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Thermo Scientific

TSQ Series II Mass Spectrometers

Hardware Manual

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ThermoFisher
SCIENTIFIC

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Release history: Rev. A September 2021

Software version: (Thermo) Foundation 3.1 SP4 and later, Xcalibur 4.4 and later, Tune 3.4 and later

Note: You can access this manual from the TSQ II Series version 3.4 instrument control software.

General Laboratory Equipment. Not for use in diagnostic procedures.

Regulatory Compliance

Thermo Fisher Scientific performs complete testing and evaluation of its products to ensure full compliance with applicable North American and European regulations. Your system meets the applicable requirements in the electromagnetic compatibility (EMC) and product safety standards described in this section.

Unauthorized changes that you make to your system will void regulatory compliance and might defeat the built-in protections for your instrument. Some examples of unauthorized changes include using replacement parts or adding components, options, or peripherals that Thermo Fisher Scientific has not qualified and authorized. Unauthorized changes can also result in bodily injury and/or damage to your system and laboratory.

Ensure continued compliance with regulatory standards:

- Follow all installation instructions provided in the documentation that comes with your system.
- Order replacement parts (as specified in the instrument manual) and additional components, options, and peripherals directly from Thermo Fisher Scientific or an authorized representative.

TSQ Endura and TSQ Quantiva Mass Spectrometers

Low Voltage Directive 2014/35/EU

This device complies with Low Voltage Directive 2014/35/EU and the harmonized safety standard IEC/EN/CSA/UL 61010, 3rd Edition.

EMC Directive 2014/30/EU and other EMC test standards

This device was tested by TÜV Rheinland of North America and complies with the following EMC standards:

47 CFR 15, Subpart B, Class A: 2011	EN 61000-3-3: 2008	EN 61000-4-8: 2010
CISPR 11: 2009 + A1	EN 61000-4-2: 2009	EN 61000-4-11: 2004
ICES-003: 2012	EN 61000-4-3: 2006 + A1 + A2	BSMI CNS 13438: 2006
EN 55011: 2009 + A1	EN 61000-4-4: 2004 + A1	VCCI V-3: 2013.04
EN 61326-1: 2013	EN 61000-4-5: 2006	
EN 61000-3-2: 2006 + A1 + A2	EN 61000-4-6: 2009	

TSQ Altis, TSQ Quantis, and TSQ Fortis Mass Spectrometers

Refer to the Thermo Fisher Scientific CE Declaration of Conformity for details.

Low Voltage Directive 2014/35/EU

This device complies with Low Voltage Directive 2014/35/EU and the harmonized safety standard IEC/EN/CSA/UL 61010-1, 3rd Edition.

EMC Directive 2014/30/EU

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

TSQ Altis Plus, TSQ Quantis Plus, and TSQ Fortis Plus Mass Spectrometers

Refer to the Thermo Fisher Scientific CE Declaration of Conformity for details.

Low Voltage Directive 2014/35/EU

This device complies with Low Voltage Directive 2014/35/EU and the harmonized safety standard IEC/EN/CSA/UL 61010-1, 3rd Edition.

EMC Directive 2014/30/EU

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

FCC Compliance Statement

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



CAUTION Read and understand the various precautionary notes, signs, and symbols contained inside this manual pertaining to the safe use and operation of this product before using the device.

Notice on Lifting and Handling of Thermo Scientific Instruments

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

Notice on the Proper Use of Thermo Scientific Instruments

In compliance with international regulations: This instrument must be used in the manner specified by Thermo Fisher Scientific to ensure protections provided by the instrument are not impaired. Deviations from specified instructions on the proper use of the instrument include changes to the system and part replacement. Accordingly, order replacement parts from Thermo Fisher Scientific or one of its authorized representatives.

WEEE Directive 2012/19/EU



Thermo Fisher Scientific is registered with B2B Compliance ([B2Bcompliance.org.uk](https://www.b2bcompliance.org.uk)) in the UK and with the European Recycling Platform ([ERP-recycling.org](https://www.eur-recycling.org)) in all other countries of the European Union and in Norway.

