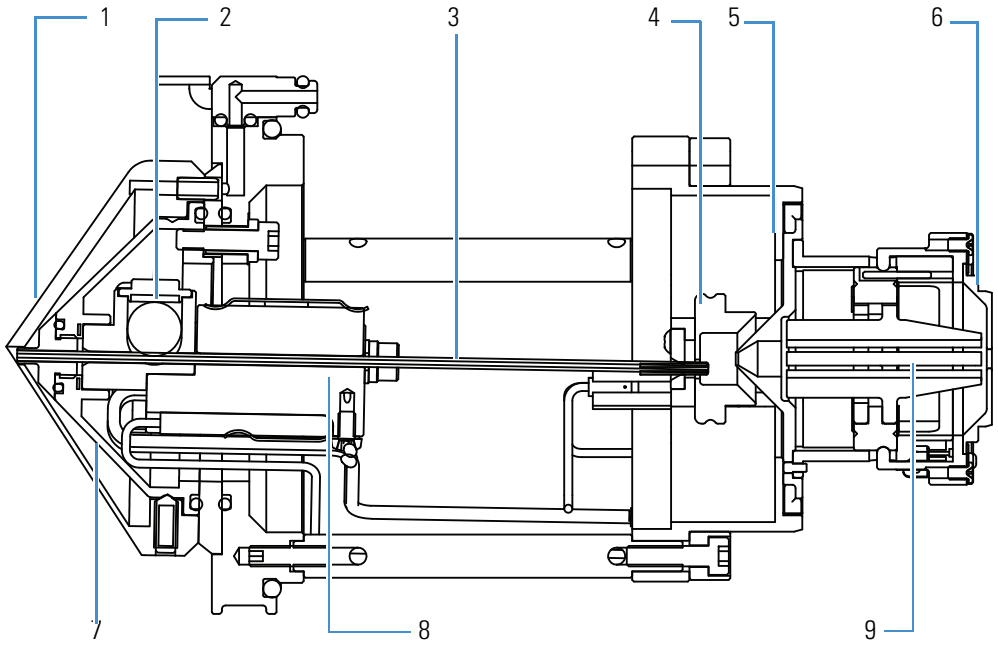
The API source interface includes an ion sweep cone, an ion transfer tube, two cartridge heaters, a heater block, a sensor, a vent prevent ball, the RF lens, and lens L0. In addition, the TSQ Altis MS and the TSQ Quantis MS also have an exit lens (Figure 5), and the TSQ Fortis MS has a skimmer and a tube lens (Figure 6). Except for the atmospheric pressure side of the ion sweep cone that is within the API source, the API source interface components are located in a vacuum chamber.

Figure 5. API source interface for the TSQ Altis MS (cross section)



No.	Description	No.	Description	No.	Description
1.	Ion sweep cone	2.	Vent prevent ball	3.	Ion transfer tube
4.	RF lens	5.	Exit lens	6.	L0 lens
7.	Spray cone	8.	Heater block	9.	MP0 multipole

Figure 6. API source interface for the TSQ Fortis MS (cross section)



No.	Description	No.	Description	No.	Description
1.	Ion sweep cone	2.	Vent prevent ball	3.	Ion transfer tube
4.	Tube lens	5.	Skimmer	6.	L0 lens
7.	Spray cone	8.	Heater block	9.	MP0 multipole

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

Ion Transfer Tube

The ion transfer tube is a metal, cylindrical tube that assists in desolvating ions produced by the API spray insert while transferring them into the vacuum system. The design of the ion transfer tube is different for each MS system (Figure 8, Figure 7, and Figure 9).

Figure 7. TSQ Altis MS ion transfer tube (1/4 turn ion transfer tube)

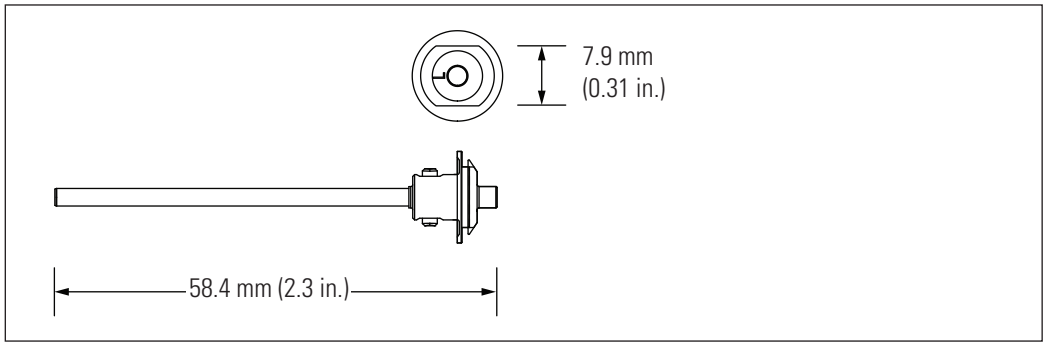


Figure 8. TSQ Quantis MS ion transfer tube (threaded nose cone)

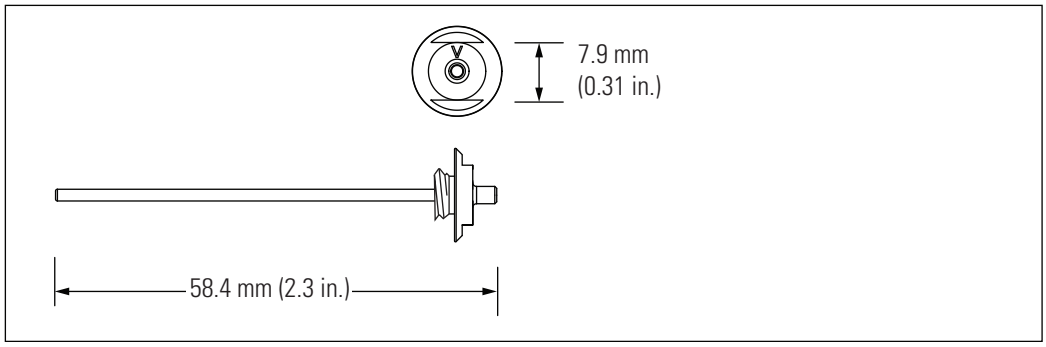
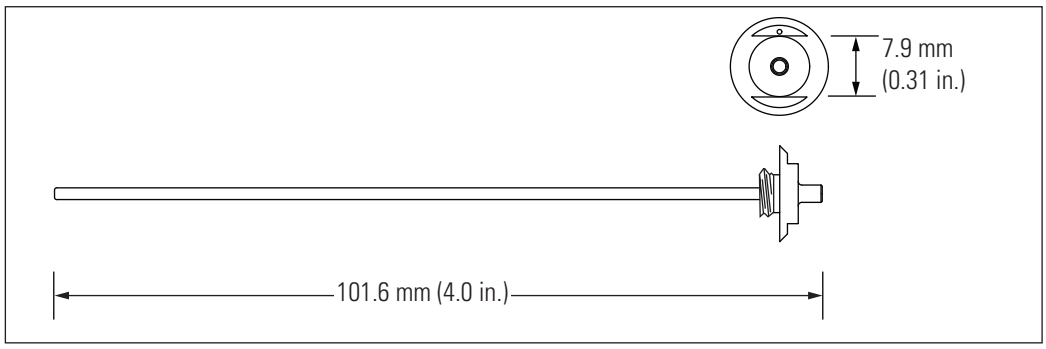


Figure 9. TSQ Fortis MS ion transfer tube (threaded nose cone)



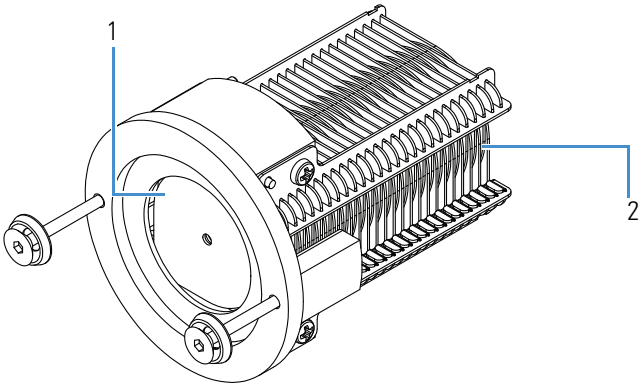
The heater block contains two heater cartridges that surround the ion transfer tube and heat the tube to temperatures up to 400 °C (752 °F). A decreasing pressure gradient draws ions into the ion transfer tube in the atmospheric pressure region. When you remove the ion transfer tube (after it has cooled to room temperature), the vent prevent ball drops into place to stop air from entering the vacuum manifold. Therefore, you can remove the ion transfer tube for cleaning or replacement without venting the system.

RF Lens and Exit Lens (TSQ Altis and TSQ Quantis)

The TSQ Altis MS (Figure 10) and TSQ Quantis MS (Figure 11) have an RF lens and an exit lens.

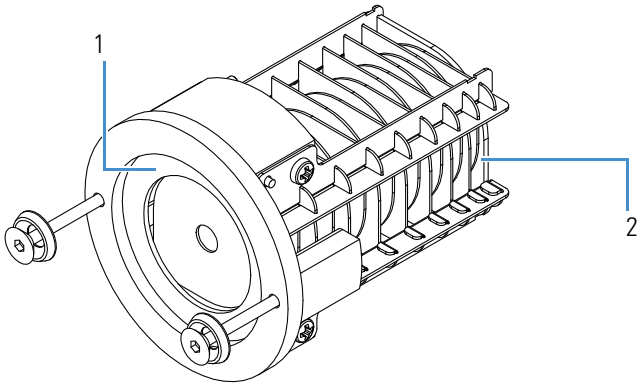
Ions from the ion transfer tube pass through the RF lens and then the exit lens (Figure 10). The RF lens is an ion transmission device consisting of progressively spaced, stainless-steel electrodes. The MS applies an RF voltage to the electrodes, and the adjacent electrodes have voltages of opposite phase. As the RF amplitude increases, ions of progressively higher *m/z* values pass through to the exit lens and move toward the MP00 multipole. The exit lens acts as a vacuum baffle between the higher pressure API source interface region and the lower pressure MP00 multipole region of the vacuum manifold.

Figure 10. TSQ Altis MS RF lens and exit lens



No.	Description	No.	Description
1.	Exit lens	2.	RF lens [Electro Dynamic Ion Funnel (EDIF)]

Figure 11. TSQ Quantis MS RF lens and exit lens



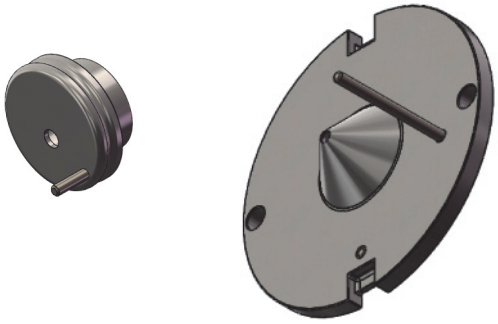
No.	Description	No.	Description
1.	Exit lens	2.	Rf lens [Stacked Ring Ion Guide (SRIG)]

Tube Lens and Skimmer (TSQ Fortis)

The TSQ Fortis MS has a Matrix Separator Ion Guide (MSIG), which consists of a skimmer and a tube lens. Ions from the ion transfer tube pass through the tubes lens and then the skimmer.

Figure 12 shows the tube lens on the left and the skimmer on the right.

Figure 12. Tube lens (left) and skimmer (right)



Ion Optics and Detector Components

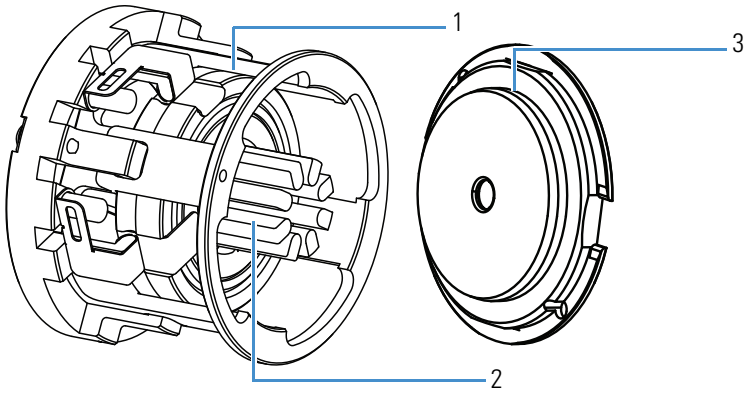
MP00 Ion Optics

The MP00 ion optics (Figure 13) include the MP00 multipole and the L0 lens.

The MP00 multipole is an array of eight metal elements. The MS applies an RF voltage to the elements to generate an electric field that guides the ions along the axis of the lens.

The lens L0 is a metal disk with a small hole in the center through which the ion beam passes. The MS applies an electrical potential (positive for positive ions and negative for negative ions) to lens L0 to transmit ions of the selected charge. Lens L0 acts as a baffle between MP00 and MP0 to isolate the lower vacuum region.

Figure 13. MP00 multipole (left) and lens L0 (right)



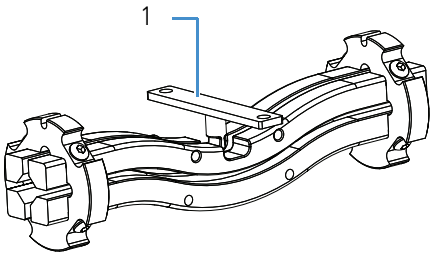
No.	Description	No.	Description
1,	MP00 assembly	2.	MP00 multipole (array of 8 metal elements)
3.	L0 lens		

MP0 Ion Optics and Neutrals Blocker

The MP0 ion optics (Figure 14) transmits ions from the MP00 ion optics to the quadrupoles.

The multipole MP0 ion optics includes multipole MP0 and lenses EL11 and EL12. The neutrals blocker (1 in Figure 14) is attached to the MP0 multipole.

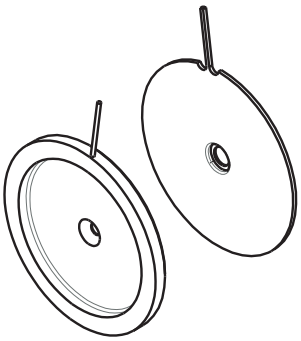
Figure 14. MP0 multipole with neutrals blocker (1)



Multipole MP0 is an array of square-metal rods that transmit ions. The MS applies an RF voltage to the elements to generate an electric field that guides the ions along the axis of the multipole. The MP0 offset voltage increases the translational kinetic energy of the ions as they leave MP00. The voltage causes the charged ions to follow the curve of the rods. Neutral species do not follow the curve; instead, they strike the neutrals blocker and are removed from the beam.

The EL11 and EL12 lenses are metal disks with a circular hole in the center through which the ion beams passes (Figure 15). They act as a two-element cone lens. The MS applies an electrical potential to the lens to accelerate (or decelerate) ions as they approach each lens. The EL11 and EL12 lenses are also a vacuum baffle between multipole MP0 and quadrupole Q1.

Figure 15. EL11 (left) and EL12 (right) lenses



Dual-Mode, Discrete-Dynode Ion Detection System

The ion detection system includes a high-voltage conversion dynode (11 in Figure 1) and an electron multiplier. Typically, the electron multiplier is set to a gain of about 5×10^5 (that is, for each ion or electron that enters, 5×10^5 electrons exit) in MS mode and 2×10^6 in MS/MS mode. The electrometer circuit converts the current that leaves the electron multiplier through the anode to a voltage, and the data system records the voltage.

7

Controls and Indicators

Become familiar with the controls and indicators on your MS.

- LEDs
- Power Entry Module
- Communications Panel
- Cooling Fans

LEDs

See Figure 16 for the LED indicators on the instrument front panel and Table 2 for their descriptions.

Figure 16. LEDs on the instrument front panel

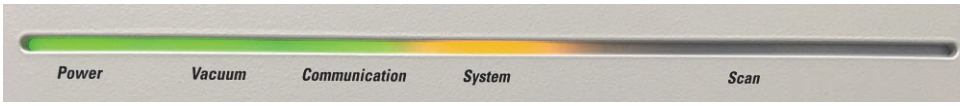


Table 2. Instrument front panel LEDs (Sheet 1 of 2)

LED	State	Description
Power	Green	The MS is receiving power. (The electronics service switch is in the Operating Mode position.)
	Off	The MS is not receiving power. (The electronics service switch is in the Service Mode position.)
Vacuum	Green	The vacuum is within the allowable operating range.
	Yellow	The vacuum is outside the allowable operating range.
	Off	The MS is either off or in the process of starting up.

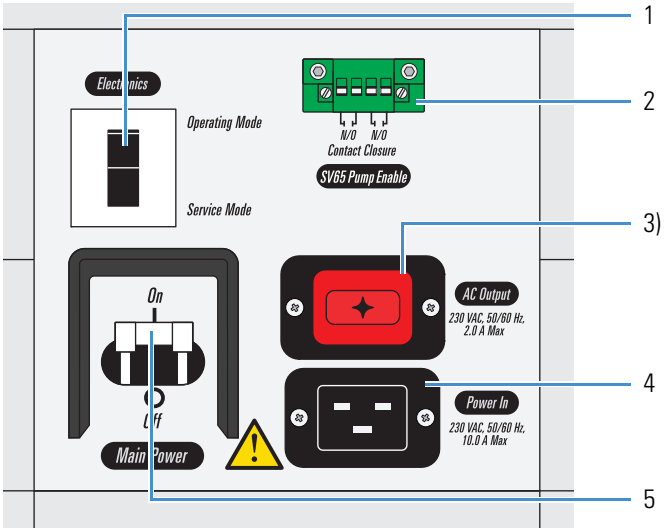
Table 2. Instrument front panel LEDs (Sheet 2 of 2)

LED	State	Description
Communication	Green	The MS and data system are communicating.
	Yellow	The MS and data system are trying to establish a communication link.
	Off	The MS is off.
System	Green	The MS is on.
	Yellow	The MS is in standby mode.
	Off	The MS is off.
Scan	Flashing blue	The MS is on and scanning.
	Off	The MS is not scanning.

Power Entry Module

The MS receives line power at 230 Vac ±10%, 5 A, 50/60 Hz through the right-side power entry module (Figure 17).

Figure 17. Power entry module



No.	Description	No.	Description
1.	Electronics service switch	2.	SV65 Pump Enable connector (forepump on/off control)
3.	AC Output receptacle (reserved for future use)	4.	Power In receptacle (230 Vac)
5.	Main Power switch		

Main Power Switch

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

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

Electronics Service Switch

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

SV65 Pump Enable Connector

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

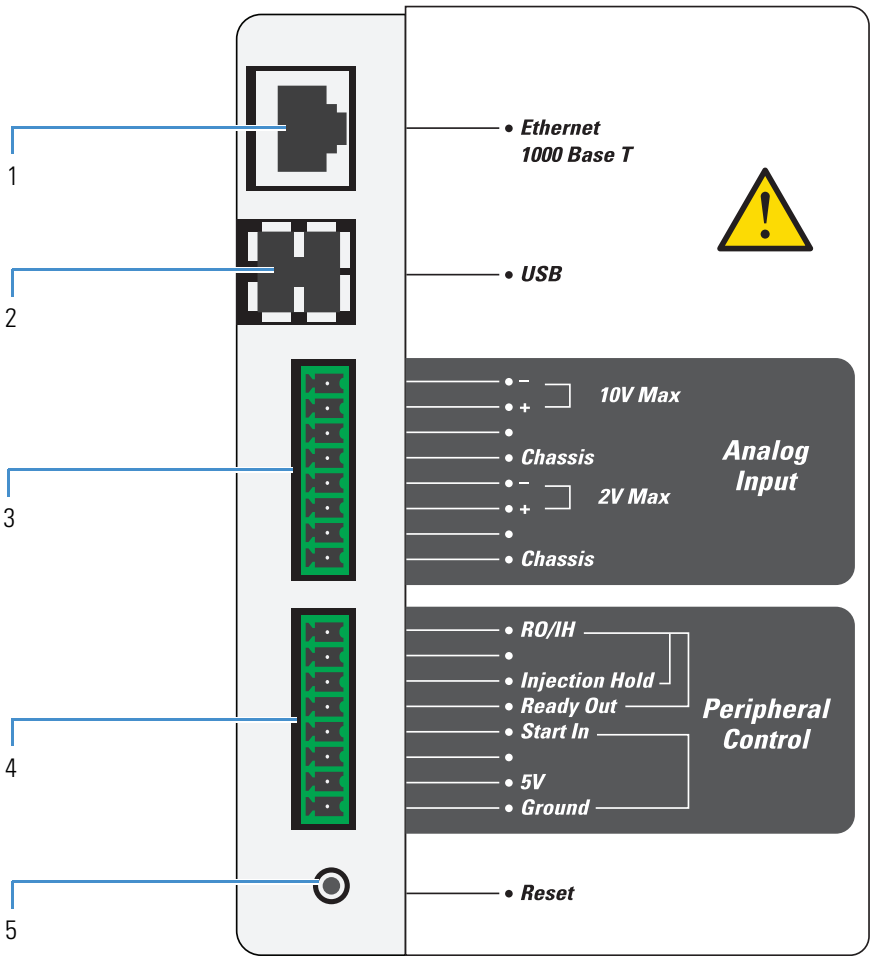
Communications Panel

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

When you briefly press the reset button, the embedded processing system and digital circuitry reset and the system software reloads from the data system. For more information about resetting the MS, see Chapter 10, “Restarting the MS System After a Shutdown.”

Figure 18 shows the communication connectors, and Table 3 describes the pin-outs for these connectors.

Figure 18. Communication connectors (right side of the MS)



No.	Description	No.	Description
1.	Ethernet port	2.	USB ports
3.	Analog Input connector	4.	Peripheral Control connector
5.	Reset button		

Table 3. Pin-out descriptions for the communication connectors (Sheet 1 of 2)

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

Table 3. Pin-out descriptions for the communication connectors (Sheet 2 of 2)

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

Cooling Fans

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

The only user-serviceable part is the air filter in front of the air intake fans. For the recommended maintenance schedule, see "Maintaining the Air Filter."

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

Using the MS Power Options

Become familiar with the power options.

Turning On the MS

1. In the Tune window, click the **System On** icon,  .

   The System LED on the front panel turns green.

2. If necessary, turn the power on to the other MS system components, such as the syringe pump, the LC pumps, and the autosampler.

Placing the MS in Standby Mode

If you are not going to use the MS for a few days, place it in standby mode.

1. Open the Tune window:

   - (Windows 7) From the Microsoft™ Windows™ taskbar, choose **Start > All Programs > Thermo Instruments > *model x.x* > *model* Tune**.
   - (Windows 10) From the Windows taskbar, choose **Start > All Apps > Thermo Instruments > *model x.x* > *model* Tune**.

2. If your LC/MS system includes LC pumps, turn off the liquid flow to the API source.

   For instructions, refer to the LC pump manual.

3. In the Tune window, place the MS in **Standby** mode,  .

The center of the selected power mode icon changes from white to green. The System LED on the front panel turns yellow. To keep the API source clean, the MS reduces the auxiliary and sheath gas flows to their standby default settings (2 arbitrary). The MS turns off the electron multiplier, conversion dynodes, 8 kV power to the API source, main RF voltage, and ion optic RF voltages. For a more complete list of the system statuses, refer to Chapter 11, "MS Components On/Off Status."

Shutting Down the LC/MS System in an Emergency

CAUTION Emergency shut down procedure.

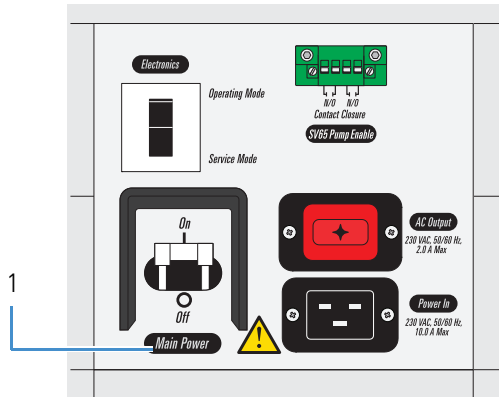
1. To shut down the MS in an emergency, turn off the main power switch (1 in Figure 19) on the power panel on the right-side of the MS (Figure 19).

   This switch turns off all power to the MS, including the forepump, without harming components within the instrument.

   If you cannot safely reach the main power switch, unplug the power cord from the outlet.