If this product is located in Europe and you want to participate in the Business-to-Business (B2B) Recycling Program, send an email request to weee.recycle@thermofisher.com with the following information:

- WEEE product class
- Name of the manufacturer or distributor (where you purchased the product)
- Number of product pieces, and the estimated total weight and volume
- Pick-up address and contact person (include contact information)
- Appropriate pick-up time
- Declaration of decontamination, stating that all hazardous fluids or material have been removed from the product

For additional information about the Restriction on Hazardous Substances (RoHS) Directive for the European Union, search for RoHS on the European language websites.

IMPORTANT This recycling program is **not** for biological hazard products or for products that have been medically contaminated. You must treat these types of products as biohazard waste and dispose of them in accordance with your local regulations.

Contents

	Preface	13
	Access documentation	13
	View the manuals	14
	View the Help	15
	View user documentation on the Thermo Fisher Scientific website	16
	Special notices, symbols, and cautions	16
	Contact us	18
Chapter 1	Introduction to the TSQ Series II product line	19
	External features of a TSQ Series II MS	19
	Front panel of the MS	20
	Right side of the MS	21
	Left side of the MS	22
	Back side of the MS	22
	Basic components of a TSQ Series II MS	23
	Models in the TSQ Series II product line	24
	First generation—Endura and Quantiva	24
	Second generation—Altis, Quantis, and Fortis	25
	Third generation—Altis Plus, Quantis Plus, and Fortis Plus	26
	Mass range, speed, and selectivity for each model	27
	Compatible ion sources	27
	Compatible FAIMS interfaces	28
	Overview of an LC/MS Analysis	28
	LED indicators	31
	Power entry module	32
	Main Power switch	33
	Electronics service switch	33
	Mechanical pump/forepump enable connector	33
	Communications panel	33
	Drainage system	37
	Cooling Fans	38

Chapter 2	Scan parameters in the Tune and Method Editor windows	39
	Scan types	39
	Quadrupole modes	40
	Summary of the quadrupole modes for the various scan types	40
	Full scan Q1 and Q3 scan types	41
	Selected ion monitoring scan type	42
	Product ion scan type	42
	Precursor scan type	43
	Neutral loss scan type	44
	Selected reaction monitoring scan type	46
	Quantitation enhanced data-dependent scan type	47
	Profile and centroid data	47
	Ion polarity modes	48
Chapter 3	Functional description of the MS components	49
	Vacuum system and inlet gases hardware and N ₂ gas flow paths	49
	Vacuum pumps	50
	Vacuum manifold	51
	Vacuum gauges	52
	Inlet gas supply hardware	52
	Sheath gas, auxiliary gas, and sweep gas flow paths	53
	Atmospheric pressure ionization source	55
	API source interface	60
	Ion sweep cone	63
	Spray cone	64
	Ion transfer tube	65
	Heater block	67
	Vent prevent ball	68
	RF lens and exit lens	68
	Tube lens and skimmer (TSQ Fortis and TSQ Fortis Plus)	69
	MP00 ion optics – MP00 multipole and L0 lens	70
	MP0 ion optics and neutrals blocker	71
	Mass analyzers and collision cell	72
	Quadrupole rod assemblies	72
	Applied RF and DC fields	75
	Mass analysis	75
	Collision cell and CID efficiency	76
	Quadrupole offset voltage	76
	Mass analyzer lenses	77
	Ion detection system	77

Chapter 4	Maintain the MS on a daily basis	78
	Before operating the mass spectrometer	78
	Check the vacuum pressure levels	78
	Find and fix air leaks	81
	Check the argon and nitrogen gas supplies	82
	After operating the mass spectrometer	83
	Flush the inlet components	83
	Purge the oil in the forepump	84
	Empty the solvent waste container	84
	Place the system in Standby mode	84
Chapter 5	System startup, shutdown, and reset	85
	Place the MS in On mode for operation	85
	Turn on the MS from the Tune window	85
	Turn on the MS from the data system	86
	Place the MS in Standby mode for short periods between use	86
	Shut down the MS system completely in an emergency	87
	Shut down the MS system completely for planned service or storage	88
	Restart the MS system after a complete shutdown	89
	Restart the data system computer	90
	Pump down and restart the MS after a complete shutdown	90
	Reset the MS if it is not communicating with the data system	92
	MS components On/Off status	94
Chapter 6	Connect the sample flow to the API source	96
	Connect the sample flow to the H-ESI source	96
	Connect the sample flow to the APCI source	97
Chapter 7	Calibrate the MS	99
	Prepare the MS system for calibration	99
	Access the system preparation instructions from the Calibration pane	100
	Set up the syringe pump with the calibration solution	101
	Position the H-ESI probe or the calibration probe for the calibration process	102
	Apply the favorites settings for the calibration process	103
	Start the flow of calibration solution to the ion source	105
	Check the full scan for missing or interfering peaks	106
	Evaluate the spray stability	107
	Run the automated System Calibration routine	113
	Run the automated System Check routine	115
	Tune and calibration parameters	117
	Calibration solution peak values	117

Chapter 8	Starting source conditions for various LC flow rates.....	120
	Check the recommended ion source settings for the LC flow rate	120
	Recommended H-ESI source settings for various LC flow rates.....	121
	Recommended LC/APCI/MS parameters	121
	Recommended LC/NSI/MS parameters	122
Chapter 9	Optimize the compound signal	123
	View the Performing Compound Optimization animation	123
	Set up the MS system for compound optimization	123
	Optimize the source parameters in the Optimization pane	124
Chapter 10	Acquire sample data.....	129
	View an animation about creating an SRM method	129
	Use the Tune application to acquire sample data	130
	Use the Xcalibur data system to acquire sample data	133
	Use the templates in the Method Editor to set up the MS experiment.....	136
Chapter 11	Maintenance	137
	Maintenance schedule	137
	Guidelines for performing maintenance.....	139
	Maintenance animations on the Thermo Fisher Scientific website.....	140
	Tools and supplies for routine maintenance procedures.....	140
	Maintain the API source housing	142
	Remove the API source housing from the MS	143
	Clean the API source housing	143
	Maintain the external components of the API source interface	144
	Remove the ion sweep cone.....	145
	Remove the ion transfer tube.....	146
	Clean the spray cone	149
	Clean the ion sweep cone and the ion transfer tube.....	150
	Reinstall the ion transfer tube	151
	Reinstall the ion sweep cone	152
	Verify the cleaning process for the external components of the API source.....	153
	Maintain the internal components of the API source interface.....	154
	Vent the mass spectrometer and remove the API source interface	155
	Remove the MP00 assembly, the RF lens, and the exit lens from the source interface cage.....	156
	Remove the MP00 assembly, the skimmer, and the tube lens (TSQ Fortis and TSQ Fortis Plus only)	159
	Clean the lenses.....	163
	Clean the MP00 multipole	165
	Reinstall the components of the API source interface cage.....	165
	Reinstall the API source interface cage.....	169

Maintain the forepumps	169
Check the level of the forepump oil before daily use	170
Purge or change the oil	170
Maintain the air filter	170
Appendix A Basic Tune functions	172
Open the Tune window	172
Set the instrument system controls	174
Set the instrument power mode.	175
Check the instrument readback status	175
Set the Tune preferences	177
Use the mass list table in the Define Scan pane	178
Add a row to the table	178
Delete a row from the table	178
Delete multiple rows from the table.	178
Add or remove scan parameters from the scan type table	179
Import a mass list from a file	179
Export a mass list to a file	180
Use the History pane.	180
Use the Favorites pane to save the system settings	181
Appendix B Set up the syringe and the syringe pump	183
Set up the syringe pump to infuse a sample from the syringe.	183
Connect the syringe union to the sample transfer line	184
Appendix C Divert/Inject valve	186
Divert/Inject valve positions	186
Divert/Inject valve configurations	187
Loop injection	187
Divert valve	188
Divert/Inject valve controls	189
Appendix D Sample introduction techniques	190
H-ESI or low-flow H-ESI direct infusion	190
Set up H-ESI direct infusion	190
Set up low-flow H-ESI direct infusion.	192
High-flow infusion without an autosampler	193
Set up loop injections for a flow-injection analysis.	195
Set up injections using the autosampler.	197
Appendix E Replaceable parts	198
Test Solution Kits	198
Calibration Kit	198
Low Flow Needle and ESI Probe Calibration Kit	199
Performance Specification Kit	200

TSQ Source Installation Kit 200
API source interface replaceable parts 201
Miscellaneous replaceable parts 202
Glossary203
Index208

Preface

The *TSQ Series II Mass Spectrometers Hardware Manual* describes how to operate and maintain the Thermo Scientific™ TSQ Series II family of triple-stage quadrupole mass spectrometers.