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

Figure 19. Main power switch on the power module



Shutting the MS System Down Completely

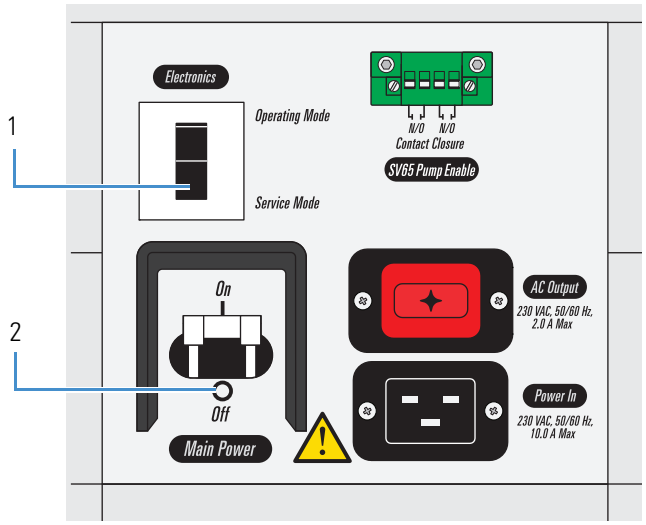
Shut down the MS system completely only when you are not using it for an extended period of time or when you must shut it down for maintenance or service. Also turn off the LC, gases, data system and autosampler.

Shutting Down the MS Completely

1. Follow the procedure, Chapter 8, "Placing the MS in Standby Mode."
2. Find the electronics service switch on the right-side power panel (Figure 20).
3. Switch it into the Service Mode (down) position.

   This turns off all LEDs on the front panel and the power to the nonvacuum system electronics.
4. Turn off the Main Power switch.
   - The ion transfer tube heater and the ion optics voltages turn off.
   - All power to the MS, including the turbomolecular pumps and the forepump, goes off.
   - After approximately 5 seconds, power to the vent valve solenoid shuts off, the vent valve opens, and the vacuum manifold vents with dry nitrogen. This creates a hissing sound.
   - After about 2 minutes, the vacuum manifold is at atmospheric pressure.

Figure 20. Electronic service switch and main power switch



No.	Description
1.	Electronics service switch- service mode
2.	Main power switch-off

5. Unplug the MS's power cord from the electrical outlet.

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

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

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

Turning off the LC, Gases, Data System, and Autosampler

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

Restarting the MS System After a Shutdown

When you restart the MS system after a complete shutdown, the sequence of tasks is important.

Restarting the Data System

If possible, use the Windows 7 or Windows 10 restart procedure for the data system so that Windows can properly close applications and save changes to any open application.

Note After you reset the data system, the communications link between the data system and the MS is automatically reestablished. When this occurs, the Communication LED turns yellow and then green. If the system is unable to reestablish the communications link, follow "Resetting the Mass Spectrometer."

Restarting the Data System Using Windows

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

Restarting the Data System Using the Power Button

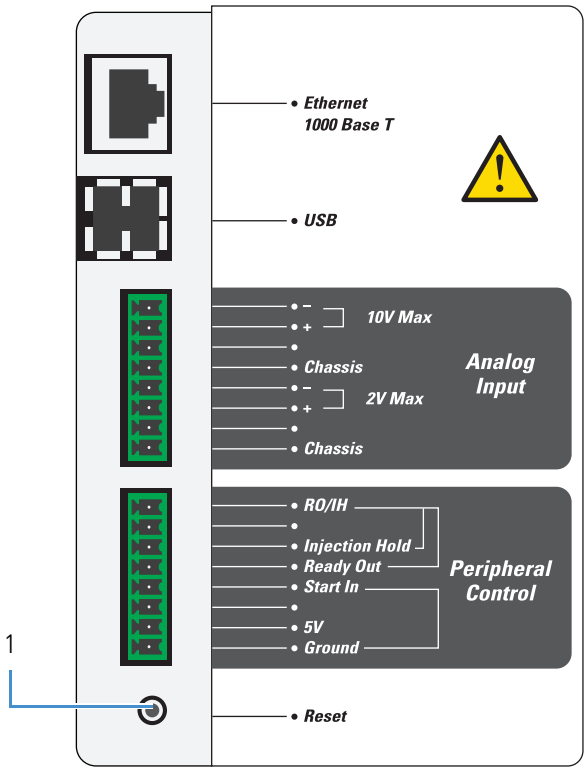
1. Press the power button on the data system computer.
2. Wait at least 20 seconds.
3. Press the power button again.

Resetting the Mass Spectrometer

In the unlikely event that communication is lost between the MS and data system computer, you can reset the MS by using the reset button (1 in Figure 21) located on the right-side communications panel.

With both the MS and data system computer on and operational, hold down the reset button on the right-side communication panel for 3 seconds.

Figure 21. Reset button (1) on the communication panel



The following occurs:

- The embedded computer restarts. All LEDs on the front panel turn off except the Power LED.
- After several more seconds, the Communication LED turns yellow and then green to indicate that the MS and the data system are communicating. The data system transfers operational software to the MS.

After a few minutes, the System LED turns yellow to indicate that the software transfer from the data system to the MS is complete and that the MS is in standby mode. When you change the mode from standby to on, the System LED turns green to indicate that the MS is functional.

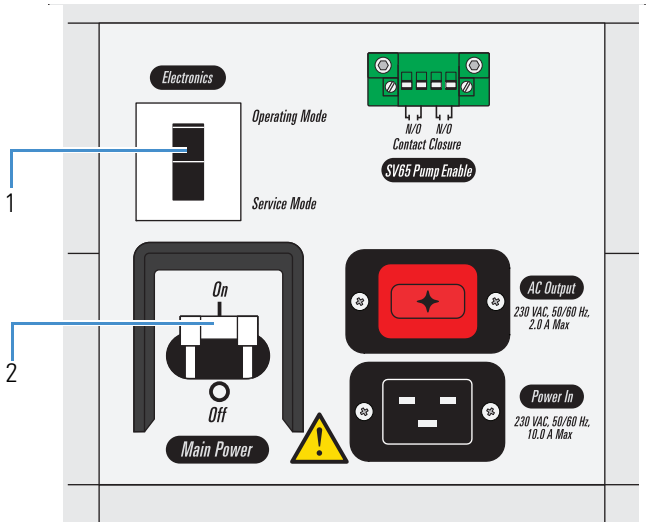
Pumping Down the MS

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

1. Ensure that the Main Power switch is off and that the electronics service switch is in the Service Mode position.
2. Plug in the power cord for the MS.
3. Turn on the Main Power switch.

   This turns on the forepump or forepumps and the turbomolecular pumps. All LEDs on the front panel are off.
4. Wait 15 minutes before you place the electronics service switch in the Operating Mode (up) position.
5. Wait at least 15 hours for the pumps to create sufficient vacuum.

Figure 22. Electronic service switch and main power switch



No.	Description
1.	Electronics service switch in service mode
2.	Main power switch turned on

The colors of the LED lights show the MS status.

MS Status	LED	Color
MS enters operating mode	Power	Green
	• Vacuum • Communication • System	Off
MS startup completed	• Vacuum • Communication	Green
	System	Yellow

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

6. In the Tune window, open the Status pane and double-click **Vacuum**.
A green square ( ) marks that the ionization gauge reading is below the maximum allowable pressure of 1×10^{-4}.

   Verify that the source pressure and analyzer pressure readback values are below the operating threshold limits.

Table 4. Vacuum pressure gauges threshold limits

MS	Source pressure	Analyzer pressure
TSQ Altis	4.5 Torr	9.0×10^{-6} Torr
TSQ Quantis	3 Torr	
TSQ Fortis	3 Torr	

Resetting Calibration Parameters

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

IMPORTANT

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

Starting the LC, Gases, and Autosampler

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

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

2. Turn on the autosampler by using its on/off power switch.

   If necessary, configure the autosampler. For procedures for placing sample vials, preparing solvent and waste containers, installing syringes, and so on, refer to the autosampler manual.

3. Check that the valves of the argon and nitrogen gases are open.

MS Components On/Off Status

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

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

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

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

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

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

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

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

Maintaining the MS on a Daily Basis

There are tasks that you can do before and after you operate the MS to prevent needless downtime.

- Before Operating the Mass Spectrometer
- After Operating the Mass Spectrometer

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

Before Operating the Mass Spectrometer

Follow these tasks to ensure that the MS is ready for operation.

- Finding and Fixing Air Leaks
- Checking the Vacuum Pressure Levels
- Checking the Argon and Nitrogen Gas Supplies

Finding and Fixing Air Leaks

A major air leak can indicate insufficient pressure levels to turn on the system. In the Tune window, a green square,( ), indicates that the readback value is good. Possible causes of a major leak might be a loose or disconnected fitting, an improperly positioned O-ring, or an open valve.

1. Listen for a rush of air or a hissing sound coming from the MS.
   - If you do not hear these sounds, there is no air leak.
   - If you hear these sounds continue with step 2.
2. Follow "Shutting the MS System Down Completely."
3. Visually inspect the vacuum system and vacuum lines for leaks.

4. Check each fitting and flange on the system for tightness and tighten any that are loose. Start with fittings that have been changed recently and fittings that have been subjected to heating and cooling.

Checking the Vacuum Pressure Levels

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

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

1. Open the Tune window.
2. Click the **Status** tab and click the **Expand** icon, , next to Vacuum.
3. Compare the current values of the pressures in the vacuum manifold with the values listed in Table 6 for the TSQ Altis MS, Table 7 for the TSQ Quantis, and Table 8 for the TSQ Fortis MS. If the values are higher than normal, you might have an air leak.

Table 6. TSQ Altis MS typical pressure readings

Conditions	Pressure (Torr)	
	Source pressure (foreline, ion transfer tube, RF lens region)	Analyzer (analyzer region after pumping for at least 12 hours)
Collision gas off, ion transfer tube orifice sealed	Less than 0.05	Less than 6×10^{-6}
Collision gas off, ion transfer tube orifice open	Less than 2.0	Less than 9×10^{-6}
Collision gas set to 1.5 mTorr, ion transfer tube orifice open	Less than 2.0	Approximately 3×10^{-5}

Table 7. TSQ Quantis MS typical pressure readings

Conditions	Pressure (Torr)	
	Source pressure (foreline, ion transfer tube, RF lens region)	Analyzer (analyzer region after pumping for at least 12 hours)
Collision gas off, ion transfer tube orifice sealed	Less than 0.05	Less than 6×10^{-6}
Collision gas off, ion transfer tube orifice open	Less than 3.5	Less than 9×10^{-6}
Collision gas set to 1.5 mTorr, ion transfer tube orifice open	Less than 3.5	Approximately 3×10^{-5}

Table 8. TSQ Fortis MS typical pressure readings

Conditions	Pressure (Torr)	
	Source pressure (foreline, ion transfer tube, Tube lens/Skimmer Region	Analyzer (analyzer region after pumping for at least 12 hours)
Collision gas off, ion transfer tube orifice sealed	Less than 0.05	Less than 6×10^{-6}
Collision gas off, ion transfer tube orifice open	Less than 2.0	Less than 9×10^{-6}
Collision gas set to 1.5 mTorr, ion transfer tube orifice open	Less than 2.0	Approximately 3×10^{-5}

4. Use the following table if the pressure is too high or is decreasing.

Table 9. Troubleshooting high or low vacuum pressure

If the pressure reading ...	Do this ...
Is high (above 5×10^{-5} Torr in the analyzer region), and you have restarted the system within the last 30 to 60 minutes	Wait an additional 30 minutes and recheck the pressure.
Decreases with time	Check the pressure periodically until it is within the typical pressure range of the MS.
Remains high	• Inspect the vacuum lines and fittings external to the MS for leaks and repair. • If you suspect an air leak within the MS, contact Thermo Fisher Scientific.

Checking the Argon and Nitrogen Gas Supplies

Check both argon and nitrogen regulators to determine how much gas is in the tank.

Table 10. Checking argon and nitrogen gas supplies

Gas	Procedure
Argon	1. Check the regulator to make sure there is sufficient gas. If necessary, replace the tank. 2. Verify that the pressure of argon gas reaching the MS is 135 ±70 kPa (20 ±10 psi). If necessary, adjust the pressure with the tank pressure regulator.
Nitrogen	1. Using the regulator of the nitrogen gas tank or liquid nitrogen boil-off tank, make sure that there is sufficient gas for the analysis. Based on 24-hour per day operation, typical nitrogen consumption is 2800 liters per day (100 ft^3/day). If necessary, replace the tank. 2. Verify that the pressure of nitrogen gas reaching the MS is 690 ± 140 kPa (100 ± 20 psi). If necessary, adjust the pressure with the tank pressure regulator.

CAUTION Before you operate the MS, verify that there is sufficient nitrogen for the API source. If you run out of nitrogen, the MS automatically turns off to prevent atmospheric oxygen from damaging the source. If oxygen is in the source when the MS is on, the source might be damaged. In addition, if the MS turns off during an analytical run, you might lose data.

For more information about gas requirements, refer to the *TSQ Altis, TSQ Quantis, and TSQ Fortis Preinstallation Requirements Guide*.

After Operating the Mass Spectrometer

Do these tasks after operating the MS.

Flushing the Inlet Components

Flush the syringe and the inlet components (sample transfer line, sample tube, and spray insert) regularly (or more often if you suspect they are contaminated). You can also use an LC pump to flush the 50:50 methanol/water solution through the inlet components to the API source at a flow rate of 200–400 µL/min for approximately 15 minutes.

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

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

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

c. Slowly depress the syringe plunger to flush the solution through the sample transfer line, sample tube, and spray insert.

d. Remove the syringe needle from the syringe adapter assembly.

Purging the Oil in the Forepump

The best time to purge (decontaminate) the oil is at the end of the working day after you flush the inlet components. Daily purging of the oil removes water and other dissolved chemicals, which can cause corrosion and decrease forepump performance over its lifetime.

Refer to the forepump's documentation. Make sure to close the purge valve before continuing normal operation.

Emptying the Solvent Waste Container

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

Placing the System in Standby Mode

After you complete the daily maintenance procedures, place the MS in standby mode as described in Chapter 8, "Placing the MS in Standby Mode."

Recommended Inlet and Flow Rates

Use the following tables for the recommended settings when operating your system in H-ESI, APCI, or NSI mode.

Recommended LC/H-ESI/MS Parameters

LC flow rate (µL/min)	Spray voltage (V)	Gas (arbitrary units)			Ion transfer tube temp (°C)	Vaporizer temp (°C)	Nitrogen use (L/min)
		Sheath	Auxiliary	Sweep			
Up to 15	Pos: 3500 Neg: –2500	5	2	0	Altis: 325 Quantis: 275 Fortis: 275	20	3.5
16–99		25	5	0		75	8.0
100–199		35	7	0	Altis: 325 Quantis: 300 Fortis: 300	275	10.5
200–500		50	10	1		350	15.0

Recommended LC/APCI/MS Parameters

LC flow rate (µL/min)	Sheath gas arbitrary units)	Auxiliary gas (arb units)	Sweep gas (arb units)	Ion transfer tube temp (°C)	Vaporizer temp (°C)	Corona discharge current (µA)
Up to 5	15	5	0	Altis: 300 Quantis: 250 Fortis: 250	275	Pos: 4 Neg: –10
5–199	25				325	
200–500	45			Altis: 325 Quantis: 275 Fortis: 275	350	

Recommend LC/NSI/MS Parameters

Spray voltage (V)	Sweep gas (arb units)	Ion transfer tube temp (°C)
Positive mode: 1200 Negative mode: –600	0	325

Connecting the Sample Flow to the Source

Connect the sample flow to the H-ESI source or the APCI source.

Note Use the fittings (PEEK or Viper™) that are appropriate for your application. The illustrations in Figure 23 and Figure 24 are examples only.

- Connecting the Sample Flow to the H-ESI Source
- Connecting the Sample Flow to the APCI Source

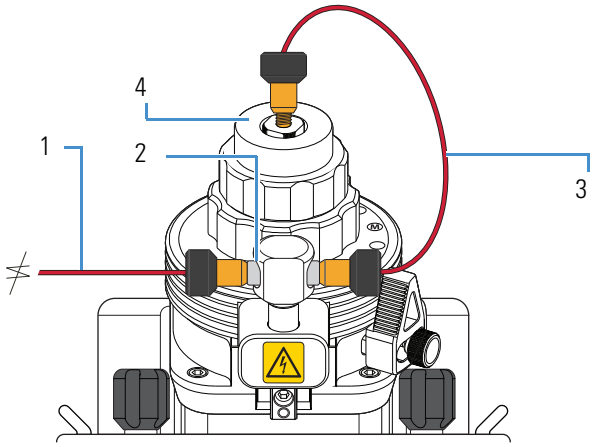
Connecting the Sample Flow to the H-ESI Source

Connect the H-ESI source or the low-flow H-ESI source to the sample flow. After making the connections, check for leaks at each of the connections before you turn the power on.

Note Refer to the *OptaMax NG Ion Source User Guide* for more information.

CAUTION If liquid is leaking out of a tube or a fitting it may be electrically live and could cause an electric shock when touched. Turn off the power to the source before fixing the leak. Turn the power off by switching the main power switch to off mode (down position) (5 in Figure 19). If you cannot safely reach the main power switch, unplug the power cord from the outlet.

Figure 23. Connection to the H-ESI or the low-flow H-ESI source



No.	Description
1.	Red PEEK tubing from the sample flow
2.	Grounding union
3.	Red PEEK tubing to the H-ESI or the low-flow H-ESI spray insert
4.	H-ESI or low-flow H-ESI spray insert

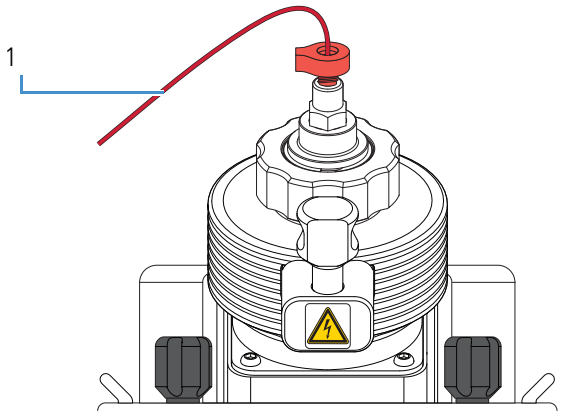
1. Use red PEEK tubing (1) (with a fingertight fitting) to connect the sample flow to the grounding union (2 Figure 23).
2. Use red PEEK tubing (3) (with a fingertight fitting) to connect to the other end of the grounding union (2).
3. Use a fingertight fitting to connect the other end of the red PEEK tubing (3) to the H-ESI or the low-flow H-ESI spray insert (4).

Connecting the Sample Flow to the APCI Source

Connect the APCI spray insert to the sample introduction method. If you have the inlet plumbed for H-ESI, you can leave the grounding union in place. You will not use it.

- Use tubing (red PEEK or natural PEEK (nano-Viper)) with a fingertight fitting to connect the sample flow to the sample inlet of the APCI spray insert (Figure 24).

Figure 24. Connection to the APCI spray insert



No.	Description
1.	Tubing from sample flow (red PEEK or natural PEEK (nano-Viper))

Calibrating the MS

Risk of electric shock: This instrument uses voltages that can cause electric shock and/or personal injury. While operating the instrument keep the covers on.

Set up the syringe pump and the MS for calibration, and then perform the calibration.

- Preparing the Syringe Pump for Calibration
- Preparing the MS for Calibration
- Determining the Initial API Source Settings
- Evaluating the Spray Stability
- Calibration Parameters
- Calibrating and Tuning the MS
- Calibration Solution Peak Values

Preparing the Syringe Pump for Calibration

Use the syringe pump to infuse the EMRS calibration solution into the H-ESI source. For a list of calibration supplies, see Appendix E, "Replaceable Parts."

Before you begin, follow the procedure in Appendix B, "Setting Up the Syringe with the Syringe Pump."

CAUTION Do not wear nitrile gloves when you are working with the calibration solution, EMRS. Nitrile gloves are made with diphenylguanidine which is soluble in EMRS. If diphenylguanidine contaminates the EMRS, the spectrum includes a peak at *m/z* 212.

IMPORTANT To prevent the EMRS from degrading, do the following:

- Do not return any EMRS back to the original vial.
- Do not store EMRS in a glass syringe. Discard unused EMRS and rinse the syringe with acetonitrile.
- If you observe degradation products in the EMRS mass spectrum, rinse the sample line (including the fittings, syringe, tubing, and union) with acetonitrile.

Observe these storage precautions for EMRS and reserpine solutions:

- Refrigerate the containers after opening.
- For long-term storage, keep the containers refrigerated at 2–8 °C (36–46 °F).

1. Load a clean, 500 µL syringe with EMRS.

   Use the following information to determine how much EMRS to use.

   - Tuning and calibrating take 30–50 minutes.
   - A full 500 µL syringe delivers sample for 100 minutes at a flow rate of 5 µL/min. Use a full syringe the first time you tune and calibrate.

2. Turn on the syringe pump's power switch (on the back of the device).
3. In the Tune window, place the MS in **Standby** mode.

CAUTION To prevent electric shock, verify that the grounding union is made of stainless steel. A grounding union made of a non-conductive material, such as PEEK, creates an electric shock hazard.

Preparing the MS for Calibration

1. In the Tune window, place the MS in **On** mode,  .
2. Click **Profile (Centroid)** and select the profile data type.
3. In the Favorites pane under System Settings, right-click **Default for EMRS Calibration with Positive Polarity,** and choose **Apply**.

   The default parameter settings appear at the top of the Favorites pane.

4. Set the syringe pump parameters as follows:

   a. Click **Syringe Off** to turn on the syringe pump.

      The button name changes to Syringe On.

   b. Click the arrow next to the Syringe On/Off button to open the syringe pump settings box (Figure 25), and then enter the following:

      Flow Rate (µL/min): **5**

      Volume (µL): **500**

Figure 25. Syringe pump settings box

c. Click **Apply**.

5. Verify that the inlet plumbing connections do not leak.
6. Open the syringe pump settings box again. Press and hold **Prime** to prime the syringe at 100 µL/min.
7. Verify that the system readback is normal, .

Determining the Initial API Source Settings

These initial setting are a starting point for calibrating and optimizing system performance.

1. In the Tune window, click the **Ion Source** tab.
2. In the Current LC Flow (µL/min) box, type the flow rate from Table 11, and then click **Get Defaults**.

Table 11. Recommended LC flow rates

Solution type	Injection type	LC flow rate (µL/min)
Calibration	Syringe	5
Sample	Syringe	3–10
	Autosampler	200

3. Click **Apply**.

The Tune application makes a change in the History pane.

Evaluating the Spray Stability

Use the Plot Chromatogram tool to evaluate the stability of the spray.

Before you begin, verify that the syringe contains the appropriate calibration solution and that the Tune window has the following settings.

Parameter	Value
Current LC Flow	5 µl/min
Syringe pump settings box	5 µL/min flow rate and a 500 µL syringe volume
Ion polarity mode	Positive
Data type	Profile

1. In the Define Scan pane (Figure 27), set the following parameters:
   - Scan Type: **SIM (Q1)**
   - Precursor (*m/z*): **622 (602 in Negative Mode)**
   - Source Fragmentation (V): **30**

   Figure 26. Define Scan parameters

2. Check the H-ESI probe position is as follows:
   - Depth: low to medium
   - Front-to-back position: closest to the MS entrance
   - Side-to-side position: center (closest to the MS entrance)
3. Place the MS in **On** mode.

The MS begins to scan and applies high voltage to the spray insert. A real-time mass spectrum appears in the Tune window.

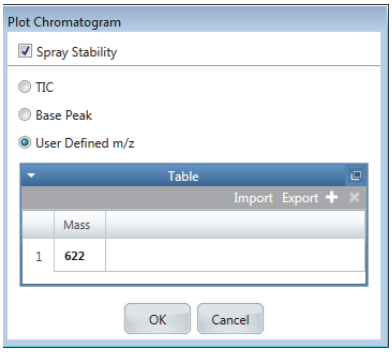
4. Click **Syringe Off** to turn on the syringe pump.

   A real-time plot of the EMRS mass spectrum appears.

5. Plot the ion chromatogram and the relative standard deviation (RSD) graphs as follows:

   a. Click the **Plot Chromatogram** icon,  , to open the Plot Chromatogram dialog box (Figure 27).