The TSQ Series II product line includes the following mass spectrometers:

- TSQ Altis™ Plus
- TSQ Altis
- TSQ Quantiva™
- TSQ Quantis™ Plus
- TSQ Quantis
- TSQ Endura™
- TSQ Fortis™ Plus
- TSQ Fortis

See these topics:

- [Access documentation](#)
- [Special notices, symbols, and cautions](#)
- [Contact us](#)

Access documentation


For details about accessing the product manuals and the Help systems, see these topics:

- [View the manuals](#)
- [View the Help](#)
- [View user documentation on the Thermo Fisher Scientific website](#)

Note For system requirements, refer to the release notes on the software DVD.

View the manuals

❖ To view the product manuals for your TSQ Series II mass spectrometer

1. From the Windows 10 taskbar, click the **Start** icon, . Then, choose **Thermo Instruments > TSQ Model 3.4 Manuals**.
2. Double-click the PDF that you want to view.

[Table 1](#) lists the PDFs that you can find in the Manuals folder for each TSQ Series II MS. The *Safety and Regulatory Guide* ships with every Thermo Scientific MS.

Table 1. TSQ Series II manuals for the mass spectrometers, ion sources, and FAIMS interfaces (Sheet 1 of 2)


MS model	Manual title
TSQ Altis Plus MS and TSQ Altis MS	1. <i>TSQ Series II Hardware Manual</i> (2021)
	2. <i>TSQ Series II Preinstallation Guide</i> (2021)
TSQ Quantis Plus MS and TSQ Quantis MS	3. <i>TSQ Series II Getting Connected Guide</i> (2021)
	4. <i>FAIMS Pro Interface and FAIMS PRO Duo Interface User Guide</i> (2021)
	5. <i>OptaMax NG Ion Source User Guide</i> (2020)
	6. <i>OptaMax Duet Ion Source User Guide</i> (2021)
	7. <i>EASY-Spray Series Ion Source User Guide</i> (2020)
	8. <i>Nanospray Flex Series Ion Source User Guide</i> (2018)
	9. <i>VeriSpray PaperSpray Ion Source Guide</i> (2019)
TSQ Fortis Plus MS and the TSQ Fortis MS (The FAIMS interfaces are not compatible with the TSQ Fortis Plus MS and the TSQ Fortis MS.)	1. <i>TSQ Series II Hardware Manual</i> (2021)
	2. <i>TSQ Series II Preinstallation Guide</i> (2021)
	3. <i>TSQ Series II Getting Connected Guide</i> (2021)
	4. <i>OptaMax NG Ion Source User Guide</i> (2020)
	5. <i>OptaMax Duet Ion Source User Guide</i> (2021)
	6. <i>EASY-Spray Series Ion Source User Guide</i> (2020)
	7. <i>Nanospray Flex Series Ion Source User Guide</i> (2018)
	8. <i>VeriSpray PaperSpray Ion Source Guide</i> (2019)

Table 1. TSQ Series II manuals for the mass spectrometers, ion sources, and FAIMS interfaces (Sheet 2 of 2)

MS model	Manual title
TSQ Endura MS and TSQ Quantiva MS	1. <i>TSQ Series II Hardware Manual</i> (2021)
	2. <i>TSQ Endura and TSQ Quantiva Preinstallation Requirements Guide</i> (2017)
	3. <i>TSQ Endura and TSQ Quantiva Getting Connected Guide</i> (2016)
	4. <i>Ion Max NG and EASY-Max NG Ion Sources User Guide</i> (2016)
	5. <i>OptaMax NG Ion Source User Guide</i> (2020)
	6. <i>EASY-Spray Series Ion Source User Guide</i> (2020)
	7. <i>Nanospray Flex Series Ion Source User Guide</i> (2018)
	8. <i>VeriSpray PaperSpray Ion Source Guide</i> (2019)
	9. <i>FAIMS Pro Interface and FAIMS PRO Duo Interface User Guide</i> (2021)