   Figure 27. Plot Chromatogram dialog box

   b. To monitor the RSD of the target ion current, select the **Spray Stability** check box.

   c. Select the **User Defined m/z** option, add a table row by clicking the + icon (upper right of the table), and type **622** (positive mode) or **602** (negative mode) in the Mass column.

   d. To plot the specified chromatogram, click **OK**.

      The Plot Chromatogram tool generates a real-time graph (plot) where you can observe the signal stability and the effects of changes to various parameters. The tool also generates a real-time graph of the RSD for a 10 Da-selected ion monitoring (SIM) scan that is centered around the most abundant mass-to-charge ratio (*m/z*) in the current spectrum.

6. Observe the RSD graph, and review the signal stability rating and %RSD value.

   Table 12 lists the criteria for a stable spray in either positive or negative ion polarity mode.

   Table 12. Recommended %RSD values and ratings for the calibration solutions

Ion polarity mode	Acceptable signal stability rating	Maximum %RSD (threshold)
Positive	Excellent or Good	15
Negative	Excellent or Good	15

7. If the signal stability rating is poor or the %RSD value is above the threshold, optimize the API source parameters as follows.

   a. Adjust the sheath gas plus or minus 1 unit.

b. Adjust the spray voltage plus or minus 250 units.

c. Change the API depth position from L/M to M.

8. Repeat this procedure for negative ion polarity mode.

Calibration Parameters

The calibration parameters affect mass accuracy and resolution.

The tune parameters affect the magnitude of the ion signal. There are two types of tune parameters:

- Mass-dependent parameters: DC offset voltages of lens L0, Turner-Kruger Lens 1 (TK1), and mass-analyzing quadrupoles and their end segments.
- Compound-dependent parameters: spray voltage (H-ESI or N-ESI), spray current (APCI), sheath gas pressure, auxiliary gas pressure, sweep gas pressure, vaporizer temperature, and ion transfer tube temperature.

Note When the MS completes a calibration, the Tune application writes the calibration parameters and the mass-dependent tune parameters to the calibration file, which overwrites the existing file. You cannot replace or modify the calibration file.

The Tune application writes the compound-dependent tune parameters to a change record in the History pane. You can rename and save the change record to the Favorites pane for future use in the Tune application or the Method Editor.

Calibrating and Tuning the MS

Successful calibration of the MS requires a steady flow rate of EMRS.

CAUTION Do not operate the system if it fails a calibration procedure. Contact a Thermo Fisher Scientific field service representative.

Note
- For optimum performance, calibrate the MS every one to three months of operation.
- To reduce the risk of potential errors, monitor quality control standards frequently.

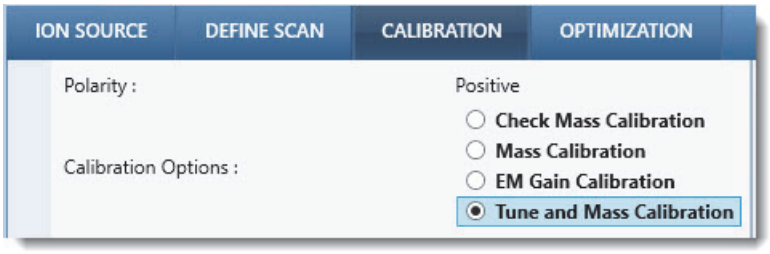
Before you calibrate the MS, follow the procedure "Evaluating the Spray Stability."

1. Set the syringe pump to infuse the EMRS at 5 µL/min into the API source.
2. Place the MS in **On** mode.
3. In the Define Scan pane, select **Full Scan (Q1)** or **Full Scan (Q3)**.

4. Set the scan range to **50–1650**.
5. Click **Calibration** to display the calibration status in the Calibration pane, and then click **Calibrate** to display the calibration options in the Calibration pane (Figure 28).

   Ensure that the calibration ions are present in the real-time spectrum. If the syringe was not primed, it may take a few minutes. For a list of the calibration ions, see "Calibration Solution Peak Values."

Figure 28. Calibration pane options



6. Select one of the Calibration options.

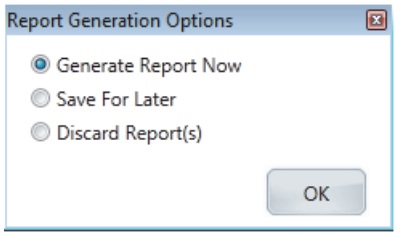
   Before you run each of these options, the system evaluates the spray stability.

   - Check Mass Calibration
   - Mass Calibration
   - EM Gain Calibration
   - Tune and Mass Calibration

7. Click **Start**.

   When the calibration is complete, the Tune application prompts you to generate a report of the calibration results.

Figure 29. Report Generation Options



8. Select an option and click **OK**.
9. After the MS completes the calibration procedure in positive mode, run the calibration procedures in negative ion mode.

IMPORTANT Check the spray and reevaluate it when it becomes unstable. If the spray is not stable, then data quality might be compromised, which can result in a poor calibration or diagnostic result.

Check Mass Calibration

Use the Check Mass Calibration option regularly (Figure 28).

To check the mass position and resolution, the Tune application uses the following calibrant masses:

- Positive Ion Mode: *m/z* 69, 622, and 1522
- Negative Ion Mode: *m/z* 69, 602, and 1634

The Check Mass Calibration routine evaluates the mass position and FWHM peak widths for the calibrant masses on a subset of the available resolutions including 0.2 Da (TSQ Altis MS only), 0.4 Da, 0.7 Da, and 1.2 Da. The routine performs the evaluation at the following scan rates: 250 Da/sec, 500 Da/sec, and 1000 Da/sec. The FWHM peak width and mass position tolerances for the calibrant masses are mass dependent and increase with mass. The results are displayed in the *Check Mass Calibration Report*.

Mass Calibration

Use the Mass Calibration option (Figure 28) if the Check Mass Calibration option fails.

During the mass and resolution calibration procedure, the RF and DC voltages are varied to achieve the targeted FWHM peak widths and mass positions. At the completion of the calibration procedure, a subset of calibrated FWHM peak widths and mass positions are evaluated and the results are displayed in the *Mass Calibration Report*.

EM Gain Calibration

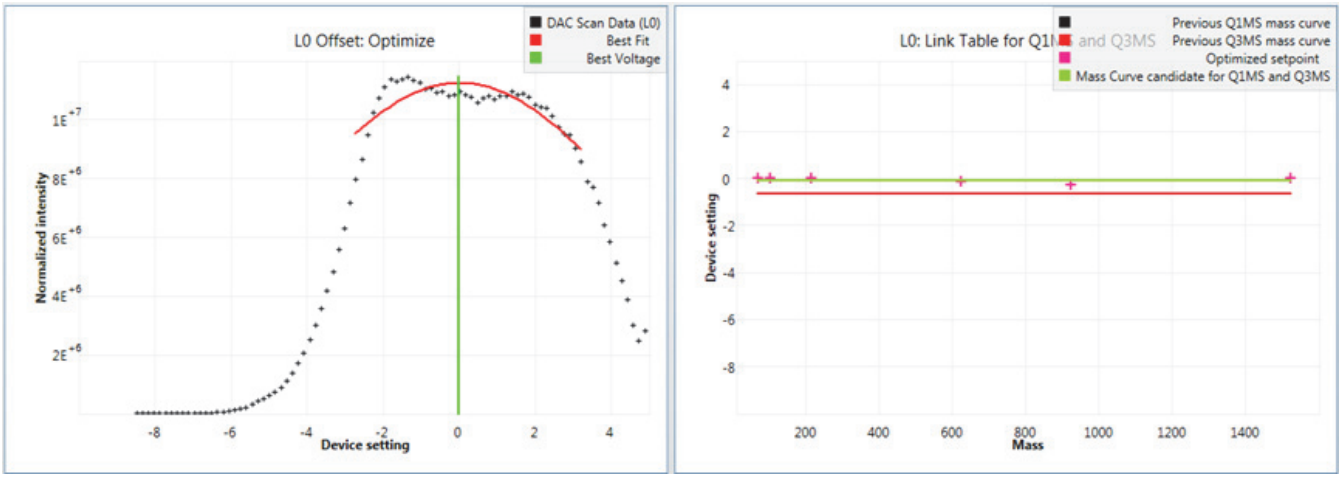
If you observe a decrease in sensitivity, run the EM Gain Calibration routine (Figure 28). This routine can be performed as frequently as needed to maintain sensitivity.

Tune and Mass Calibration

When you select the Tune and Mass Calibration option (Figure 28), the MS maximizes the ion signal by optimizing the DC offset voltages of the lenses and other optical elements.

Figure 30 shows the lens L0 offset voltage optimization for EMRS. After the optimizations are complete, the system performs a full mass position and resolution calibration.

Figure 30. Ion signal intensity as a function of the lens L0 offset voltage



Calibration Solution Peak Values

The mass spectra of the EMRS in positive and negative ion polarity modes (Figure 31 and Figure 32, respectively) have peaks at *m/z* values close to the theoretical values in Table 13 and Table 14.

IMPORTANT If you observe interfering peaks in the EMRS spectrum that are within ±10 Da of any of these calibration masses, follow the procedure "Flushing the Inlet Components," on page 45. Ensure that the interfering masses show less than 25 percent of the intensity of the calibrant ions.

Table 13. Mass spectral peaks $[M+H]^+$ for EMRS in the positive ion polarity mode

Component	Positive mode (*m/z*)
Imidazole	69.04
Triethylamine	102.13
1,8-Bis(diethylamino) napthalene	215.15
Hexakis(2,2-difluoroethoxy)phosphazene	622.03
Hexakis(2,2,3,3-tetrafluoropropoxy) phosphazene	922.01
Hexakis(1h,1h,5h-octafluoropentoxy) phosphazene	1521.97

Figure 31. Mass spectrum of EMRS in positive ion mode

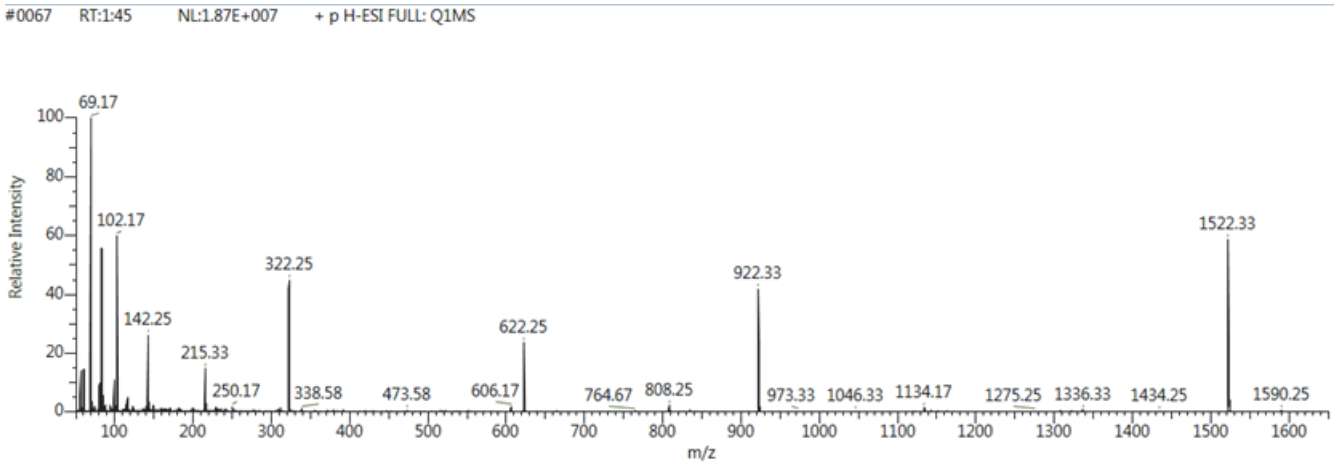


Table 14. Mass spectral peaks for EMRS in the negative ion polarity mode

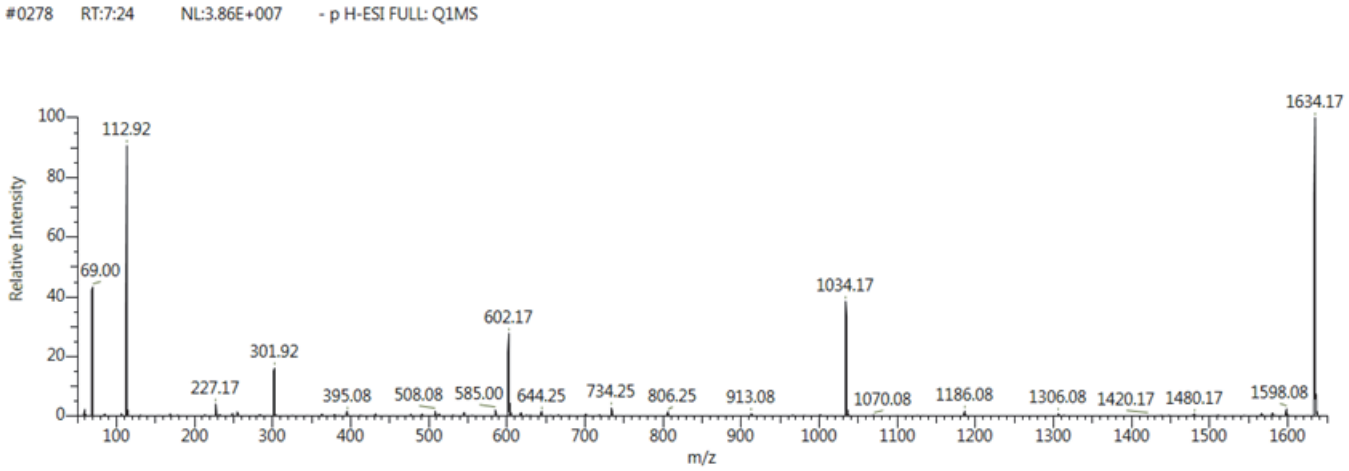
Component	Negative mode (*m/z*)
Fragment of TFA	69.00
Trifluoroacetic acid (TFA)	112.99[a]
2,4,6-Tris(trifluoromethyl)-1,3,5-triazine	302.00[b]
2,4,6-Tris(heptafluoropropyl)-1,3,5-triazine	601.98[b]
Hexakis(2,2,3,3-tetrafluoropropoxy) phosphazene	1033.99[c]
Hexakis(1h,1h,5h-octafluoropentoxy) phosphazene	1633.95[c]

[a] $[M–H]^-$

[b] $[M+OH]^-$

[c] $[M+TFA]^-$

Figure 32. Mass spectrum of EMRS in negative ion mode



Optimizing the Compound Signal

You can increase the signal from your analyte, by using the Optimization pane in the Tune application to optimize the MS parameters.

Performing Compound Optimization (Animation)

1. To view the animation, go to thermofisher.com.
2. In the search field, type **TSQ Altis**, **TSQ Quantis**, or **TSQ Fortis**.
3. Click the **Catalog** tab and then the instrument name.
4. Scroll down until you see the Product overview, Videos, and Documents tabs.
5. Click the **Videos** tab and on the right, click **Performing Compound Optimization**.

Setting Up for Compound Optimization

You optimize the signal of the compound with the LC conditions used to analyze it. This is a high-flow infusion technique, in which a Tee union directs the analyte from the syringe pump into an LC flow.

For plumbing instructions see "Setting Up High-Flow Infusion Without an Autosampler," in Appendix D, "Setting Up Sample Introduction Techniques."

Optimizing Parameters in the Optimization Pane

IMPORTANT Thermo Fisher Scientific recommends that you optimize system parameters if the spray becomes unstable and also after restarting the sample flow into the system.

1. Make sure that the syringe has enough of the sample solution.
2. In the Tune window, click **Syringe Off** to turn on the syringe pump.

   The button name changes to Syringe On. If your LC/MS system includes an LC device, prepare an LC method before you turn on the liquid flow to the API source.
3. In the Optimization pane (Figure 33), do the following:
   a. In the Sample Injection Type list, select **Syringe**.
   b. In the Mass List Type list, make a selection.

      If you select the Formula mass list type, you can select one or both ion polarity modes and specify the adducts to include. For descriptions of the Optimization parameters, refer to the Tune Help.

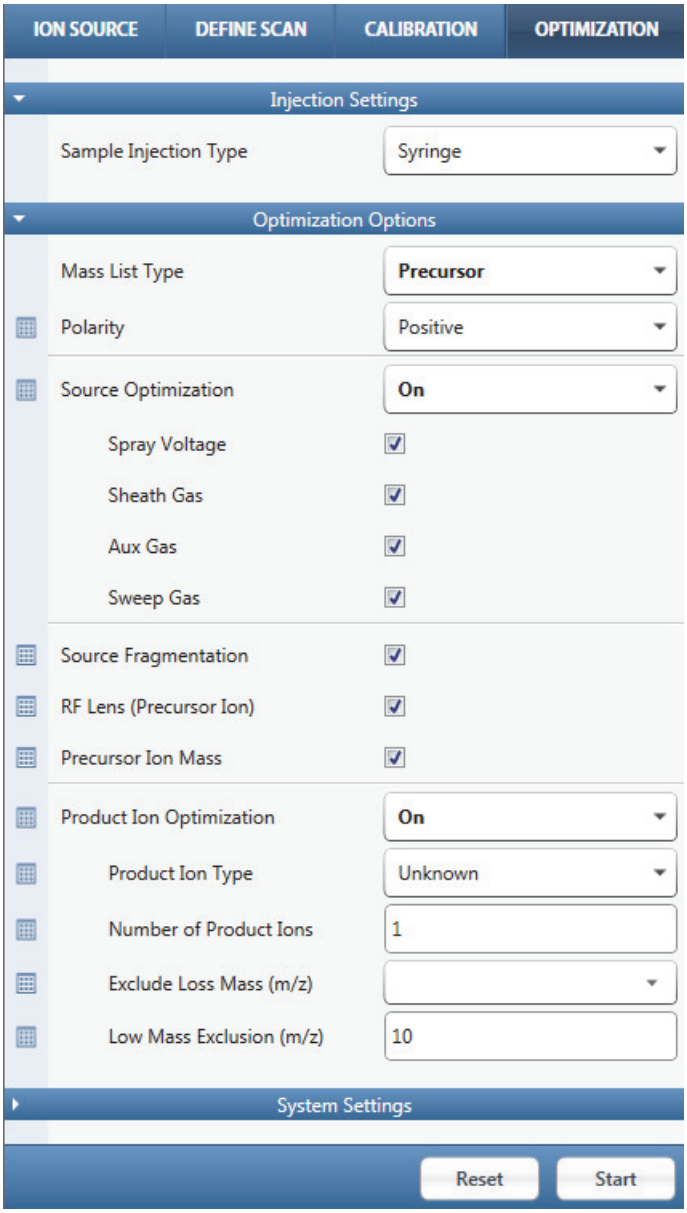
   c. In the Source Optimization list, select **On** and then select the **Spray Voltage**, **Sheath Gas**, **Aux Gas**, and **Sweep Gas** check boxes that appear.
   d. For a SIM scan, select the **Source Fragmentation**, **RF Lens**, and **Precursor Ion Mass** check boxes. For an SRM scan, also select **On** in the Product Ion Optimization list.

      Note The default values are sufficient for most experiments.

   e. Click the **Add/Remove Table Column** icon,  , next to the parameters that you want to customize per compound. Otherwise, the MS applies the parameter setting to all compounds.

      When selected, the icon changes color, from  to  , and the parameter appears in the Optimization Table (not shown here).

Figure 33. Optimizing the source parameters in the Optimization pane



4. In the Optimization Table, add a row for each compound and modify the column values as applicable.

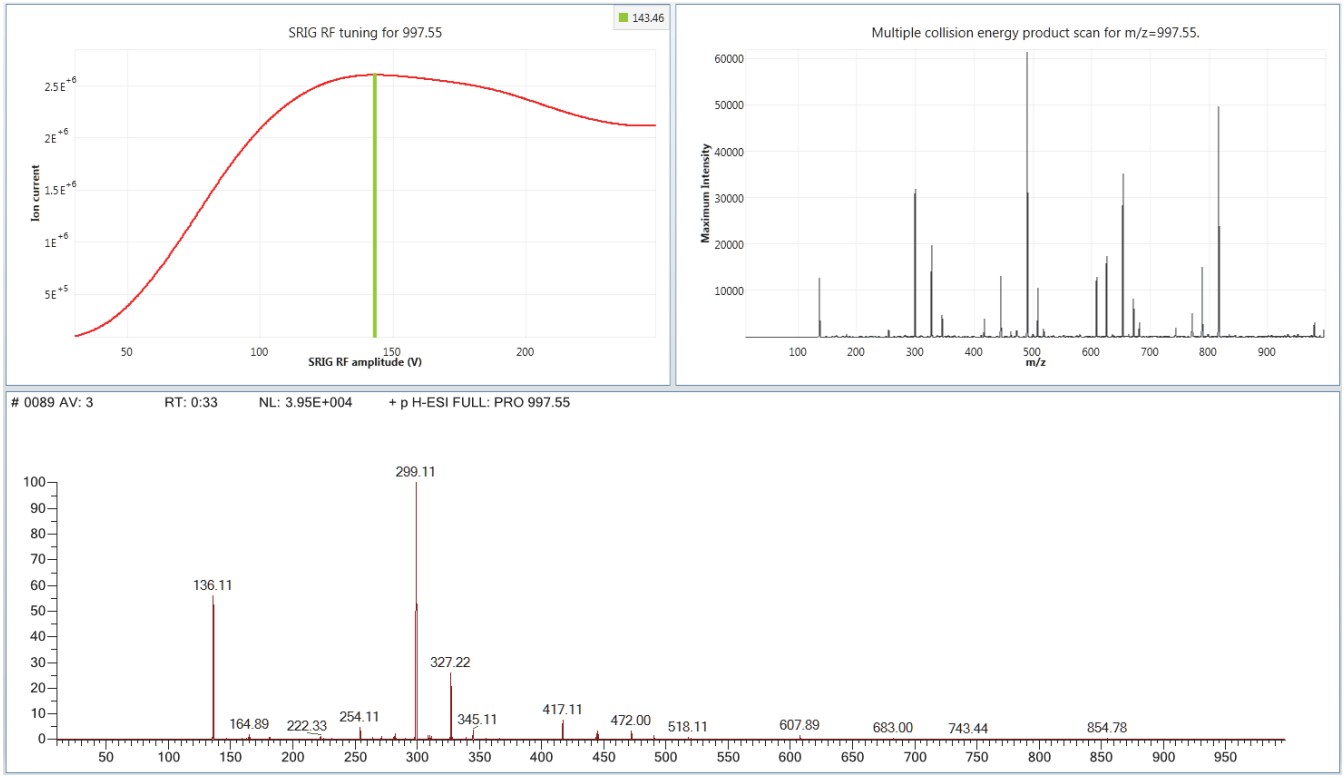
> **Tip** If there are multiple syringes, enter the syringe number in the Injection ID column.

5. Place the system in **On** mode, and then click **Start**.

   After the compound optimization is complete, you can view and save the generated report for each compound. Figure 34 shows an example of "in progress" graphs and spectra. Figure 35 shows the Optimization Results table.

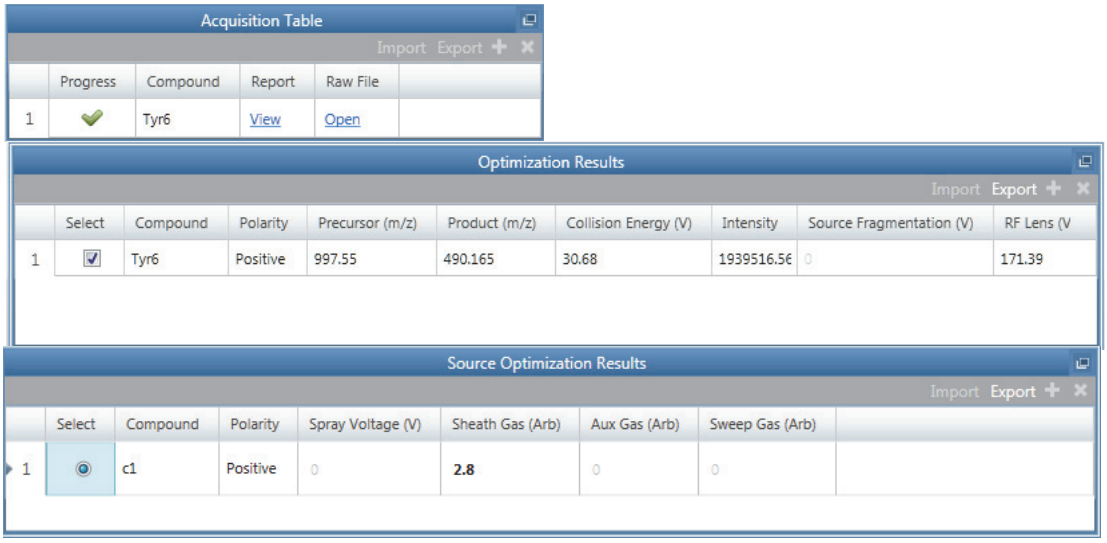
6. Right-click on the Optimization Results table, click **Copy**, and then paste it in the Xcalibur Method Editor. Figure 34 shows the Optimization Results Table.

Figure 34. Example optimization of the RF lens (SRIG RF) tuning for *m/z* 997.55



After the optimization is complete, the Acquisition Table appears, which contains links to an optimization report and raw data file for each optimized compound. The Optimization Results and Source Optimization Results tables also appear, displaying the optimized parameter values (Figure 35).

Figure 35. Examples of the optimization results tables



Scan Types

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

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

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

Quadrupole Capacities

The mass analyzers have three rod assemblies. 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 *m/z* values (that is, virtually all ions that are present).

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

On the MS, the quadrupole rod assemblies can operate with both RF and DC voltages or with only RF voltage. That is, Q1 and Q3 can act as either mass analyzers or ion transmission devices. The Q2 rod assembly operates exclusively with RF voltage. Therefore, Q2 is always an ion transmission device.

Summary of Scan Types

Table 15. Summary of scan types

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

[a] Full scan or transmission of selected ions.

[b] Pass ions or fragments within a wide range of *m/z* values.

[c] Set to pass ions of a single *m/z* or a set of *m/z* values.

[d] Collisions with argon gas cause ions to fragment.

Full Scan Q1 and Q3 Scan Types

Note For ease of documenting the first, second, and third rod assemblies as separate pieces of hardware, this manual refers to them as Q1, Q2, and Q3, respectively.

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

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

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

Before you perform a SIM or an SRM experiment, you must know what ions or reactions you are looking for. Therefore, you might use a full scan for SIM to determine the identity of an analyte and to obtain its mass spectrum, and a full scan for SRM to determine the mass spectrum and product mass spectra for precursor ions of interest. Then, you might use SIM or SRM to do routine quantitative analysis of the compound.

Selected Ion Monitoring Scan Type

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

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

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

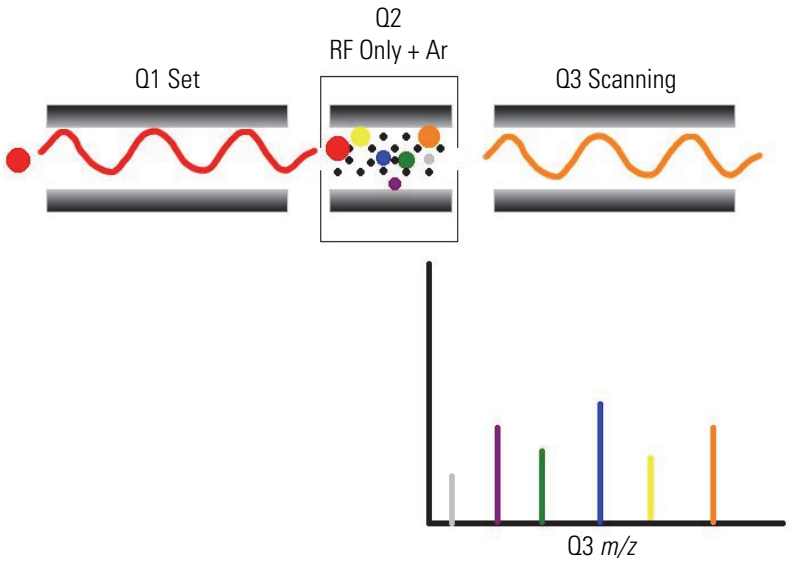
Product Scan Type

Product scan type performs two stages of analysis (Figure 36). In the first stage, the ion source forms ions that enter Q1, which is set to transmit ions of one *m/z*. Ions selected by this first stage of mass analysis are called precursor ions. (As a result, Q1 is referred to as the precursor mass analyzer, and the *m/z* of ions transmitted by the precursor mass analyzer is referred to as the precursor set mass.) After Q1 selects the precursor ions, they enter Q2, which is surrounded by the collision cell.

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

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

Figure 36. Illustration of the product scan type



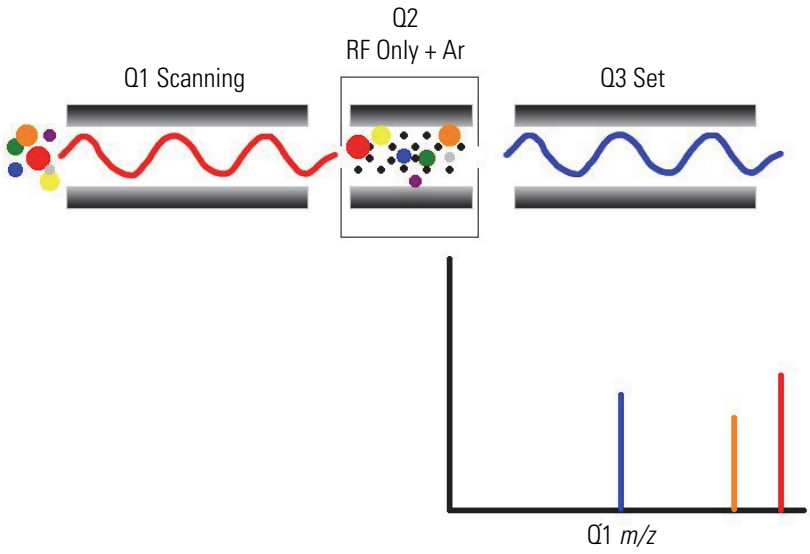
Precursor Scan Type

The precursor scan type also uses two stages of analysis (Figure 37). In the first stage, the ion source forms ions that are introduced into the precursor mass analyzer, which is scanned to transmit precursor ions sequentially into the collision cell.

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

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

Figure 37. Illustration of the precursor scan type



You can use experiments that employ the precursor scan type (precursor experiments) in structure and fragmentation studies as well as in survey analyses of mixtures. In general, precursor experiments detect all compounds that decompose to a common fragment. You can use the experiments for the rapid detection of a series of structural homologs (for example, substituted aromatics, phthalates, steroids, or fatty acids) that have a common fragment ion (for example, *m/z* 149 for the phthalates).

Neutral Loss Scan Type

In the neutral loss scan type (Figure 38), the two mass analyzers (Q1 and Q3) link together so that they are scanned at the same rate over mass ranges of the same width. However, the respective mass ranges, are offset by a selected mass so that the product mass analyzer scans a selected number of mass units lower than the precursor mass analyzer.

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

In the second stage of analysis, ions in the collision cell can fragment further by metastable ion decomposition or by CID to produce product ions. The product mass analyzer then separates these product ions by their *m/z* value.

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

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

For a neutral loss (or neutral gain) mass spectrum, as for a precursor mass spectrum, Q1 (the precursor ion) provides data for the *m/z* axis, whereas Q3 (the product ion being monitored) provides data for the ion intensity axis.

You can use experiments that use the neutral loss scan type (neutral loss experiments) when surveying a large number of compounds for common functionality. However, you frequently lose neutral moieties from substituent functional groups (for example, CO_2 from carboxylic acids, CO from aldehydes, HX from halides, and H_2O from alcohols). Figure 39 shows a common fragment ion.

Figure 38. Illustration of the neutral loss scan type

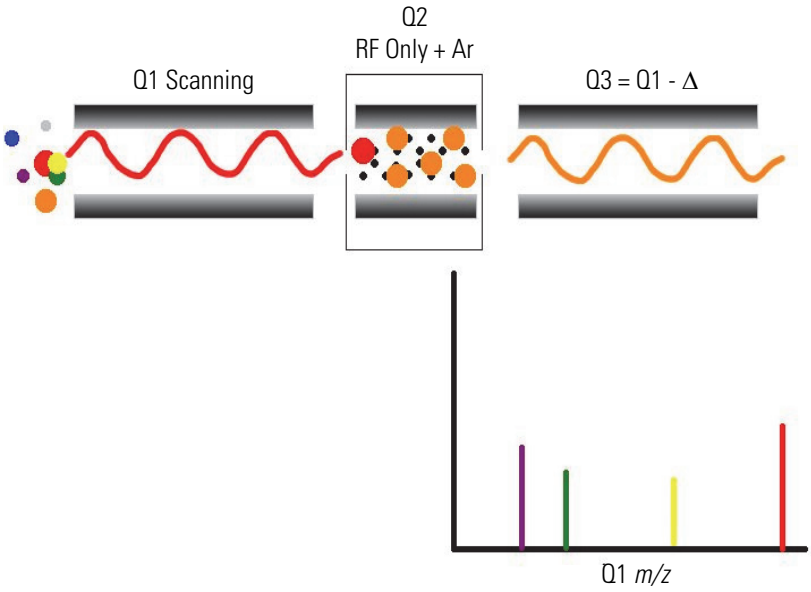
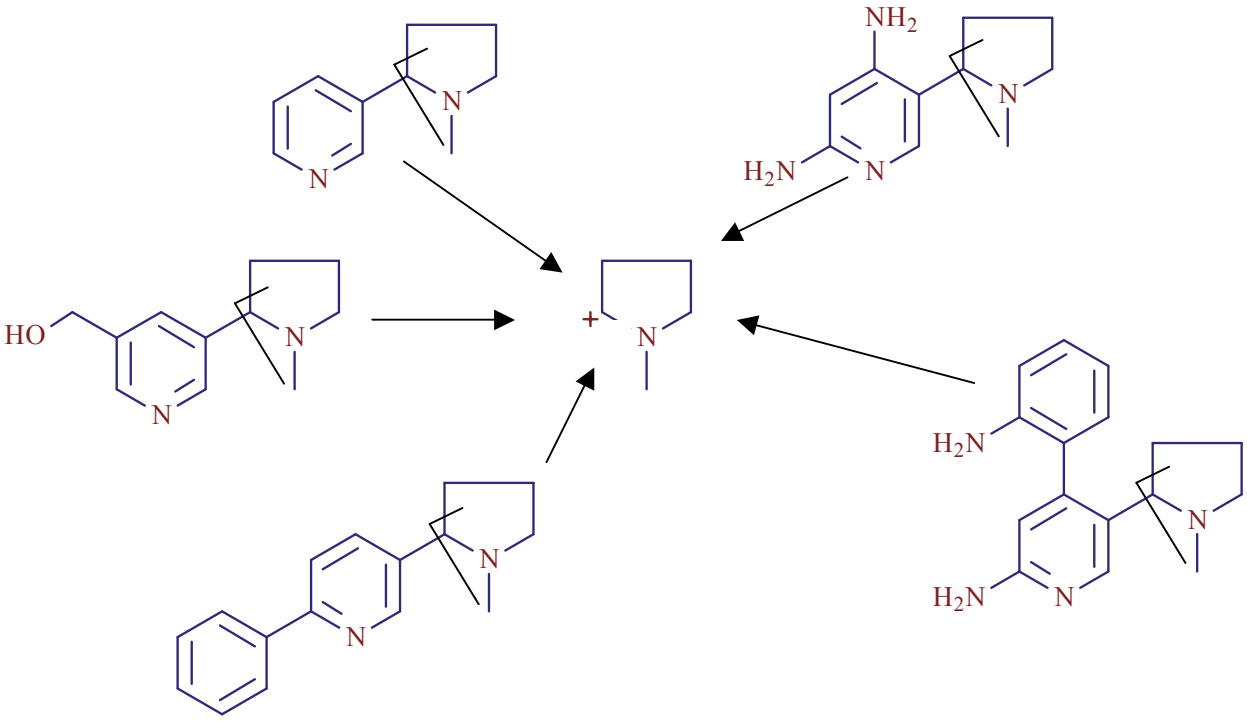


Figure 39. Examples of compounds with a common fragment



Selected Reaction Monitoring Scan Type

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

As does SIM, SRM provides for the very rapid analysis of trace components in complex mixtures. However, because SRM selects two sets of ions, it obtains greater selectivity compared to SIM. Any interfering compound would have to form a precursor ion of the same *m/z* as the selected precursor ion from the target compound. Furthermore, that precursor ion would have to fragment to form a product ion of the same *m/z* as the selected product ion from the target compound.

Data Types

You can acquire data in profile or centroid mode and you can detect positive and negative ions.

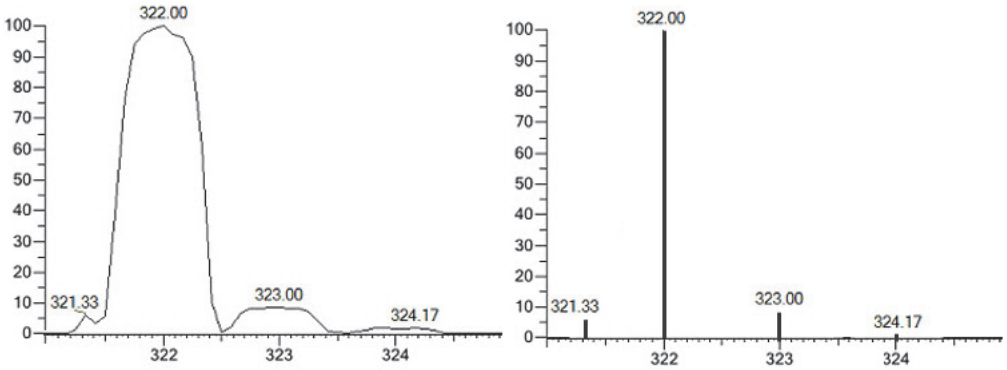
Profile and Centroid Data

You can acquire and display mass spectral data (intensity versus *m/z*) as profile data or as centroid data.

- Profile data—With profile data, you see the inherent shape of the peaks in the mass spectrum. The mass spectrum divides each atomic mass unit into several sampling intervals. The intensity of the ion current is determined at each sampling interval. The intensity at each sampling interval is displayed with the intensities connected by a continuous line. Profile data is a good way to see the isotopic distribution, especially for higher charged ions.
- Centroid data—With centroid data, you see the mass spectrum as a bar graph. Centroid gives you a reliable readback of the measured *m/z*. This scan data type sums the intensities of each set of sampling intervals. This sum is displayed versus the integral center of mass of the many sampling intervals. An advantage of centroid data it that it requires about one-tenth the computer disk space of profile data.

  When you do SRM methods, the data is automatically collected in centroid mode.

Figure 40. Examples of profile (left) and centroid (right) data



Ion Polarity Modes

The TSQ Altis, TSQ Quantis, and TSQ Fortis MSs can operate in either positive or negative ion polarity mode. You can obtain positive ion, negative ion, or positive/negative ion mass spectra.The MS controls whether positive ions or negative ions are transmitted to the mass analyzer for mass analysis by changing the polarity of the voltage potentials applied to the API source, ion optics, and ion detection system.

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

Acquiring Sample Data

To manually acquire sample data, use either the Tune application or the Xcalibur data system (Method Editor).

Note Before you begin, check the following:

- In the Calibration pane, ensure that all calibrations are up to date.
- Connect the Ready Out cable (not provided) and the contact closure cable to help prevent sample loss. Refer to the *TSQ Altis, TSQ Quantis, and TSQ Fortis Getting Connected Guide*.

Creating an SRM Method (Animation)

1. To view the animation, go to thermofisher.com.
2. In the search field, type **TSQ Altis**, **TSQ Quantis**, or **TSQ Fortis**.
3. Click the **Catalog** tab and then the instrument name.
4. Scroll down until you see the Product overview, Videos, and Documents tabs.
5. Click the **Videos** tab and on the right, click **Creating an SRM Method**.

Using Tune to Acquire Sample Data

1. Open the Data Acquisition pane (Figure 41), and then do the following:

   a. (Optional) To change the destination folder for the raw data file, click the **Browse** icon,  .

      The default folder location is in *drive*:\Thermo\Data.

   b. In the File Name box, type **reserpine** (or the name of the analyte).

      If the base file name already exists in the save location, the Tune application adds a time-stamp suffix that consists of the year (*YYYY*), month (*MM*), day (*DD*), and time (*HHMMSS*).

   c. In the Sample Name box, type the name of the analyte (or other suitable label).

   d. In the Comment box, type a comment about the experiment.

      For example, describe the ionization mode, scan type, scan rate, sample amount, or method of sample introduction. The data system includes the comment in the header information for the raw data file.

      You can also add this information to reports created with the Xcalibur XReport reporting application. To open this application, choose **Start > All Programs > Thermo Xcalibur > XReport**.

   e. Under Timed Acquisition, select the **Continuous Acquisition** option from the dropdown list (acquires data until you stop the acquisition) (1 in Figure 41).

2. Click **Record** to start data acquisition.

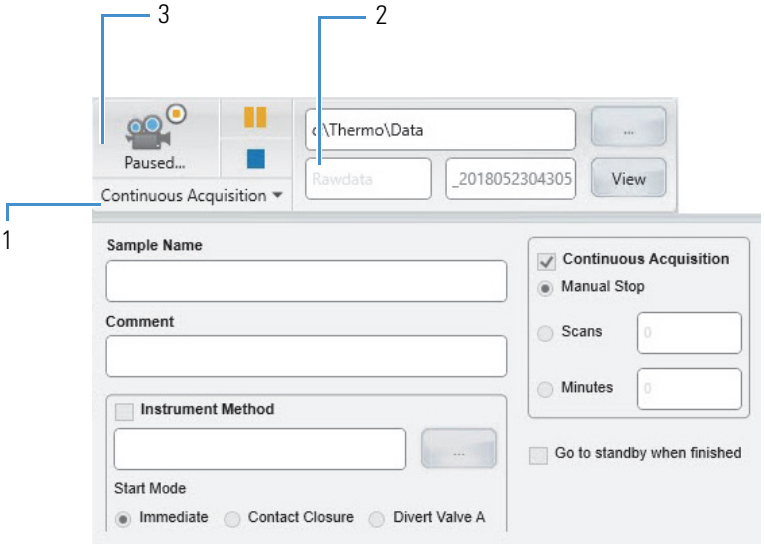
   After the Tune parameters reach their specified settings, the data acquisition process begins and the small circle on the Record button turns red ().

3. When you are ready, click **Record** again to stop the acquisition.

   The small circle on the Record button turns gray (not recording).

For more information about reviewing the acquired data, refer to the *Thermo FreeStyle User Guide* or the FreeStyle Help.

Figure 41. Data Acquisition pane in the Tune window



No.	Description
1.	Click to open/close the Data Acquisition pane.
2.	File name box
3.	Start/stop/pause the data acquisition recording.

Using the Xcalibur Data System to Acquire Sample Data

Thermo Scientific mass spectrometry applications, such as the Xcalibur data system, can control other devices in addition to the MS.

- If it can control the autosampler as part of your LC/MS system, it selects the autosampler as the default start (trigger) instrument for a sequence run.
- If the software instrument configuration does not include an autosampler, the data system selects the MS as the start instrument, which means that you must change the start instrument to the appropriate instrument as part of the Xcalibur sequence setup.

> **Note** For example, for a TSQ Series II MS with a paper spray ion source, the Xcalibur data system selects the MS as the start instrument. To run the sequence, you must make sure that no instrument is selected as the start instrument.

Follow these procedures:

1. Selecting the External Start Instrument
2. Acquiring Data Files with the Xcalibur Data System

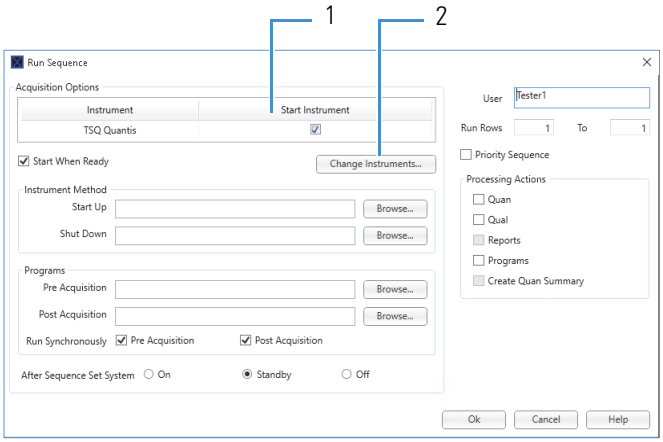
Selecting the External Start Instrument

1. Open the Xcalibur data system, and then choose **View > Sequence Setup View** to open the Sequence Setup window.
2. Open the sequence that you want to run as follows:
   a. Click the **Open** button and browse to the appropriate folder.
   b. Select the sequence (.sld) file and click **Open**.

3. Choose **Actions > Run Sequence or Actions > Run This Sample** to open the Run Sequence dialog box (Figure 42).

   The check mark in the Start Instrument column indicates the default start instrument for the sequence run.

   Figure 42. Run Sequence dialog box (partial) showing the selected start instrument

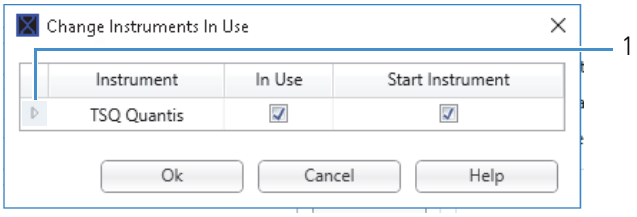


No.	Description	No.	Description
1.	Start Instrument	2.	Change Instruments button

4. If the correct instrument is not selected as the start instrument, do the following:

   a. Click **Change Instruments** to open the Change Instruments In Use dialog box (Figure 43).

      Figure 43. Change Instrument in Use dialog box



   b. In the Start Instrument column, select the check box for the start instrument. If the MS is selected as the start instrument, clear its check box in the Start Instrument column.

   c. Click **OK**.

5. In the Run Sequence dialog box, complete the remaining selections.

6. Click **OK**.

This completes the start instrument setup.

Acquiring Data Files with the Xcalibur Data System

For instructions, refer to the Instrument Setup and Sequence Setup topics in the Xcalibur Help.

Using Templates in Thermo Xcalibur Instrument Setup

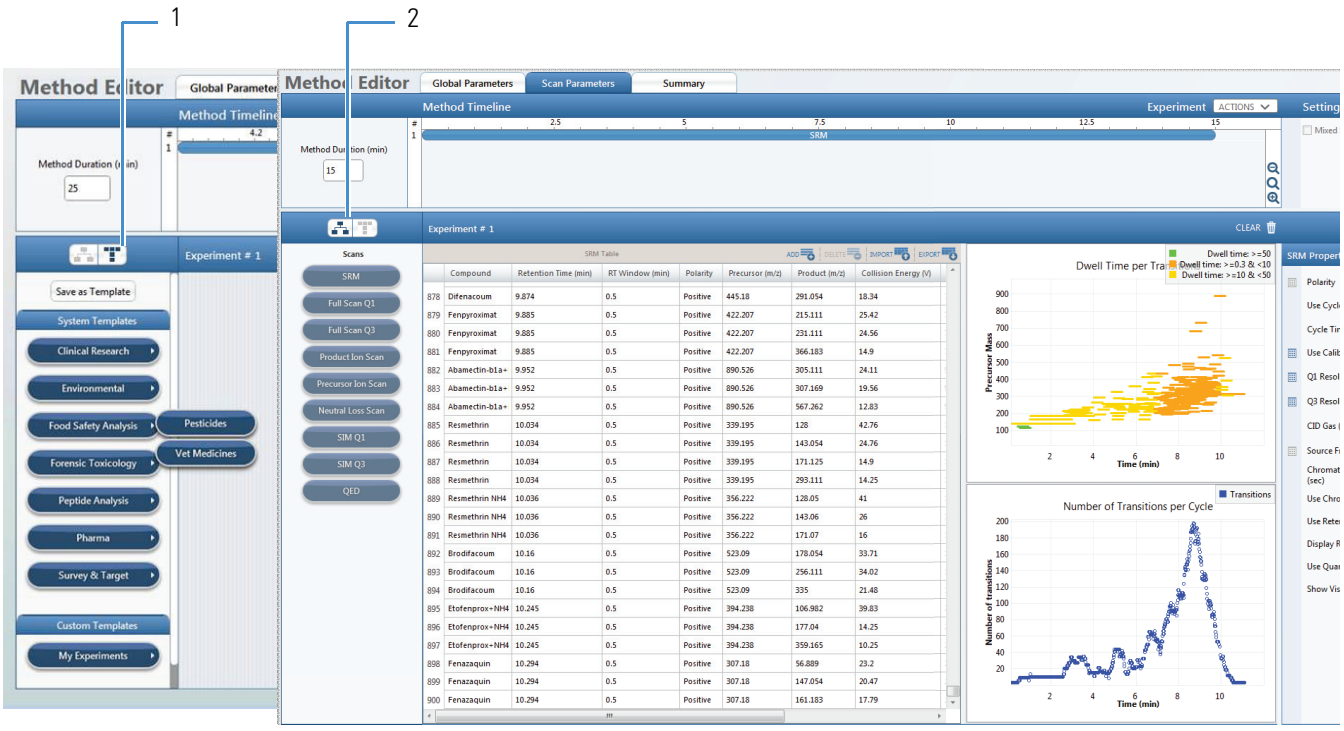
The Method Editor in the Xcalibur Instrument Setup window (Figure 44) has templates for different experiment types, including environmental and food safety (EFS) and peptide analysis (PA).