View the Help

To view the Help system, do the following as applicable:

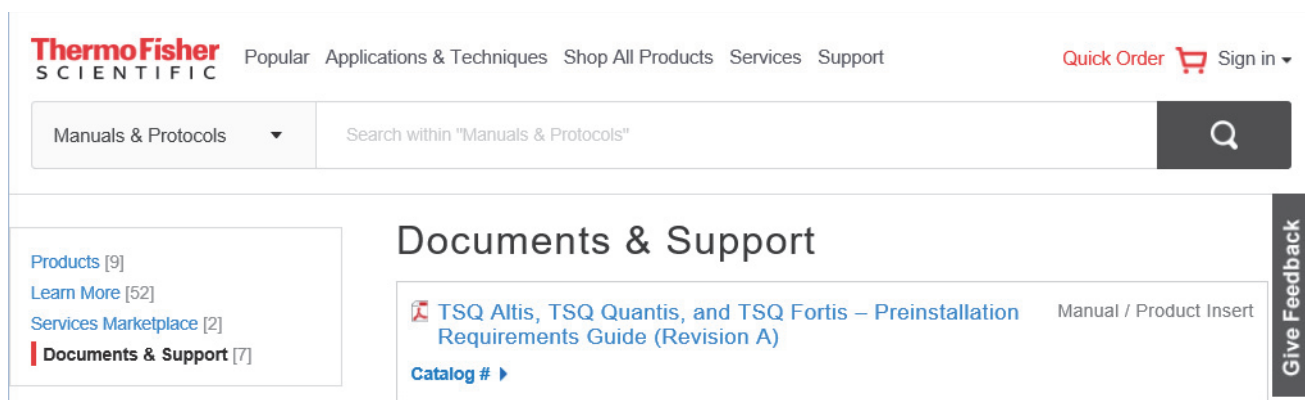
- From the Thermo Scientific Tune application, click the settings icon, , and choose **Tune Help**.
- From the Thermo Xcalibur™ Method Editor, choose an option from the (Instrument Setup window) Help menu.
- To view the context-sensitive Help topic for a specific page, pane, or dialog box in the Tune window or the Method Editor window, open the item of interest. Then, press the F1 key (or the key on your keyboard that opens Help if the F1 key is set to a different function).

View user documentation on the Thermo Fisher Scientific website

The following instructions are subject to change.

❖ To download user guides for various Thermo Scientific products

1. Go to thermofisher.com.
2. Point to **Support** and click **Manuals** on the left.
3. In the Search within Manuals & Protocols box, search by the product name.



4. From the results list, click the title to open the document in your web browser. Then, save or print the document.

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 2](#).




Table 2. 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 2. 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 atmospheric pressure ionization (API) source assembly, give the heated components time 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.

Contact us

Contact	Email	Telephone	QR Code
U.S. Technical Support	us.techsupport.analyze@thermofisher.com	(U.S.) 1 (800) 532-4752	
U.S. Customer Service and Sales	us.customer-support.analyze@thermofisher.com	(U.S.) 1 (800) 532-4752	
Global Support	<ul style="list-style-type: none"> ❖ To find global contact information 1. Go to thermofisher.com. 2. Sign in. 3. Choose Support > Contact Us. 4. At the How Can We Help prompt, type the product name. 5. Use the phone number or complete the online form. <ul style="list-style-type: none"> ❖ To find product support, knowledge bases, and resources Go to thermofisher.com/us/en/home/technical-resources. <ul style="list-style-type: none"> ❖ To find product information Go to thermofisher.com/us/en/home/brands/thermo-scientific. 		

Introduction to the TSQ Series II product line

These topics describe the basic features of the TSQ Series II product line of triple-stage quadrupole mass spectrometers:

- External features of a TSQ Series II MS
- Basic components of a TSQ Series II MS
- Models in the TSQ Series II product line
- Mass range, speed, and selectivity for each model
- Compatible ion sources
- Compatible FAIMS interfaces
- Overview of an LC/MS Analysis
- LED indicators
- Power entry module
- Communications panel
- Drainage system
- Cooling Fans

External features of a TSQ Series II MS

The TSQ Series II mass spectrometers are triple-stage quadrupole mass spectrometers and are part of the Thermo Scientific family of mass spectrometers.