From the Xcalibur Instrument Setup window, you can use the Method Editor to create an instrument method for your experiment:

1. Open the system template designed for the experiment type that you want to perform.
2. Enter the parameters specific to the experiment.
3. Save the entries as part of an Xcalibur instrument method (.meth file name extension).

For additional information, refer to the Help.

Figure 44. Templates in Method Editor



No.	Description	No.	Description
1.	Click this icon to display the templates.	2.	Click this icon to display scan types.

Maintenance Schedule and Supplies

Performing routine maintenance procedures ensures optimum performance of the MS system.

- MS Parts
- Maintenance Schedule
- Guidelines
- Tools and Supplies

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

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

MS Parts

While the procedures may be similar for all three systems, the TSQ Altis MS, TSQ Quantis MS, and TSQ Fortis MS might use different parts. The required parts for each MS system are noted in each procedure. For a list of replaceable parts, see Appendix E, "Replaceable Parts."

Maintenance Schedule

Table 16 lists the maintenance procedures, their location, and their recommended frequency.

Table 16. Mass spectrometer maintenance procedures and frequency

MS component	Procedure	Recommended frequency	Reference
API source	Flush (clean) the sample transfer line, sample tube, and spray insert.	Daily	page 45
	Clean the API source housing.	As needed	page 91
	Clean the APPI fan filter.		*OptaMax NG Ion Source User Guide*
	Replace the APPI lamp.		
	Replace the H-ESI needle insert.	If the metal needle is obstructed	
	Replace the APCI fused-silica tubing.	If the tubing is obstructed	
API source interface	Clean the ion sweep cone and spray cone.	Daily, or more often depending on analytical conditions	page 93
	Remove and clean the ion transfer tube.	Weekly, or if the ion transfer tube bore is contaminated or obstructed	
	Replace the ion transfer tube.	If the bore becomes corroded or blocked	
	Clean the exit lens or RF lens.	As needed, depending on analytical conditions	
	Clean MP00 RF lens and lens L0.	As needed, depending on analytical conditions	
Forepump (each)	Purge (decontaminate) the oil and check for leaks.	Daily	Manufacturer's manual
	Add oil.	As needed, based on oil level	
	Change the oil.	Every 12 months of typical use, or if the oil is cloudy or discolored	
Cooling fans	Clean the air filter.	Every 4 months	page 115

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

Guidelines

These guidelines prepare you to do maintenance efficiently.

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

IMPORTANT Make sure that you do not introduce any scratches or surface abrasions while handling the API source interface components. Even small scratches can affect performance if they are close to the ion transmission path. Avoid using tools, such as metal pliers, that might scratch these components.

Note Before you continue, read the precautions in "Special Notices, Symbols, and Cautions," xvi.

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

Tools and Supplies

The MS requires few tools to perform routine maintenance procedures. You can remove and disassemble many of the components by hand. Table 17 lists the necessary chemicals, tools, and equipment for maintaining the instrument. (One of the tools is in the TSQ Source Installation Kit.) In addition, you can use the contents of the PM Cleaning Kit (P/N 70111-62112).

CAUTION Avoid exposure to potentially harmful materials.

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

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

Table 17. Chemicals, tools, and equipment (Sheet 1 of 2)

Description	Part number
Chemicals	
Detergent (for example, Liquinox™)	(Liquinox) Fisher Scientific™ • 16-000-125 (1 quart) • 16-000-126 (1 gallon)
Methanol, UHPLC/MS-grade	Fisher Scientific A458-1
Nitrogen gas, clean and dry	–
Water, UHPLC/MS-grade	Fisher Scientific W8-1
Tools	
Ion transfer tube removal tools for these MSs	(in the TSQ Source Installation Kit)
• TSQ Altis MS (ion transfer tube with quarter-turn pin)	70005-20972
• TSQ Quantis MS (ion transfer tube w/threaded nose cone)	70111-20258
• TSQ Fortis MS (ion transfer tube w/threaded nose cone)	70111-20258
Screwdriver, Phillips #2 (M3)	–
(Optional) Toothbrush, soft (or similar tool)	–
(Optional) Tweezers, plastic (or similar tool)	–
Equipment	
Beaker or graduated cylinder (for use with methanol)	–

Table 17. Chemicals, tools, and equipment (Sheet 2 of 2)

Description	Part number
Chamois-tipped swabs	00725-01-00028
Gloves, lint-free and powder-free	Fisher Scientific 19-120-2947 Unity Lab Services: • 23827-0008 (size medium) • 23827-0009 (size large)
Industrial tissues, lint-free	–
Magnification device	–
MICRO-MESH™ polishing swabs, 6000 grit (light purple color), 2.25 in. long	00725-01-00027
Sonicator	–

21

Maintaining the API Source Housing and Replacing the H-ESI Needle

Cleaning the API Source Housing

Clean the housing as necessary. Follow all safety precautions in the *OptaMax NG Ion Sources User Guide* regarding the installation and removal of the API source. For any additional service, contact your local Thermo Fisher Scientific service engineer.

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

Replacing the H-ESI Needle

Refer to the *OptaMax NG Ion Source User Guide* or view the video on the Thermo Fisher Scientific website. Go to thermofisher.com.

Maintaining the External Components of the API Source Interface

Clean the ion sweep cone, the spray cone, and the ion transfer tube at the same time, since they are closely connected.

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

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

Perform these tasks in order:

1. Removing the Ion Sweep Cone and the Ion Transfer Tube
2. Cleaning the Spray Cone and Seal
3. Cleaning the Ion Transfer Tube
4. Cleaning the Ion Sweep Cone

Maintenance Animations

1. To view the animations, go to thermofisher.com.
2. Open the product page for your MS as follows:
   a. In the Search All field, type **TSQ Altis**, **TSQ Quantis**, or **TSQ Fortis**.
   b. Under Products, click the product name to open the product page for the selected mass spectrometer.
3. On the product page, scroll down to the Product overview, Videos, and Documents tabs.
4. Click the **Videos** tab and select the video to view.

Note (Subject to change) The *Removing and Cleaning the Ion Transfer Tube* video for the TSQ Altis MS shows you how to remove, clean, and reinstall the ion transfer tube.

Removing the Ion Sweep Cone and the Ion Transfer Tube

Because buffer salts or high concentrations of samples can cause blockages in the bore of the ion transfer tube, you must clean it.

If pressure in the ion transfer tube and RF lens region (Source Pressure gauge) drops below 2 Torr (TSQ Altis) or 1 Torr (TSQ Quantis or TSQ Fortis), a blocked ion transfer tube is probably the cause.

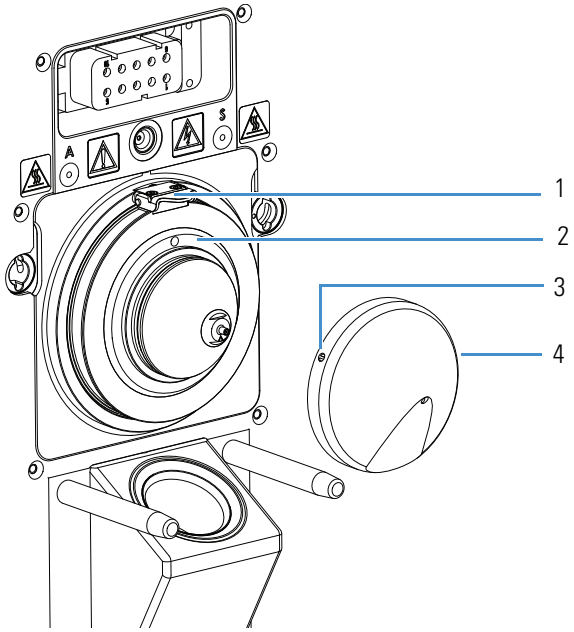
CAUTION Hot surface. The external surface of the spray insert, API source housing, and entry to the ion transfer tube can be hot enough to burn your skin. Allow the parts to cool to room temperature (approximately 20 minutes) before you touch it.

1. Turn off the liquid flow to the API source.
2. In the Tune application, place the MS in **Standby** mode.
3. In the Ion Source pane, set the Ion Transfer Tube Temperature and Vaporizer Temperature to 50 °C or less and observe the readback temperatures.
4. Place the MS in the **Off** mode.
5. After the source cools to room temperature, remove the source housing, refer to the *OptaMax NG Ion Source User Guide*, Chapter 2 section *Removing and Installing the API Source.*
6. Remove the ion sweep cone by grasping its outer ridges and pulling it off (Figure 45). If necessary, loosen the screws on the ion sweep cone.

CAUTION

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

Figure 45. Ion sweep cone removed from the MS mount assembly



No.	Description	No.	Description
1.	Release lever for the API source interface	2.	API cone seal
3.	Ion sweep cone screw	4.	Ion sweep cone

7. Depending on the MS model, do the following:

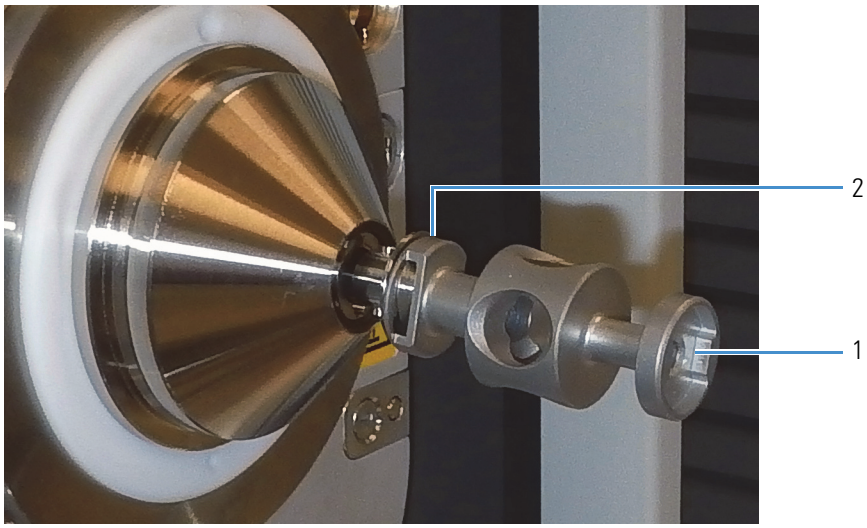
   a. For the TSQ Altis MS, align the flat end of the 1/4 turn ion transfer tube removal tool with the flat edges on the ion transfer tube's nose cone.

   b. Rotate the tube counterclockwise by a quarter turn to release the pins behind the nose cone that secure the tube to the spray cone.

   Figure 46. Turning the nose cone counterclockwise by a quarter turn (TSQ Altis MS)

c. Use the other end of the tool to pull the tube out of the API source interface.

Figure 47. Pulling the transfer tube out of the API source interface (TSQ Altis MS)



No.	Description
1.	Use this end of the tool to rotate the tube by a 1/4 turn, releasing it from the spray cone (not shown).
2.	Use this end of the tool to hook onto the released tube and pull it out of the spray cone (as shown in figure).

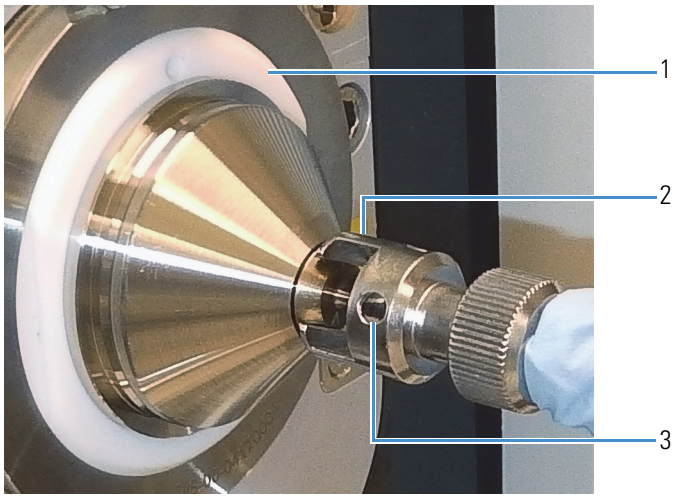
–or–

a. For the TSQ Quantis MS or the TSQ Fortis MS, align the hook end of the ion transfer tube removal tube with the flat edges of the ion transfer tube's nose cone.

b. Rotate the ion transfer tube counterclockwise until its threaded nose cone is free of the API interface.

Tip If necessary, insert a hex key through the side hole in the tool, and use it for leverage.

Figure 48. Ion transfer tube removal tool (TSQ Quantis MS and TSQ Fortis MS)

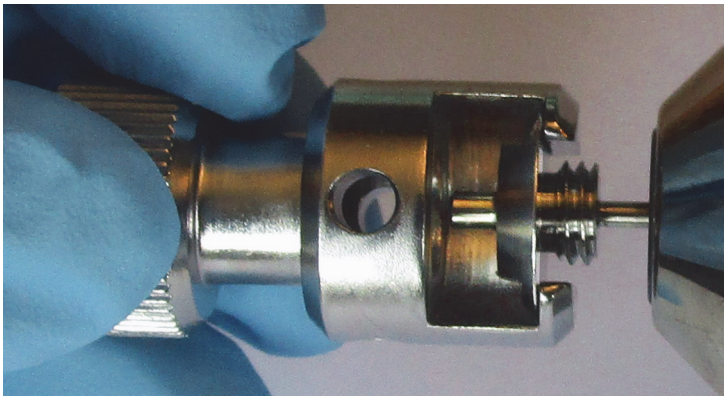


No.	Description
1.	API source interface
2.	Hook end of the tool aligned to the flat edges of the ion transfer tube's nose cone
3.	Side hole for leveraging tool

c. Hook the tool onto the back of the ion transfer tube's nose cone, and then pull the tube out of the spray cone.

Figure 49 shows how to pull the ion transfer tube out of a TSQ Quantis MS or a TSQ Fortis MS.

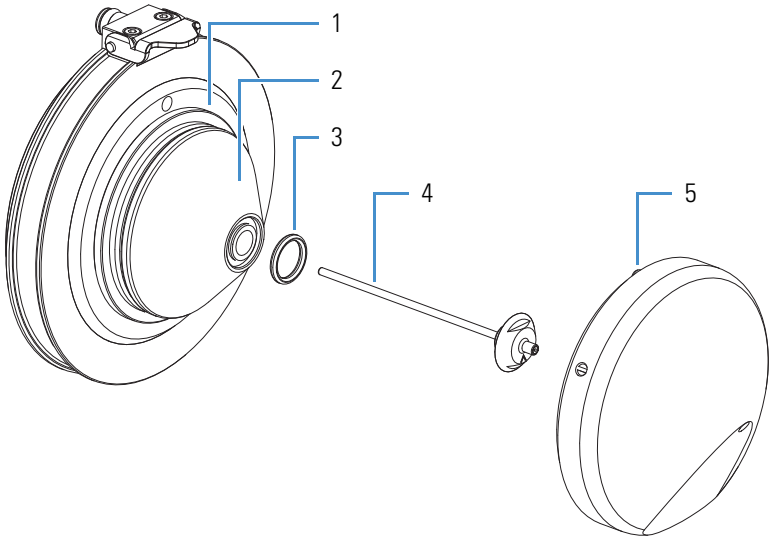
Figure 49. Pulling the tube out of the spray cone



Cleaning the Spray Cone and Seal

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

Figure 50. Spray cone, seal, ion transfer tube, and ion sweep cone



No.	Description	No.	Description
1.	API cone seal	2.	Spray cone
3.	Graphite Vespel™ seal	4.	Ion transfer tube
5.	Gas inlet on the ion sweep cone		

3. Clean the seal with a wipe with methanol or replace the seal, if necessary.
4. Using a magnification device, inspect the components for any residual lint or particulates.

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

5. Reinstall the seal in the spray cone.

Cleaning the Ion Transfer Tube

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

1. For extreme contamination, follow these steps. Otherwise, start with step 2.
   a. Overnight, sonicate the component in a 10% solution of Liquinox in water.
   b. Rinse the component with water, and then for 2 minutes force a strong stream of water through the orifice.
   c. For 30 minutes, sonicate the component in water.
2. For 30 minutes, sonicate the component in a 50:50 solution of methanol/water that contains 20% formic acid.
3. Rinse the component thoroughly with water.
4. For 15 minutes, sonicate the component in deionized water.
5. Rinse the component with methanol.
6. For 15 minutes, sonicate the component in methanol.
7. Dry the component thoroughly with nitrogen gas.

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

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

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

Reinstalling the Ion Transfer Tube

1. Make sure that the API source housing is cooled to room temperature.
2. Insert the tube at a 0 degree angle into the API source housing and gently push the vent ball out of the way.

   Note As you insert the tube, you feel a slight resistance from the vent ball. After you push the vent ball out of the way, the system vacuum draws the tube further into the API source housing.
3. Depending on the MS model, do one of the following:
   a. For the TSQ Altis MS, align the tube's pin with the slot in the API source interface.

b. Use the flat end of the 1/4 turn ion transfer tube removal tool to turn the tube clockwise by a quarter turn.

–or–

- For the TSQ Quantis MS or TSQ Fortis MS, align the ion transfer tube removal tool with the flat edges of the ion transfer tube's nose cone, and then rotate the tube clockwise until you completely tighten the nose cone to the spray cone.

Cleaning the Ion Sweep Cone

1. Soak lint-free tissues or chamois-tipped swabs in a 50:50 solution of methanol/water, and then clean both sides of the ion sweep cone.
2. For 10 minutes, sonicate the component in either a 50:50 solution of methanol/water or a 1% solution of Liquinox in water.
3. Rinse the component thoroughly with water.
4. Sonicate the component in water for 10 minutes.
5. Sonicate the component in methanol for 10 minutes.
6. Rinse the component with methanol.
7. Dry the component thoroughly with nitrogen gas.
8. Using a magnification device, inspect the component for any residual lint or particulates.
9. After you clean and reinstall these components, turn on the nonvacuum system voltages by placing the MS's electronics service switch in the Operating Mode (up) position.
10. To determine if you have successfully unblocked the ion transfer tube, check that the Source Pressure reading has increased to a normal value.

Table 18. Vacuum specification with ion transfer tube installed and open

Region	TSQ Altis	TSQ Quantis	TSQ Fortis
Source Pressure	less than 3.8 Torr	less than 2.0 Torr	less than 2.0 Torr

11. If the ion transfer tube is still blocked, replace it.

Maintaining the API Source Interface Lenses

Chemicals can accumulate on the surfaces of the API source interface lenses and the MP00 multipole. These components require cleaning less often than the ion sweep cone and the ion transfer tube. How frequently you clean these components depends on the type and quantity of the compounds that you analyze. To clean these components, you must vent the system and remove the API source interface cage from the MS.

MS Model	Lenses and multipole
TSQ Altis	RF lens (EDIF), Exit lens, MP00 multipole, and L0 Lens
TSQ Quantis	RF lens (SRIG), Exit lens, MP00 multipole. and L0 lens
TSQ Fortis	Skimmer and Tube lens (MSIG), MP00 multipole, and L0 lens

To clean the lenses and the MP00 multipole, follow these procedures in order:

- Removing the API Source Interface
- Removing the MP00 Assembly, the RF Lens, and the Exit Lens (TSQ Altis and TSQ Quantis)
- Removing the MP00 Assembly, the Skimmer, and the Tube Lens (TSQ Fortis)
- Cleaning the Lenses
- Cleaning the MP00 Multipole
- Reinstalling the API Source Interface Cage Components
- Reinstalling the API Source Interface

Removing the API Source Interface

You must remove the API source interface so that you can remove and clean the lenses and the multipole.

CAUTION To avoid an electric shock, be sure to follow the instructions in "Shutting the MS System Down Completely," before you start this procedure.

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

   Venting the MS can take several minutes.

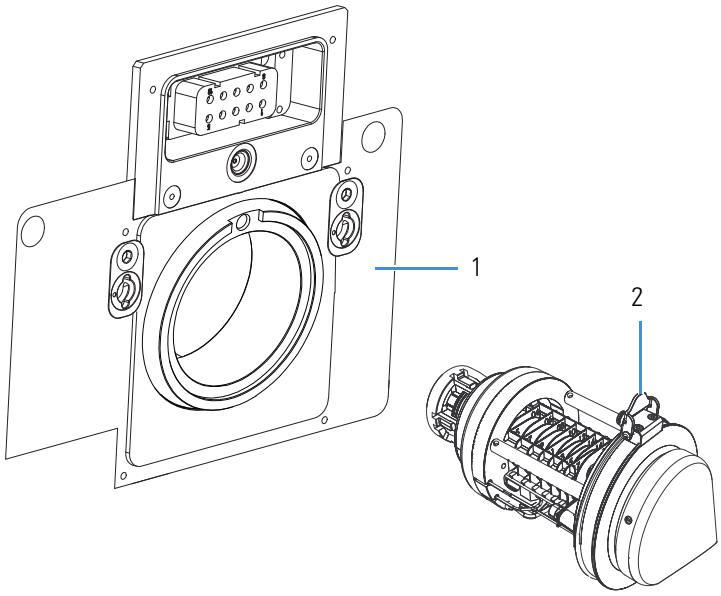
CAUTION Hot surface. The external surface of the spray insert, API source housing, and entry to the ion transfer tube can become hot enough to burn your skin. Before you touch or remove heated parts, allow the part to cool to room temperature (approximately 20 minutes) before you touch it.

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

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

3. Remove the API source housing, refer to the *OptaMax NG Ion Source User Guide*, Chapter 2 section *Removing and Installation the API Source.*
4. Lift up the release latch and firmly push it to unseal the API source interface from the vacuum manifold.
5. Grasp the API source interface with your fingers, and then carefully pull it out of the vacuum manifold (Figure 51).