A TSQ Series II MS is a relatively compact instrument that sits on a laboratory workbench or table capable of supporting twice the weight of the MS and any installed hardware (for example, the ion source, the syringe pump, the inject/divert valve, and the optional FAIMS interface). The MS by itself weighs 131 kg (289 lb).

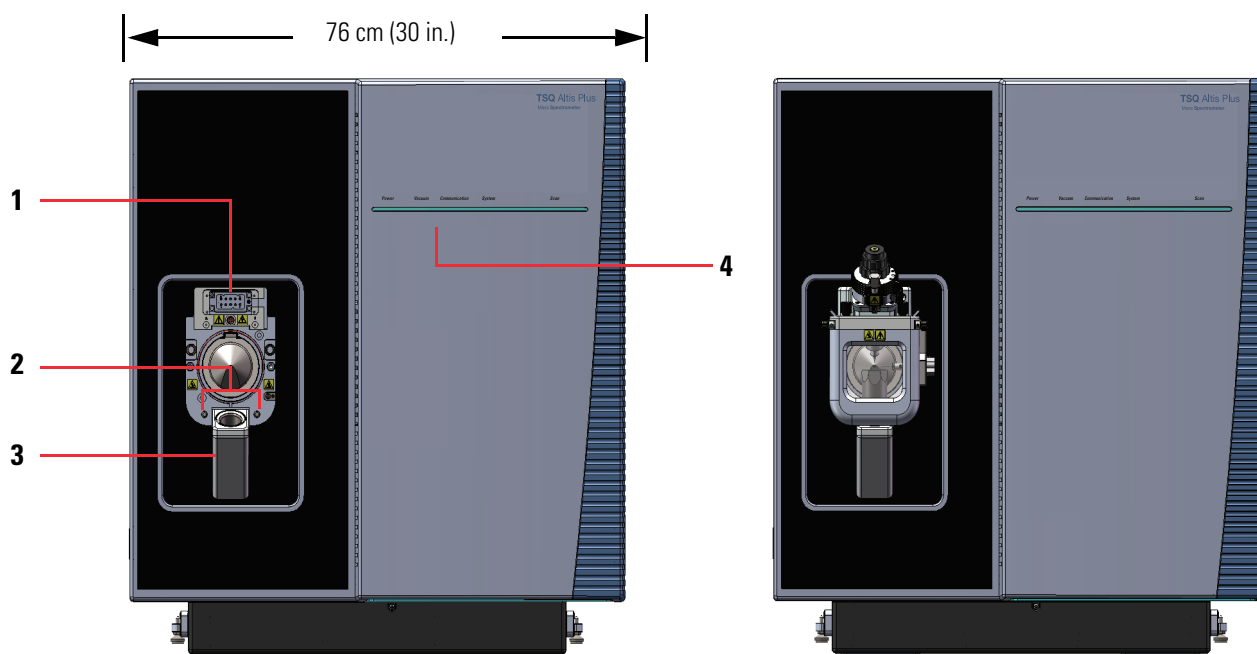
These topics describe the front, right, and left panels of the instrument as well as the back:

- [Front panel of the MS](#)
- [Right side of the MS](#)
- [Left side of the MS](#)
- [Back side of the MS](#)

Front panel of the MS

The front of the MS includes the API source interface with electrical connections and the mounting posts for the API ion source housing, a built-in drain system, and LEDs that indicate the status of the MS.

Figure 1. Front of the MS (without and with the OptaMax NG ion source)



No.	Description	No.	Description
1	Electrical connections	2	Mounting posts
3	Built-in drain system	4	LEDs

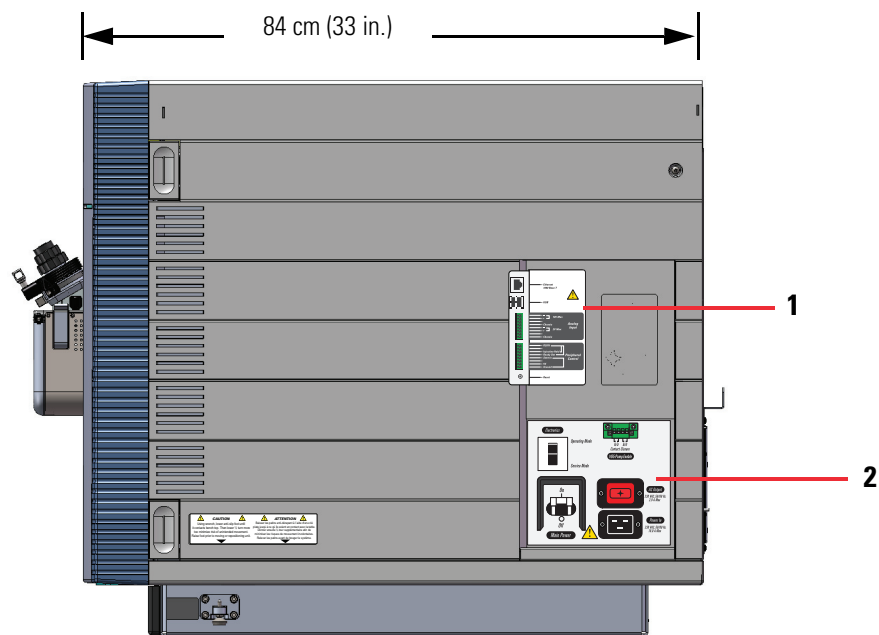
Related Topics

- [LED indicators](#)
- [Drainage system](#)
- [Atmospheric pressure ionization source](#)

Right side of the MS

The right side of the MS includes a recessed area with the communications panel and the power entry module.

Figure 2. Right side of the MS (shown with the OptaMax NG ion source housing)



No.	Description	No.	Description
1	Communications panel	2	Power module

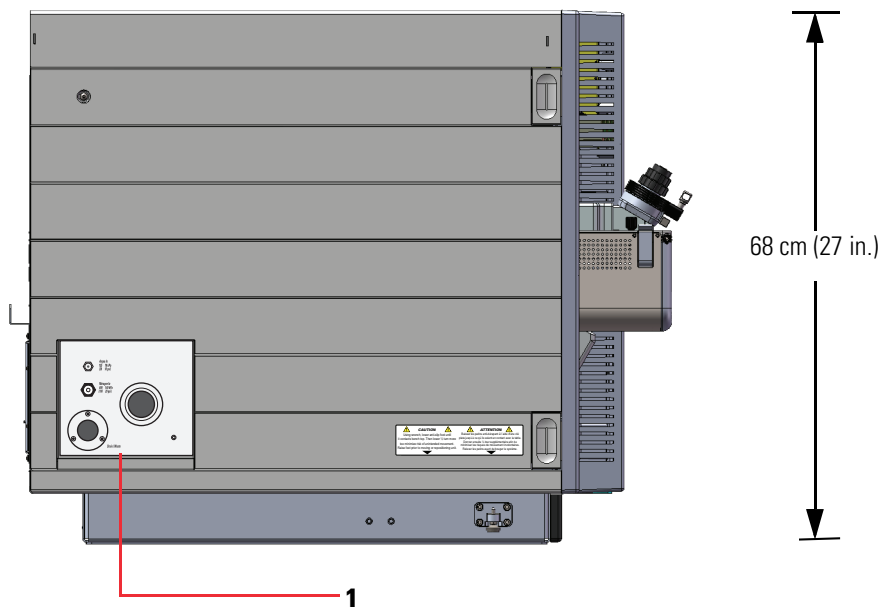
Related Topics

- [Communications panel](#)
- [Power entry module](#)

Left side of the MS

The left side of the MS includes the vacuum, gas, and solvent waste connections.

Figure 3. Left side of the MS (shown with the OptaMax NG ion source housing)



No.	Description
1	Vacuum, gas, and solvent waste connections

Related Topics

- [“Drainage system” on page 37](#)
- [“Vacuum system and inlet gases hardware and N2 gas flow paths” on page 49](#)

Back side of the MS

The back side of the MS includes grates that cover the cooling fans. The filter for the cooling fans is behind the front panel of the MS.