Figure 51. API source interface removed from the vacuum manifold



No.	Description
1.	Vacuum manifold
2.	Release latch on the API source interface

Removing the MP00 Assembly, the RF Lens, and the Exit Lens (TSQ Altis and TSQ Quantis)

Required tools: 2 mm Allen wrench and L0 lens removal tool

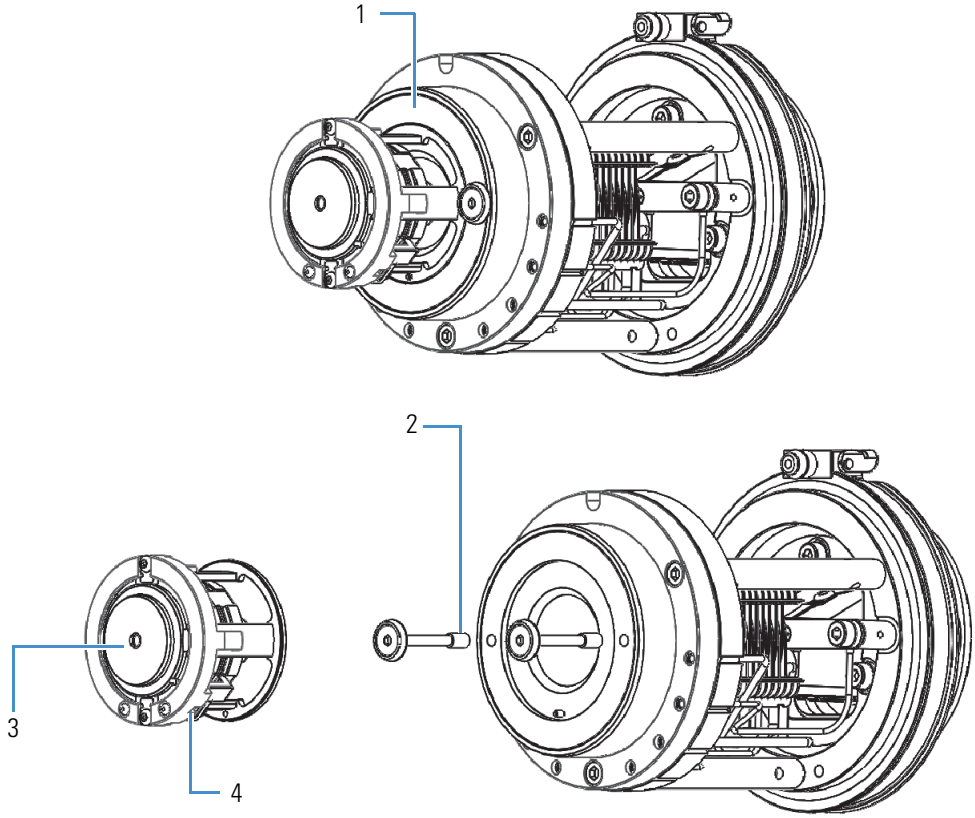
1. Remove the API source interface.
2. Wearing clean, lint-free and powder-free gloves, use a 2-mm Allen wrench to loosen and extend (if captive) or remove the two Allen screws that secure the exit lens, the MP00 multipole, and the L0 lens to the cage.

   Note In older TSQ Series II mass spectrometers, two captive screws secure the MP00 assembly to the cage.

3. Pull the MP00 assembly off of the API source interface cage. Place the assembly on a clean, lint-surface.

   See Figure 52 for the TSQ Altis.

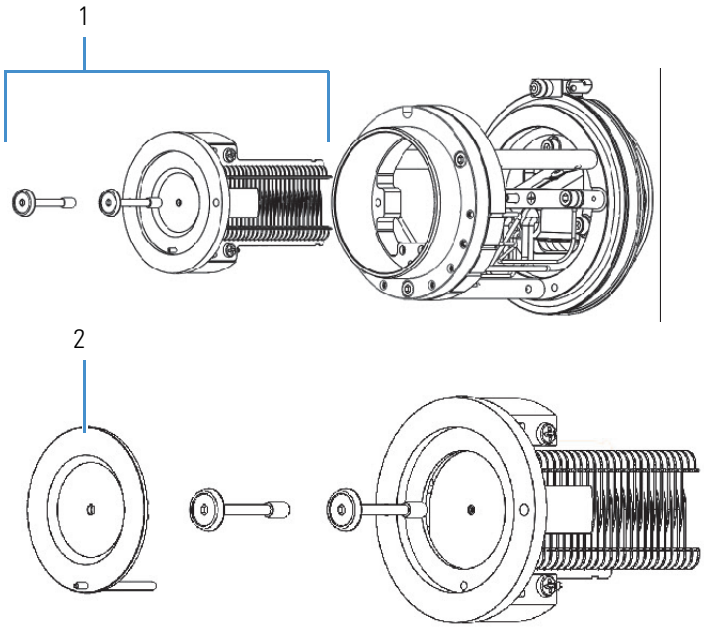
Figure 52. Removing the multipole MP00 and lens L0 assembly (TSQ Altis MS)



No.	Description	No.	Description
1.	API source interface cage	2.	Allen screws loosened and extended
3.	L0 Lens	4.	MP00 assembly

See Figure 53 for the TSQ Quantis.

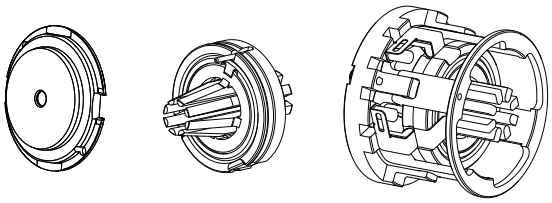
Figure 53. Removing the RF lens and the exit lens (TSQ Quantis MS)



No.	Description	No.	Description
1.	Rf lens and exit lens assembly	2.	Exit lens

4. If the Allen screws are captive, grasp them and carefully pull the RF lens with the exit lens straight out of the API source interface cage. Otherwise, push the RF lens out of the cage.
5. Separate the exit lens from the RF lens. Place both on a clean surface.
6. Using the L0 lens removal tool (or plastic tweezers), rotate the L0 lens counterclockwise to free it from the assembly, and then push the MP00 multipole out of the mount cage (Figure 54). Place the components on a clean surface.

Figure 54. Lo lens, MP00 multipole, and mount cage with multipole (from left to right)



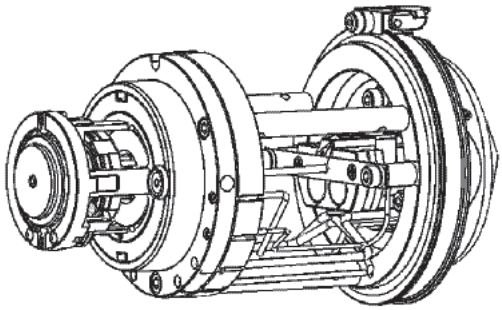
Removing the MP00 Assembly, the Skimmer, and the Tube Lens (TSQ Fortis)

Required tools:

- 2 mm Allen wrench
- Lens L0 removal tool
- Small flat-head screwdriver

1. Wearing clean, lint- and powder-free gloves, remove the API source interface from the MS.

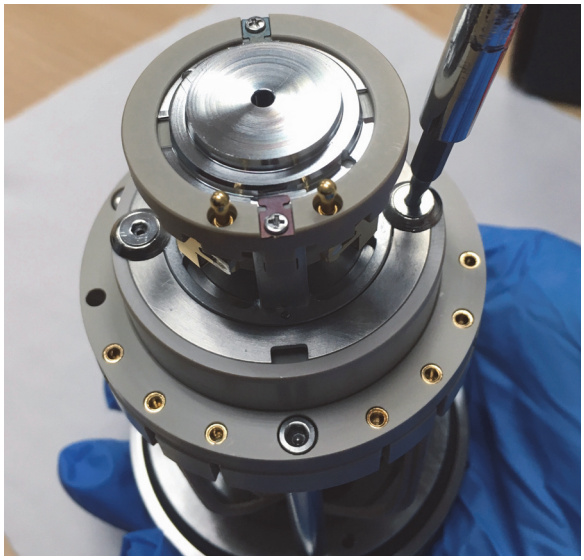
Figure 55. API source interface for the TSQ Fortis MS



2. To remove the two Allen screws that secure the MP00 assembly to the cage, use a 2 mm Allen wrench.

Note In older TSQ Series II mass spectrometers, two captive screws secure the MP00 assembly to the cage.

Figure 56. Removing the Allen screws that secure the MP00 assembly to the cage



3. Pull the MP00 assembly off of the API source interface cage. Place it on a clean, lint-free surface.

Figure 57. MP00 assembly removed from the cage

4. To remove the skimmer from the API source interface cage, use a small flat-head screwdriver (Figure 58).

Figure 58. Removing the skimmer (TSQ Fortis MS)

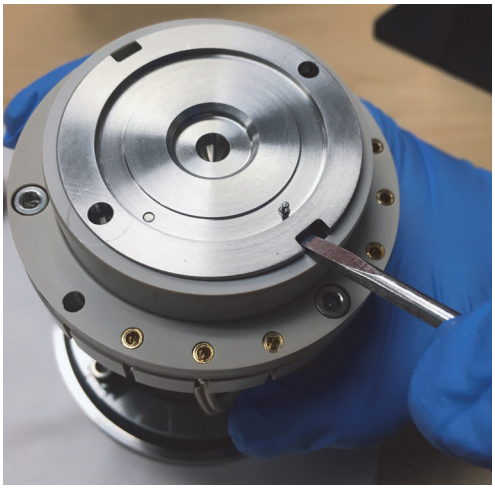
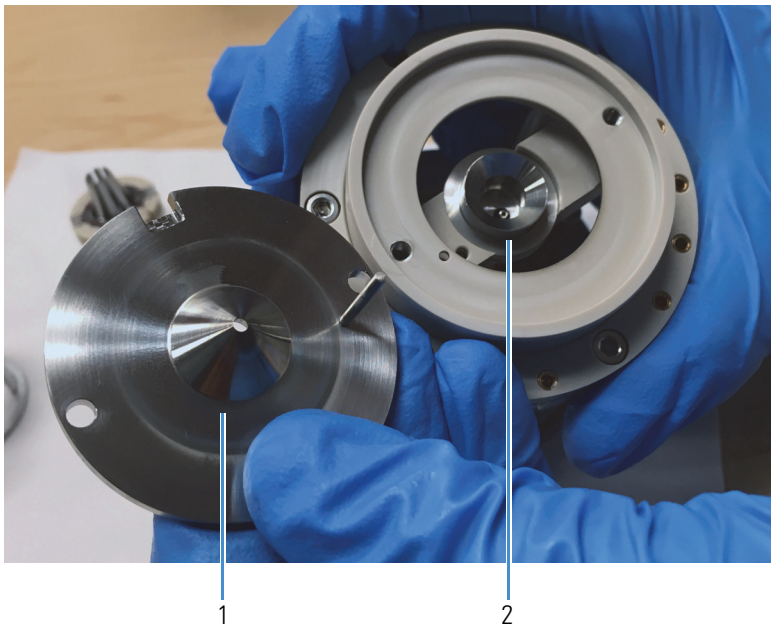


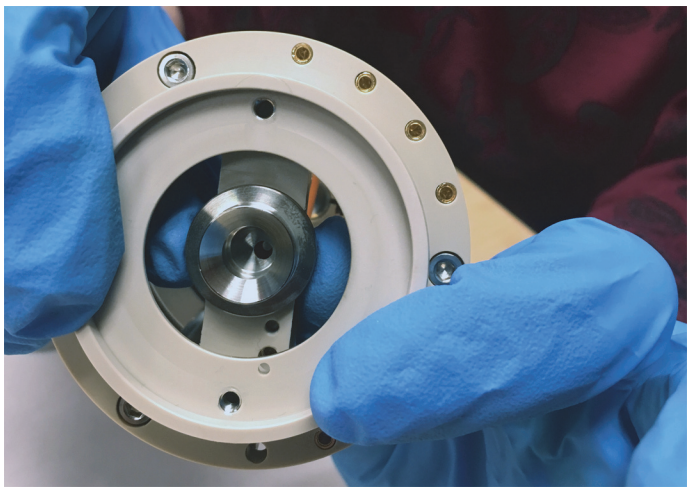
Figure 59. Skimmer removed from the cage



No.	Description	No.	Description
1.	Skimmer	2.	Tube lens

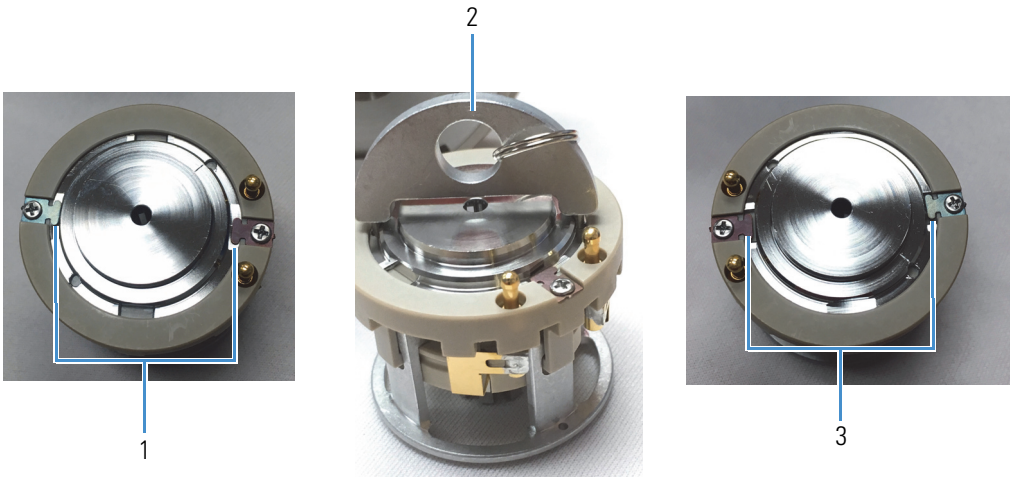
5. To remove the tube lens, push it out of the cage (Figure 60).

Figure 60. Pushing the tube lens out of the cage



6. To remove the L0 lens from the MP00 assembly, use the L0 lens removal tool or a plastic tweezers. Rotate the lens by a quarter turn to release it from the tabs.

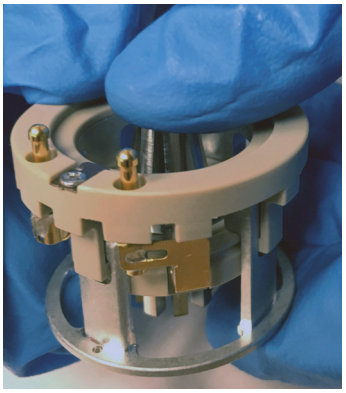
Figure 61. Using the L0 lens removal tool to rotate the L0 lens



No.	Description
1.	L0 lens secured to the MP00 assembly
2.	Rotating the L0 lens by a quarter turn
3.	L0 lens released from the MP00 assembly

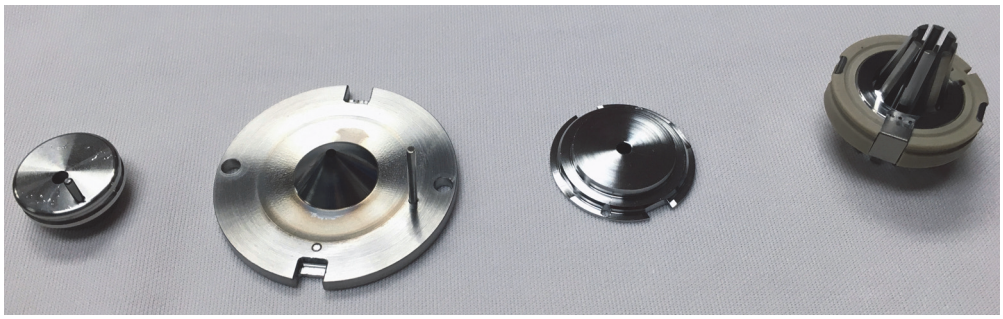
7. Push the MP00 multipole out of the mounting cage.

Figure 62. Pushing the MP00 multipole out of the mounting cage



8. Place the components on a clean surface.

Figure 63. Tube lens, skimmer, L0 lens, and MP00 multipole (from left to right)



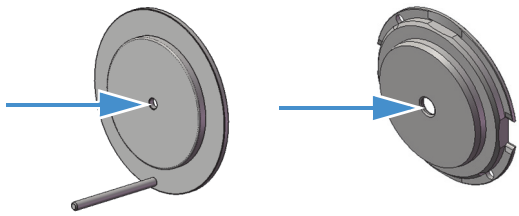
Cleaning the Lenses

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

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

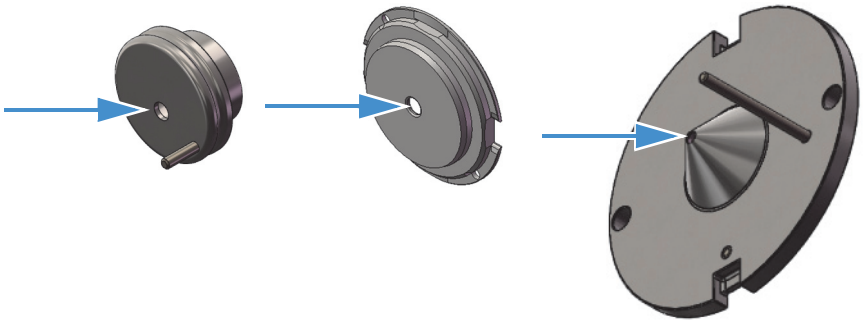
1. Using a magnification device, inspect the components for any lint, particulates, and sample buildup or coatings.
2. For 10 minutes, sonicate the components in either a 50:50 solution of methanol/water or a 1% solution of Liquinox in water.
3. If a sonicator is not available, do the following:
   - To clean the RF lens, use chamois-tipped swabs with a 1% solution of Liquinox in water. To clean the areas that you cannot reach with the swab, use the 6000 grit MICRO-MESH polishing swabs.
   - To clean the exit lens, use a soft toothbrush with a 1% solution of Liquinox in water.
4. Do the following:
   - TSQ Altis and TSQ Quantis: For the exit and L0 lenses, use the 6000 grit MICRO-MESH polishing swabs to clean the bore.

Figure 64. Exit lens on the left and L0 lens on the right



- TSQ Fortis: For the tube lens, L0 lens, and skimmer, use the 6000 grit MICRO-MESH polishing swabs to clean the bore.

Figure 65. Tube lens, L0 lens, and skimmer (from left to right)



5. Rinse the components thoroughly with water.
6. Sonicate the components in water for 10 minutes.
7. Sonicate the components in methanol for 10 minutes.
8. Rinse the components with methanol.
9. Dry the components thoroughly with nitrogen gas.
10. Using a magnifying device, inspect the components for any residual lint or particulates.

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

Cleaning the MP00 Multipole

1. Use a soft toothbrush to scrub the MP00 multipole with a 1% solution of Liquinox in water. Clean both the entrance and exit sides of the multipole.
2. Use a swab to clean between the rods.
3. Rinse the multipole thoroughly with water.
4. Rinse the multipole with methanol.
5. Thoroughly dry the multipole with a stream of nitrogen gas.
6. Verify that the multipole is clean by examining it with a loupe.

Reinstalling the API Source Interface Cage Components

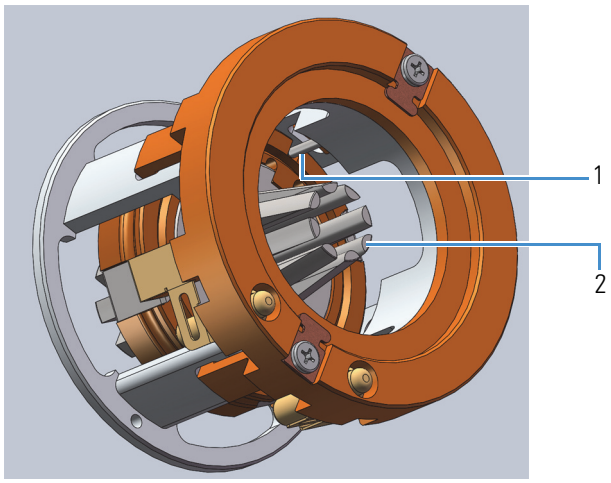
Follow these topics as needed:

- Reassembling the MP00 Assembly
- Reinstalling the Lenses and the MP00 Assembly in a TSQ Altis or TSQ Quantis MS
- Reinstalling the Lenses and the MP00 Assembly in a TSQ Fortis MS

Reassembling the MP00 Assembly

To reassemble the MP00 assembly, align the MP00 multipole with the alignment pin in the mounting cage, and then insert it into the cage.

Figure 66. Inserting the MP00 multipole into the mounting cage



No.	Description	No.	Description
1.	Alignment pin	2.	MP00 multipole

Reinstalling the Lenses and the MP00 Assembly in a TSQ Altis or TSQ Quantis MS

This procedure describes how to reinstall the RF lens, the exit lens, the MP00 assembly, and lens L0 in a TSQ Altis MS or TSQ Quantis MS.

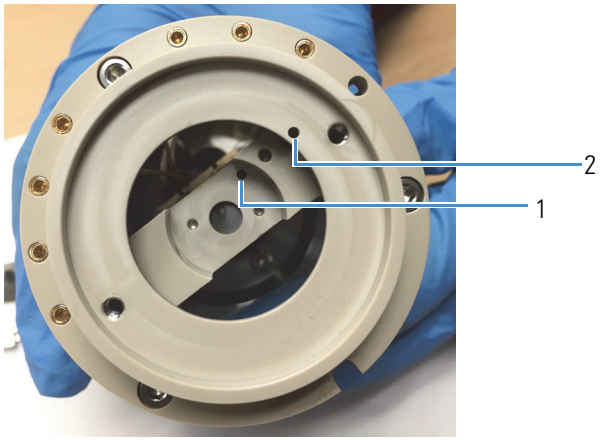
1. Reassemble the MP00 assembly.
2. Attach the exit lens to the RF lens, and then reinsert the RF lens into the API source interface cage (Figure 53).
3. Attach the MP00 assembly to the API source interface cage, and then attach lens L0.

Reinstalling the Lenses and the MP00 Assembly in a TSQ Fortis MS

Follow this procedure to reinstall the lenses and MP00 multipole in a TSQ Fortis MS.

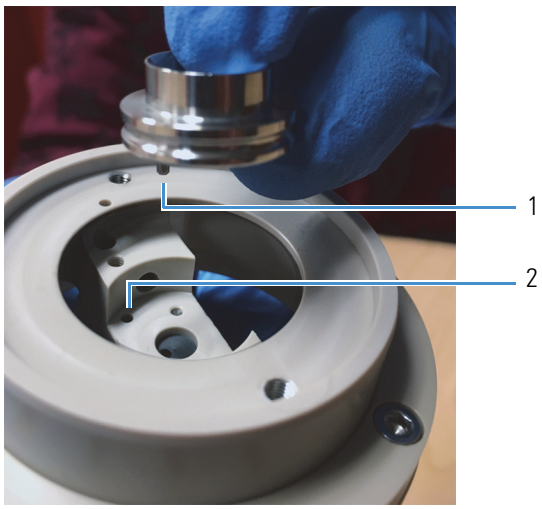
1. Reassemble the MP00 assembly.
2. Align the two slots in the outer ring of the L0 lens with the tabs on the mounting cage. Then, use the L0 lens removal tool to turn the L0 lens by a quarter turn.
3. Align the tube lens pin to the port in the inner circle of the API source interface cage, and then insert the lens into the cage and snap it into place.

Figure 67. API source interface cage with the lenses removed



No.	Description	No.	Description
1.	Mounting port for the tube lens	2.	Mounting port for the skimmer

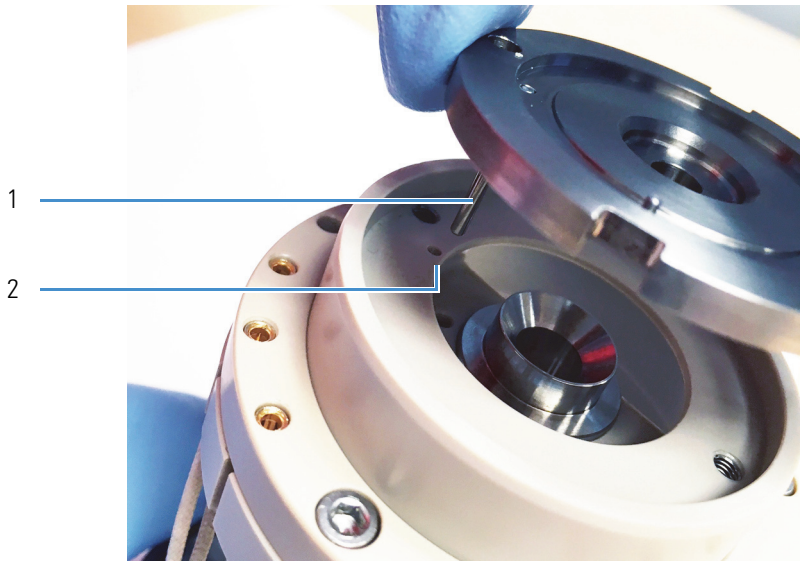
Figure 68. Installing the tube lens



No.	Description	No.	Description
1.	Tube lens pin	2.	Mounting port for the tube lens

4. Align the skimmer pin to the mounting port in the cage, and then insert the skimmer into the cage.

Figure 69. Inserting the skimmer into the cage



No.	Description	No.	Description
1.	Skimmer pin	2.	Mounting port for the skimmer

5. Reconnect the MP00 assembly to the cage. Use a 2 mm Allen wrench to tighten the two screws that secure the assembly to the cage.

Reinstalling the API Source Interface

1. Orient the API source interface with the release latch at the top (Figure 51).
2. Carefully insert the API source interface into the vacuum manifold.
3. Reinstall the API source housing.
4. Start up the system as described in Chapter 10, “Restarting the MS System After a Shutdown.”

Maintaining the Forepumps and the Air Filter

Maintaining the Forepumps

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

Check the forepump oil often. 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.

New oil has a translucent, light amber color. If the oil is cloudy or discolored, purge the oil to decontaminate dissolved solvents. If the pump oil is still discolored, change it.

Plan to change the pump oil every 10 000 hours (or about every 12–13 months) of operation.

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

Maintaining the Air Filter

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

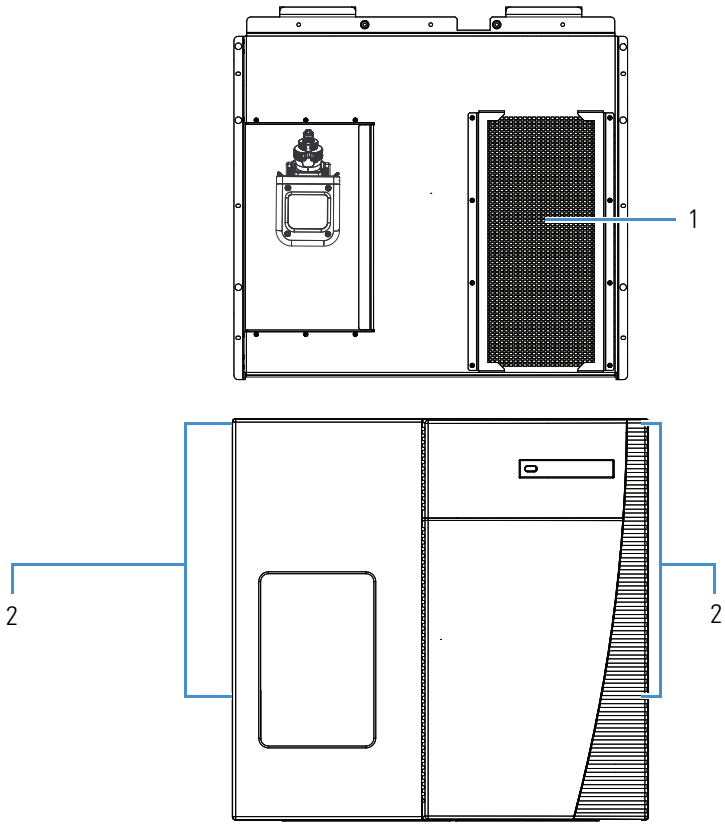
Note You do not need to remove the API source to remove the front cover of the MS.

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

d. Remove the filter from the filter bracket (Figure 70).

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

Figure 70. Air filter location in the MS with the front cover removed



No.	Description	No.	Description
1.	Air filter	2.	Spring catches

A

Using Basic Tune Functions

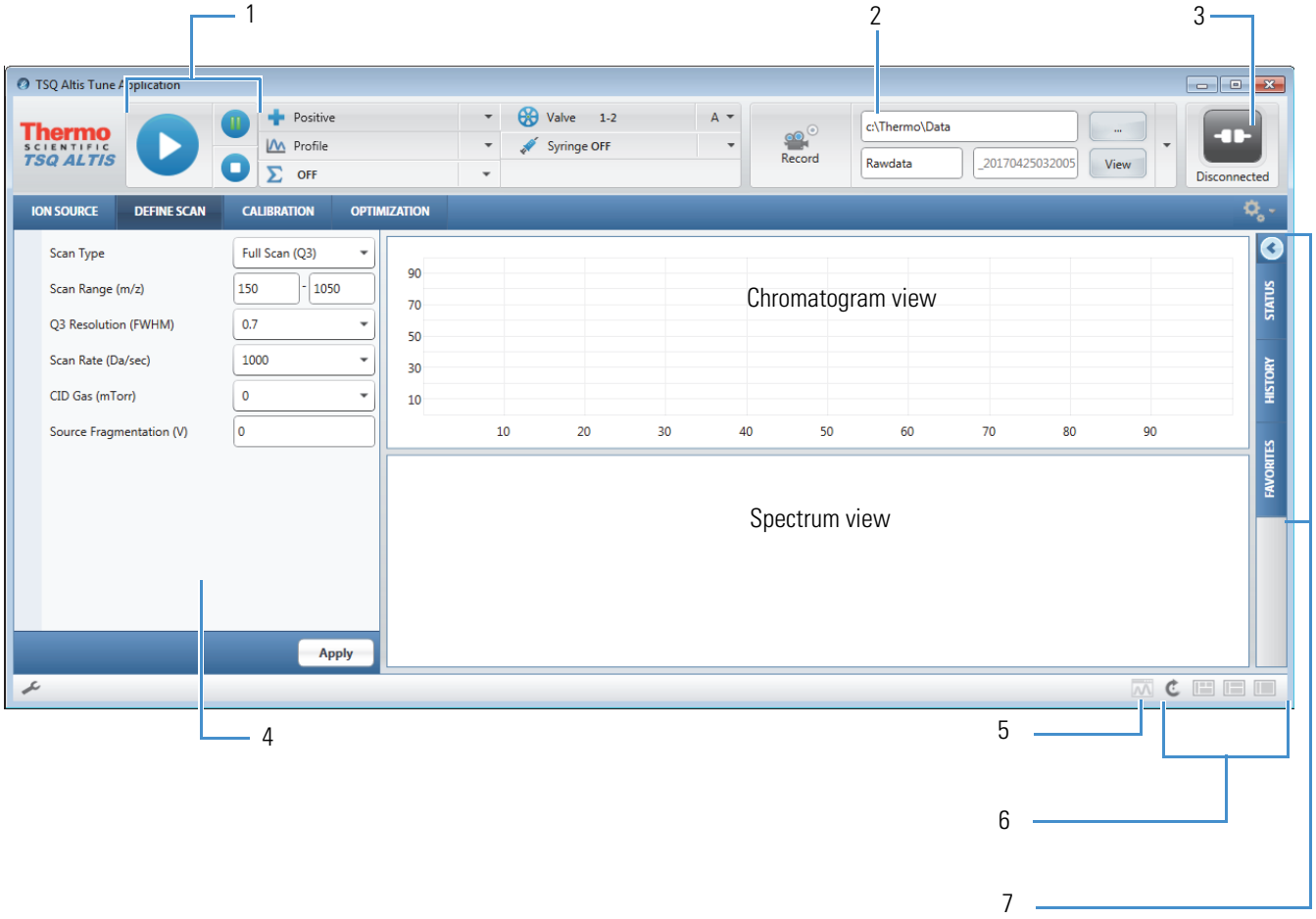
This appendix describes basic Tune functions that are referenced throughout this guide. For additional information about the Tune window, refer to the Tune Help.

Opening the Tune Window

- (Windows 7) From the Microsoft Windows taskbar, choose **Start > All Programs > Thermo Instruments > *model x.x,*** and then open the Tune window (Figure 71).
- (Windows 10) From the Windows taskbar, choose **Start > All Apps > Thermo Instruments > *model x.x***, and then open the Tune window (Figure 71).

  For information about the buttons and icons in the Tune application and what they control, refer to the Tune Help.

Figure 71. Tune window showing the Define Scan pane



No.	Description	No.	Description
1.	Three power mode icons (on/standby/off)	2.	Manual data acquisition
3.	Instrument readback status	4.	Define Scan pane
5.	Plot Chromatogram tool	6.	Controls for the graphs
7.	Panes: Status, History, and Favorites		

Setting the Instrument System Controls

Table 19 shows the options for each of the system control buttons at the top of the Tune window.

Table 19. Procedures for using the instrument control buttons (Sheet 1 of 2)

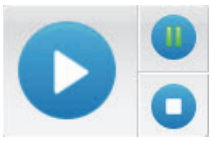
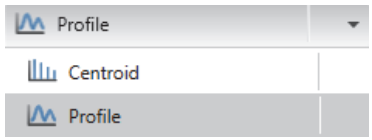
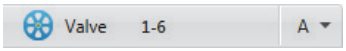
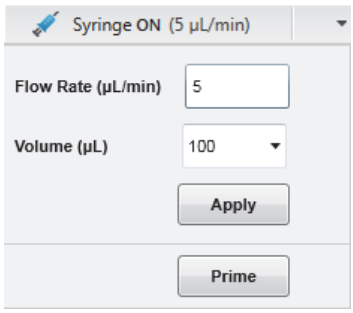
Button	Function	Procedure
	Power mode	❖ **To set the instrument power mode** Click the icon for the applicable power mode. The center of the selected icon changes from white to green. See Setting the Instrument Power Mode.
	Ion polarity mode	❖ **To set the ion polarity mode** Click **Positive (Negative)** and select the ion polarity mode.
	Data type	❖ **To set the data type** Click **Centroid (Profile)** and select the data type.
	Spectrum scan averaging	❖ **To turn the scan averaging on or off** Click the button to switch between on and off. ❖ **To set the scan averaging value** Click the down arrow to enter the value, and then click **Apply**.

Table 19. Procedures for using the instrument control buttons (Sheet 2 of 2)

Button	Function	Procedure
	Divert/inject valve	❖ **To set the divert/inject valve module and position** Click the down arrow to select the valve, and then click **Valve** to set the position.
	Syringe pump	❖ **To turn the syringe pump on or off** Click **Syringe On (Off)** to switch between on and off. ❖ **To set the syringe pump parameters** 1. Click the down arrow, and then type the values. The Tune application automatically saves the values. 2. (Optional) Press and hold **Prime** to prime the syringe at 100 µL/min. 3. Click the down arrow again or click elsewhere to close the box.

Setting the Instrument Power Mode

Use the three power mode icons in the Tune window (Figure 71) to set the MS's power mode (on, standby, or off).

When you remove the API source housing or the spray insert, the MS automatically switches to off mode.

In standby mode, the System LED on the front panel turns yellow and the MS turns off the electron multiplier, conversion dynodes, 8 kV power to the API source, main RF voltage, and ion optic RF voltages. The auxiliary, sheath, and sweep gas flows remain on and return to their standby default settings (2 arbitrary). See Chapter 8, "Using the MS Power Options."

Checking the Instrument Readback Status

The system readback icon is located in the top right of the Tune window. Table 20 lists the various readback states.

Table 20. Instrument readback icons and their meanings

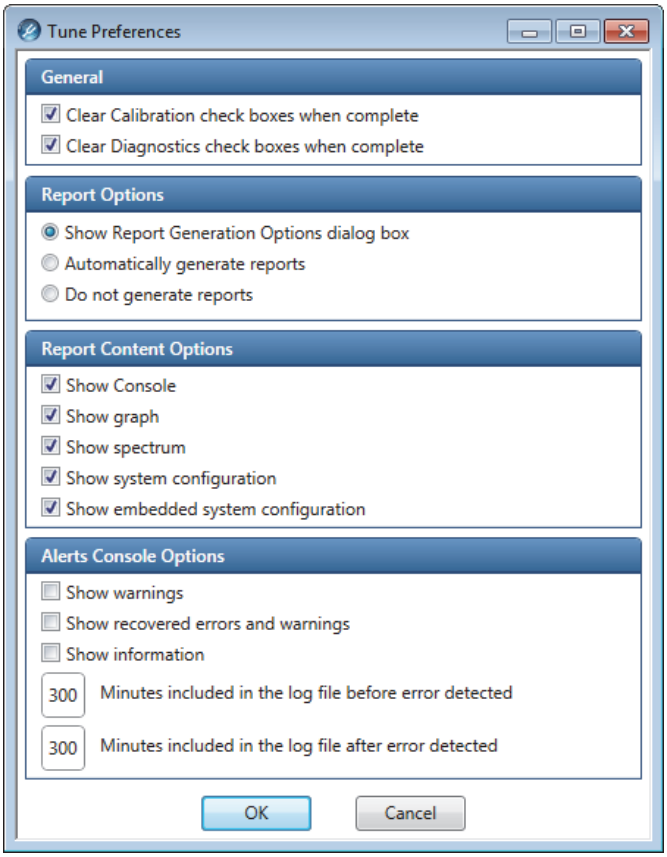
Icon	Background color	Meaning
	Green	The system parameters are within tolerance.
	Green	The system is initializing.
	Amber	One or more settings are changing.
	Red	An error has occurred.
	Gray	The API source is off.
	Gray	There is no communication between the MS and the data system.

Setting the Tune Preferences

You can set a few preferences for how the Tune application works.

1. Click the **Options** icon,  , and then choose **Preferences** to open the Tune Preferences dialog box (Figure 72).

Figure 72. Tune Preferences dialog box



2. Select all check boxes that apply.
3. Under Report Options, select one of the options, and then click **OK**.

Using the Mass List Table in the Define Scan Pane

The mass list table appears when you select the SIM Scan (Q1), SIM Scan (Q3), or SRM scan type in the Define Scan pane. To set different scan parameters for the precursor ions, add the parameters to the table.

Adding a Row to the Table

Do one of the following:

- Click the **Add Row** icon, .
- Right-click the table, and then choose **Add Row**.

Deleting a Row from the Table

1. Select the row number to highlight the entire row.
2. Do one of the following:
   - Click the **Delete Selected Rows** icon, .
   - Right-click the selected row, and then choose **Delete Selected Rows**.
   - Press the DELETE key on your keyboard.

Deleting Multiple Rows from the Table

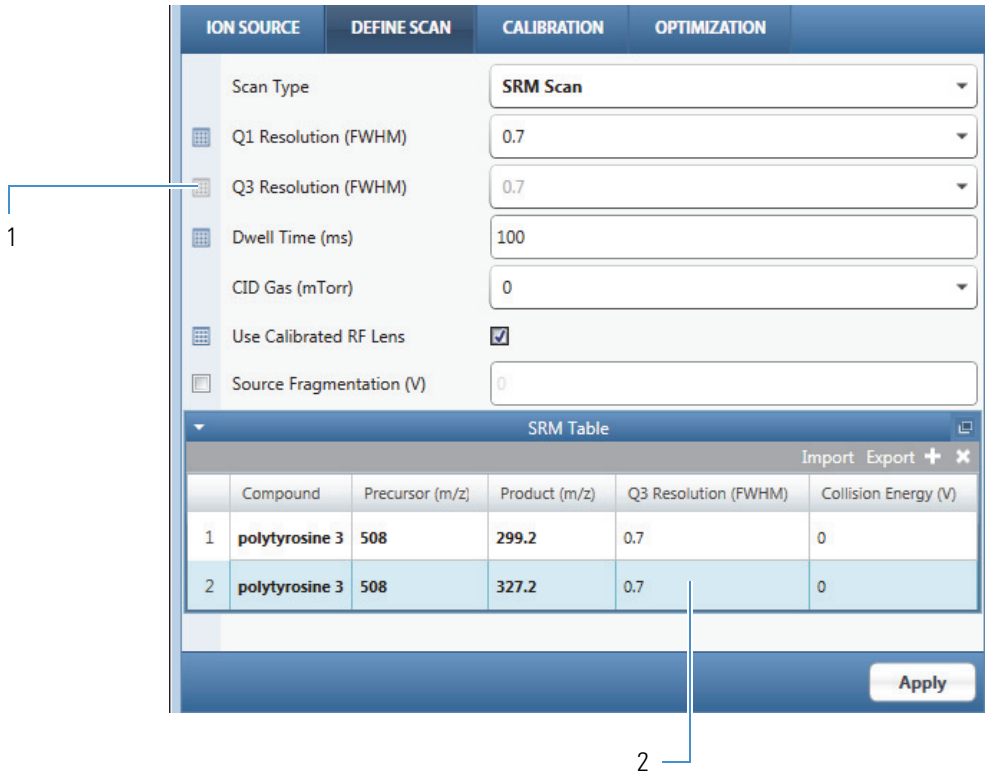
1. Select the first row's number to highlight the entire row.
2. Do one of the following:
   - For an adjacent row or group of sequential rows, use the SHIFT key as you make your selections.
   - For an adjacent row or non-sequential rows, use the CTRL key as you make your selections.
3. Do one of the following:
   - Click the **Delete Selected Rows** icon, .
   - Right-click the selected row, and then choose **Delete Selected Rows**.
   - Press the DELETE key on your keyboard.

Adding or Removing Scan Parameters from the Table

Click the **Table** icon, , once to add the adjacent scan parameter to the table. Click it again to remove the parameter from the table.

Figure 73 shows an example with Q3 Resolution added to the SRM Table.

Figure 73. Q3 Resolution selected and added to the SRM Table



No.	Description
1.	Q3 Resolution is selected (appears gray)
2.	Q3 Resolution appears in the table.

Importing a Mass List from a File

1. Click **Import** to open the Open dialog box.
2. Browse to a CSV (Microsoft Excel™), a TXT, or an XML file, and then click **Open**.

   The list of *m/z* values appears in the table.

Exporting a Mass List to a File

1. Complete the list of *m/z* values.
2. Click **Export** to open the Save As dialog box.
3. Browse to a location, enter a file name, and then select a file type (**CSV**, **TXT Only**, or **XML Data**).
4. Click **Save**.

Using the History Pane

To add a change record to the History pane, click **Apply** in the Ion Source or the Define Scan pane.

The Tune application adds a change record to the History pane. The change record records all changes to the instrument state that originated from the Tune application.

Change records in the History pane work as follows:

- The Tune application creates a change record when you change parameters in the Ion Source or Define Scan pane and then click Apply.
- The History pane displays the change records as sub-items under the date that they were created. The maximum number of change records is 100.
- You can display a change record's parameters: either double-click the record or right-click it and choose Load. Parameters that are colored red differ from their default values.
- You can submit a change record's parameters to the MS: either double-click the record or right-click it and choose Apply.
- A change record is inactive if the API source type of the change record differs from the current API source type.

Using the Favorites Pane to Save System Settings

You can manually save the current settings for the API source and scan parameters in the Favorites pane.

- To create a favorite state
- To load settings only or apply a favorite state
- To rename a favorite state
- To delete a favorite state

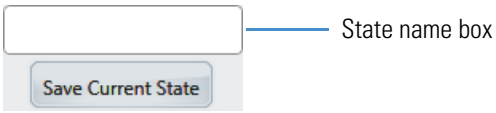
❖ To create a favorite state

1. In the Tune window, modify the parameters in the Ion Source or Define Scan pane.
2. Click **Apply** or **Export**.
3. Click the **Favorites** tab to display the Favorites pane (Figure 74).

Figure 74. Favorites pane

4. Click **Save Current State**, and then type a unique name in the box (Figure 75).

Figure 75. State name box



5. Click **Save Current State** again to save the state.

   The new favorite state appears first in the Favorites list. You can enter up to 100 states.

❖ To load settings only or apply a favorite state

Under User Settings, right-click the state name, and then choose one of the following:

- **Load** to only display the key parameters in the applicable parameter boxes.
- **Apply** to submit the key parameters to the MS.

  You can click Apply without first loading the parameters.

❖ To rename a favorite state

1. Under User Settings, right-click the state name, and then choose **Rename**.
2. Type a different name and press ENTER.

❖ To delete a favorite state

Under User Settings, right-click the state name, and then choose **Delete**.

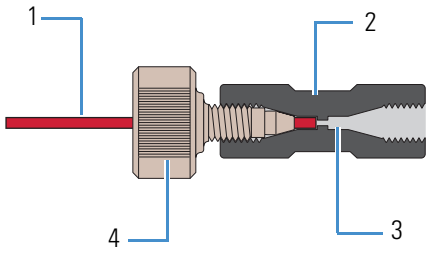
Setting Up the Syringe with the Syringe Pump

Connecting the Syringe Union to the Syringe

Connect the syringe of the syringe pump to a syringe union.

1. Cut the ends of red PEEK tubing so that they are square (Figure 76). For best results, use a polymeric tubing cutter. Poorly cut tubing can cause flow restrictions.
2. Make sure that the PEEK tubing is not crimped, kinked, or otherwise damaged.
3. Connect the PEEK tubing so that it contacts the bottom of the LC union's 10-32, coned-bottom receiving port. Tubing that is not properly seated can add dead volume to a chromatographic system.
4. Tighten the PEEK fittings by only using your fingers. If you overtighten the PEEK fittings, they can cause leaks.

Figure 76. PEEK tubing connection to syringe union



No.	Description	No.	Description
1.	Red PEEK tubing	2.	Syringe Union (cross-sectional view)
3.	10-32 coned-bottom receiving port	4.	PEEK fingertight fitting

Setting Up the Syringe Pump

Use the syringe pump to infuse samples into the API source, to infuse sample into the solvent stream that is produced by an LC pump, or to load sample into the divert/inject valve.

CAUTION Sharp object. The syringe needle can puncture your skin. Handle it with care.

IMPORTANT To minimize the possibility of cross-contamination, do the following:

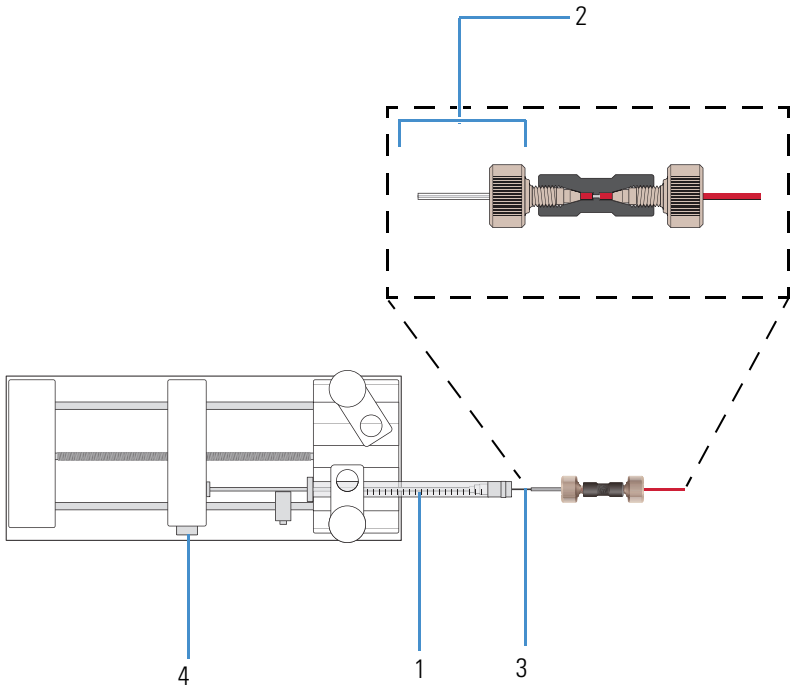
- Use a dedicated syringe and length of PEEK tubing for the calibration solution and another syringe and length of PEEK tubing for sample solutions.
- Wipe off the needle tip with a clean, lint-free tissue before reinserting the syringe into the syringe union adapter assembly.

1. Load a clean, 500 µL syringe with the sample solution (1 in Figure 77).
2. Use a fingertight fitting to connect 4 cm (1.5 in.) of Teflon tubing to the (black) syringe union adapter (2 in Figure 77).
3. Hold the plunger of the syringe in place and carefully insert the tip of the syringe needle (3) into the free end of the Teflon tubing. Then, place the syringe on the syringe pump.

Note If necessary, use the syringe needle tip to slightly enlarge the opening in the end of the Teflon tubing.

4. Squeeze the syringe pump's release button and slowly move the pusher block until it contacts the flange on the end of the syringe plunger (4).

Figure 77. Syringe pump with syringe



No.	Description
1.	Syringe with sample solution
2.	Teflon tubing connection to the union (cross-sectional, exploded view)
3.	Syringe connection to the Teflon tube
4.	Syringe pump release button on the pusher bar

C

Divert/Inject Valve

You can plumb the divert/inject valve as a loop injector for flow injection analysis or as a divert valve.

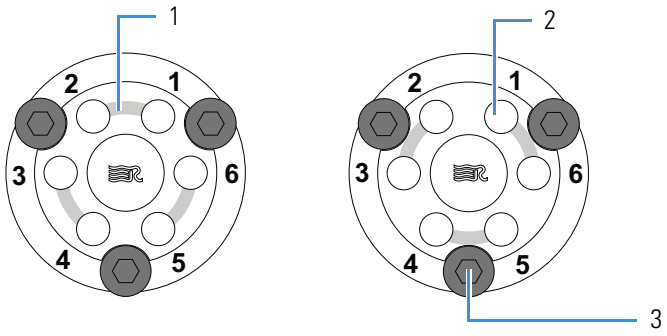
About the Divert/Inject Valve

The external Rheodyne™ MX Series II™ divert/inject valve is a 6-port motorized valve that switches between two positions. The ports use the standard 10-32 fitting for high pressure and 1/16 in. OD tubing. Figure 78 shows the internal flow paths for both positions.

- In the first position, port 1 connects internally to port 2, port 3 connects to port 4, and port 5 connects to port 6.
- In the second position, the valve rotates clockwise one position so that port 1 connects internally to port 6, port 2 connects to port 3, and port 4 connects to port 5.

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

Figure 78. Divert/inject valve positions



Position 1–2 Position 1–6

No.	Description
1.	Position 1-2: Internal connection path in light gray
2.	Position 1-6: The rotor switches between position 1-2 to 1-6.
3.	Valve screw

Divert/Inject Valve Configurations

You can configure (plumb) the divert/inject valve as a loop injector (for flow injection analysis) or as a divert valve. The divert valve can switch the solvent front, gradient endpoint, or any portion of the LC run to waste. Figure 79 shows the divert valve configuration.

Loop Injection

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

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

Inject (position 1–6)—The sample loop is open to the solvent stream. The solvent flow from the LC pump flushes sample out of the sample loop, and then exits through port 6 into the API source.

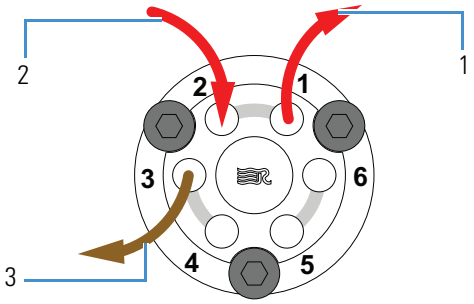
Divert Valve

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

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

Waste (position 1–6)—Solvent flow from the LC pump enters the valve through port 5 and exits through port 4 to waste.

Figure 79. Divert/Inject valve plumbed as a divert valve



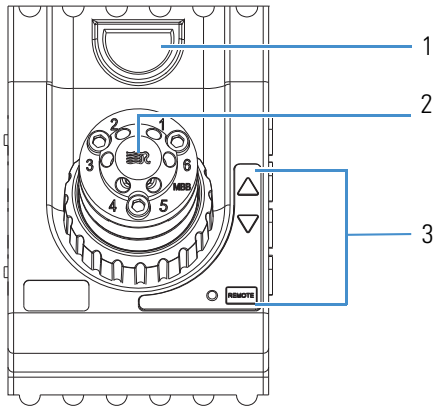
No.	Description
1.	Port 1 to API Source
2.	Port 2 from LC Pumps
3.	Port 3 to Waste

Divert/Inject Valve Controls

You can control the divert/inject valve by using the MS's data system or the control buttons on the valve.

- Use the MS's data system to specify the parameters in the Divert Valve Properties pane of the Method Editor. For instructions, refer to the Xcalibur Method Editor Help.
- Use the valve's control buttons (Figure 80) to divert the LC flow between the MS and waste when the valve is in the divert valve configuration, or switch between load and inject modes when the valve is in the loop injector configuration. For instructions, refer to the manufacturer's manual.

Figure 80. Divert/inject valve (front view)



No.	Description
1.	Valve position indicator
2.	Six-port, two-position valve
3.	Valve control buttons

D

Setting Up Sample Introduction Techniques

You can introduce samples into the MS using the external syringe pump, divert/inject valve, and LC pumps to infuse or inject samples.

- Setting Up H-ESI or Low Flow H-ESI Direct Infusion
- Setting Up High-Flow Infusion Without an Autosampler
- Setting Up Loop Injections for Flow-Injection Analysis
- Setting Up Injections Using the Autosampler

Setting Up H-ESI or Low Flow H-ESI Direct Infusion

The sample is infused from the syringe pump into the API source. You use this technique to calibrate the MS and infuse samples. Before you do this procedure, complete Appendix B, "Setting Up the Syringe with the Syringe Pump."

See the following:

- Setting Up H-ESI Direct Infusion
- Setting Up Low Flow H-ESI Direct Infusion

Setting Up H-ESI Direct Infusion

If you are going to do a calibration, follow these precautions.

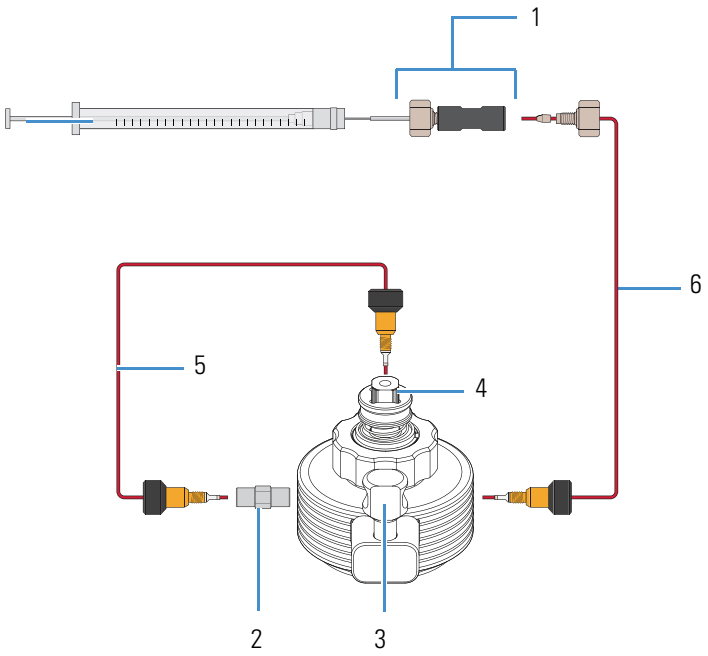
CAUTION Do not wear nitrile gloves when you are working with EMRS. Nitrile gloves are made with diphenylguanidine, which is soluble in EMRS. If diphenylguanidine contaminates the EMRS, a peak at *m/z* 212 will be in the spectrum.

IMPORTANT To prevent the EMRS from degradation, observe the following precautions:

- Do not return any EMRS back to the original vial. Once the EMRS is out of the vial, either use it or discard it.
- Use acetonitrile as a rinse solvent.
- Do not store the EMRS in a glass syringe. You may transfer the EMRS in a glass syringe, but always discard any unused EMRS and rinse the syringe with acetonitrile.
- If you observe degradation products in the mass spectrum of the EMRS, rinse everything in the sample line with acetonitrile (the fittings, syringe, tubing, and union).
- Take these storage precautions for calibration and reserpine solutions: Refrigerate the containers after opening. For long-term storage, keep refrigerated at 2–8 °C.

1. With sample in the syringe (1 in Figure 81), follow the procedures in Appendix B, "Setting Up the Syringe with the Syringe Pump." The syringe pump is not shown.
2. Insert the grounding union (2) into the grounding union holder (3).
3. Use PEEK fittings to connect the red PEEK tubing (5) to the grounding union (2) and the H-ESI spray insert (4).
4. Use a PEEK fingertight fitting to connect another length of red PEEK tubing (6) with the syringe union adapter (1).
5. Use a PEEK fighertight fitting (not shown) to connect the other end of the red PEEK tubing (6) to the grounding union (3).

Figure 81. H-ESI direct infusion



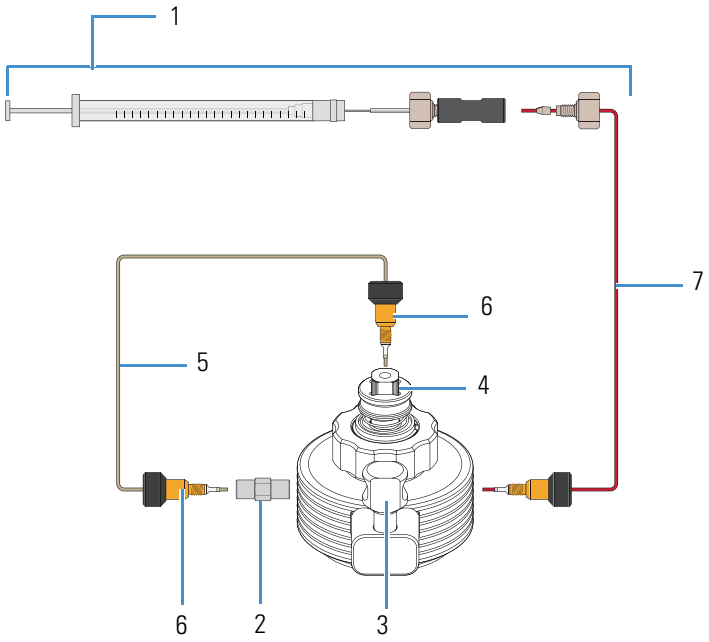
No.	Description
1.	Syringe union
2.	Grounding union
3.	Grounding union holder
4.	H-ESI spray insert
5.	Red PEEK tubing connecting grounding union to the H-ESI source
6.	Red PEEK tubing connecting the syringe to the grounding union

Setting Up Low Flow H-ESI Direct Infusion

Note Use Viper fittings on the natural-colored PEEK tubing (the nano-Viper capillary). The other fitting should be PEEK.

1. Place sample in the syringe (1 in Figure 82). The syringe pump is not shown.
2. Insert the grounding union (2) into the grounding union holder (3).
3. Use Viper fittings to connect the natural colored PEEK tubing (5) between the left side of the grounding union (2) and the H-ESI spray insert (4).
4. Use PEEK fingertight fittings to connect a length of red PEEK tubing (7) between the syringe union adapter (1) and the grounding union (2).

Figure 82. Low-flow H-ESI direct infusion



No.	Description
1.	Syringe and syringe adapter
2.	Grounding union
3.	Grounding union holder
4.	Low flow H-ESI needle in H-ESI spray insert
5.	Natural PEEK tubing (nano-Viper capillary)
6.	Viper fitting
7.	Red PEEK tubing

Setting Up High-Flow Infusion Without an Autosampler

The high-flow infusion method uses an LC Tee union to direct the solvent flow from the syringe pump into the solvent flow produced by an LC pump. The combined solvent flow goes through the divert/inject valve into the API source. Use this infusion method to perform experiments at a higher flow rate with an LC system. The high-flow infusion method allows you to optimize the source parameters (such as sheath gas and vaporizer temperature) at the flow rate and mobile phase composition of the assay.

Before you begin, complete the procedures in Appendix B, "Setting Up the Syringe with the Syringe Pump."

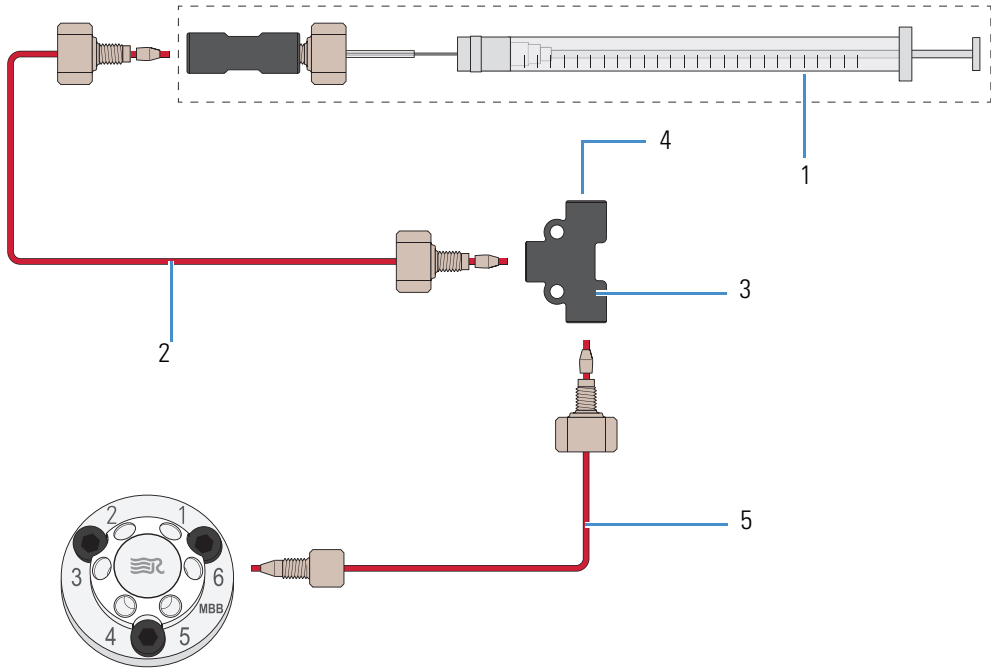
After you set up the Tee union, connect the API source.

- For H-ESI or low-flow H-ESI, see "Setting Up H-ESI or Low Flow H-ESI Direct Infusion."
- For APCI, see "Connecting the Sample Flow to the APCI Source."

Note The inject/divert valve in Figure 84 is an example. The valve in your system might be different.

1. Fill the syringe with your sample (1 in Figure 83) and connect it to the syringe pump (not shown).
2. Using red PEEK tubing (2) and fittings, connect the syringe union adapter to the base of the Tee union (3). This is the infusion line.
3. Use a fingertight fitting to connect a piece of red PEEK tubing (not shown), to one side of the Tee union (3). This adds the flow from the LC pumps to the flow from the syringe pump.
4. Using red PEEK tubing and fittings (5), connect the open end of the Tee union to the API source at Port 6. This brings the flow to the MS.
5. (Not Shown) Using a Rheodyne fitting, connect one end of the Teflon tubing to Port 3. Place the other end into an appropriate waste container.

Figure 83. HPLC infusion Tee valve



No.	Description
1.	Syringe and union
2.	Red PEEK tubing infusion line
3.	Tee union
4.	(not shown) PEEK tubing from the LC
5.	Red PEEK tubing connecting the Tee valve to Port 6 (to the MS)

Setting Up Loop Injections for Flow-Injection Analysis

When you have a limited amount of sample, use manual loop injections with or without an LC column. You can use this technique in H-ESI or APCI mode.

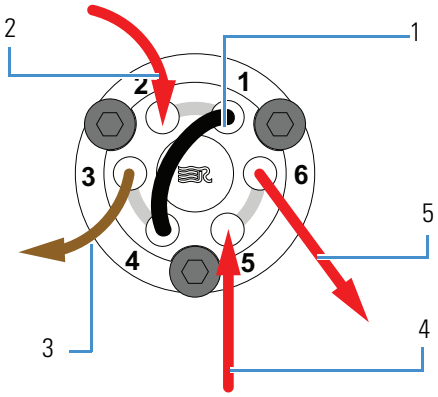
This technique requires attaching a sample loop, an injection port fitting (needle port), and an LC pump to the divert/inject valve, and then connecting the valve to the API source. With the valve in the Load position, you use a syringe to load sample through the injection port fitting into the sample loop, and then switch the position of the inject valve to the Inject position. Switching the valve to the Inject position allows the solvent flow from the LC pump to backflush the sample out of the loop and into the API source.

Figure 84 shows the flow directions for the valve when it is plumbed as an injector valve. The following procedure shows you how to plumb the valve.

1. Connect a sample loop (1 in Figure 84) across Ports 1 and 4 of the valve.

2. Connect a loop filler (needle port) (2) to Port 2.
3. Use a Rheodyne fitting to connect one end of the Teflon tubing (3) to Port 3. Place the other end in a waste container, not shown.
4. Use red PEEK tubing (5) and a fingertight fitting to connect Port 5 to the LC.
5. Connect the red PEEK tubing (6) from Port 6 to the API source.
   - To connect to the H-ESI source, see "Connecting the Sample Flow to the H-ESI Source."
   - To connect to the APCI source, see "Connecting the Sample Flow to the APCI Source."

Figure 84. Injector valve



No.	Description
1.	Sample loop (across Port 1 and 4)
2.	Sample input flows into Port 2.
3.	Teflon tubing takes waste from Port 3.
4.	LC pump flows into Port 5.
5.	Flow goes into the API source from Port 6.

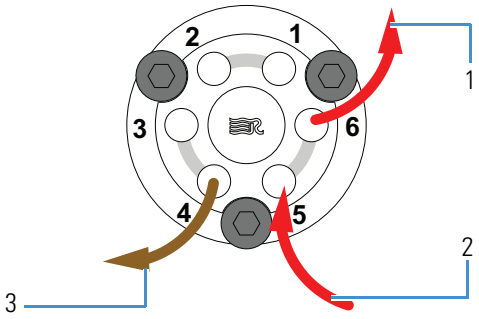
Setting Up Injections Using the Autosampler

You can use the data acquisition software automatically inject samples from an autosampler. In a typical LC/MS experiment, solvent flow goes through an LC column to separate the compounds of a mixture before they are directed into the API source, either H-ESI or APCI.

1. Use red PEEK tubing, and a Rheodyne fitting to connect Port 2 of the divert/inject valve to one of the following:
   - The outlet of the autosampler (not shown), or
   - The outlet of a column that is attached to the autosampler (not shown)

2. Use a Rheodyne fitting to connect one end of the Teflon tubing to Port 4. Place the other end in a waste container (not shown).
3. Connect red PEEK tubing to Port 6 and the other end to the API source.

Figure 85. Divert/Inject valve plumbed as a divert valve



No.	Description
1.	Port 6 flow goes to the API source.
2.	Port 5 flow comes in from the LC pumps.
3.	Port 4 Teflon tubing is connected to waste.

E

Replaceable Parts

The TSQ Altis MS, TSQ Quantis MS and TSQ Fortis MS arrive with the following kits and replaceable parts. The exception is the Test Solution Kit, which arrives separately as part of the preinstallation kit. Use the provided part numbers when ordering replacement parts.

Test Solutions

EMRS (extended mass range solution) calibrant (1 ea) HAZMAT-01-00099
TSQ Reserpine Solution Kit 80100-62033

Calibration Kit

Table 21. Source LC Connection Kit (P/N 80000-62057)

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

Table 22. Syringe Adapter Kit (P/N 70005-62011)

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

MS Setup Kit

MS Setup Kit {Rev G} 80100-62003
Drain hose adapter with 0-ring 70111-20971
Connector plug, MINI-COMBICON™, 8-pin, 26.67 mm (1.05 in.) long, rated 160 V, 8 A (contact closure, 2 provided) 00004-21512
Container, Nalgene™, 4 L heavy-duty; filling/venting cap 80100-20265
Ethernet cables, shielded Category 5e, 2.1 m (7 ft) long (2 provided) 00302-99-00036
Ethernet power supply (rated 100–240 Vac, 50/60 Hz, 0.6/0.3 A input; 18 W, 12 Vdc, 1.5 A output) 00012-01-00039
Ethernet switch, 5-port Gigabit 00825-01-00111
Ferrule, brass, front, 1/4 in. ID (2 provided) 00101-10000
Ferrule, brass, front, 1/8 in. ID (2 provided) 00101-08500
Ferrule, brass, back, 1/4 in. ID (2 provided) 00101-04000
Ferrule, brass, back, 1/8 in. ID (2 provided) 00101-02500
Swagelok™-type nut, brass, 1/4 in. ID (2 provided) 00101-12500
Swagelok-type nut, brass, 1/8 in. ID (2 provided) 00101-15500
Tubing, precleaned copper, 1/8 in. OD, 0.030 in. thick, 4.6 m (15 ft) long (for the UHP argon and nitrogen gases) 00301-22701
Tubing, Teflon PFA, 1/4 in. (6.35 mm) OD, 0.062 in. (1.57 mm) thick, 4.6 m (15 ft) long (for the HP nitrogen gas) 00101-50100
Tubing, Tygon™, 1-3/8 in. OD, 1 in. ID, 3 m (10 ft) (for the drain/waste line) 00301-01-00020

Performance Specification Kit

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

Single Mechanical Pump Kit

Single Mechanical Pump Kit {Rev C} 80100-62004
Forepump, Oerlikon Leybold Vacuum™, SOGEVAC™ SV 65 BI, single-phase 230 Vac, 50/60 Hz 00108-01-00032
Forepump oil tray, stainless steel, caster wheels 00201-99-00549
Accessories Single Mechanical Pump Kit (Table 23) 80100-62015

Table 23. Accessories Single Mechanical Pump Kit (P/N 80100-62015)

Item	Part number
90-Degree Elbow Installation Kit (2 provided, Table 24)	97055-62036S
Relay control cable, single pump, 2.4 m (8 ft) long (preassembled)	80000-63139
Single pump vacuum hose assembly, KF40, 2.4 m (8 ft) long (preassembled)	80000-60229
Tubing, Tygon, 3/4 in. (19.1 mm) OD, 0.5 in. (12.7 mm) ID, 3 m (10 ft) long	00301-22920

Table 24. 90-Degree Elbow Installation Kit (P/N 97055-62036S)

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

Dual Mechanical Pumps Kit

Dual Mechanical Pumps Kit {Rev B} 80100-62013
Forepump, Oerlikon Leybold Vacuum, SOGEVAC SV 65 BI, single-phase 230 Vac, 50/60 Hz (2 provided) 00108-01-00032
Forepump oil tray, stainless steel, caster wheels (2 provided) 00201-99-00549
Accessories Dual Mechanical Pump Kit (Table 25) 80100-62016

Table 25. Accessories Dual Mechanical Pump Kit (P/N 80100-62016) {Rev C}

Item	Part number
90-Degree Elbow Installation Kit (3 provided, Table 24)	97055-62036S
Dual relay control cable, 2.4 m (8 ft) long (preassembled)	80100-63146
Dual pump vacuum hose assembly (preassembled)	80100-60049
Fitting Tee, barbed, nylon, for 0.5 in. (12.7 mm) ID tubing	00103-01-00012
Tubing, Tygon, 3/4 in. (19.1 mm) OD, 0.5 in. (12.7 mm) ID, 6 m (20 ft) long	00301-22920

TSQ Source Installation Kit

TSQ Source Installation Kit {Rev A}

Ion transfer tube removal tool, TSQ Altis 70005-20972
Ion transfer tube removal tool, TSQ Quantis 70111-20258
L0 lens removal tool 70005-20900
Viper Capillary Kit (5 provided) 00109-99-00068
Capillary length tool 80000-20957

API Source Interface

TSQ Altis MS

API source interface assembly
MP00 multipole 80100-20070
Ion sweep cone 80100-20646
Ion transfer tube (58 mm tube length, L-etched and 1/4 turn nose cone) 80500-20045
Lens L0 80100-20548
O-ring, Vespel, graphite, 0.325 in. ID, 0.046 in. thick
(under ion transfer tube) 97055-20442
SRIG lens stack (ion funnel) 80100-60036

TSQ Quantis MS

API source interface assembly
MP00 multipole 80100-20070
Ion sweep cone 80111-20646
Ion transfer tube (58 mm tube length, V-etched and threaded nose cone) 70005-20606
Lens L0 80100-20548
SRIG lens stack (S-lens) 80100-60136

TSQ Fortis MS

API source interface assembly
Ion transfer tube (101.6 mm tube length, threaded nose cone) 80100-20062
Skimmer 80111-20064
Tube lens 80111-20162
Ion sweep cone 80111-20646
Lens L0 80100-20548

Miscellaneous Parts

Divert/Inject Valve and Syringe Pump Assembly

Divert/inject valve, Rheodyne MXT715-004 Valve 00109-99-00046
Holder, divert valve and syringe pump 80100-60258
Syringe pump, Chemyx™ Fusion 100T 00109-99-00045

Sample Loop

2 µL, PEEK. 00110-16012

Air Filter

Air filter, metal mesh. 80000-10355

Forepump Accessories

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

Power Supply Cords

Mass Spectrometer

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

Forepump

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

Glossary

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

A

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

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

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

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

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

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

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

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

C

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

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

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

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

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

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

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

D

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

E

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

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

F

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

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

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

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

H

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

I

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

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

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

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

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

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

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

L

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

M

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

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

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

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

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

mass-to-charge ratio (*m/z*) An abbreviation used to denote the quantity formed by dividing the mass of an ion (in Da) by the number of charges carried by the ion. For example, for the ion $C7H7^{2+}$, $m/z = 45.5$.

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

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

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

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

N

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

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

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

P

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

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

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

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

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

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

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

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

Q

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

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

R

relative standard deviation (RSD) A measure of the dispersion of a group of measurements relative to the mean of the group. Related standard deviation is expressed as a percentage of the average value. The percent standard deviation is calculated as:

$$\%\text{RSD} = 100 \times (S/\bar{X})$$

where S is the standard deviation and $\bar{X}$ is the sample mean.

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

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

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

S

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

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

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

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

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

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

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

T

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

V

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

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

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