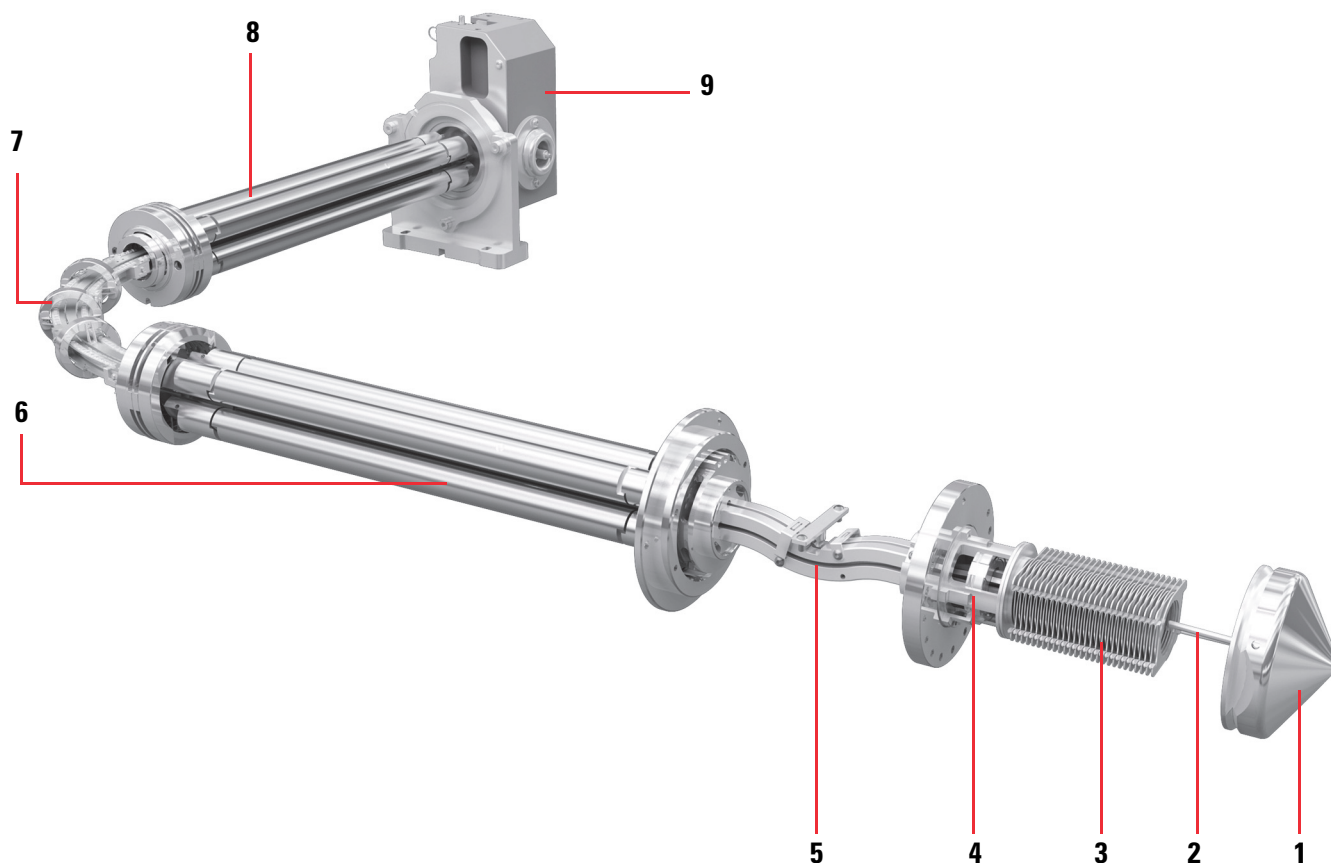
Related Topics

- [“Cooling Fans” on page 38](#)
- [“Maintain the air filter” on page 170](#)

Basic components of a TSQ Series II MS

The basic components of a mass spectrometer are the ion source, the mass analyzer, and the ion detector. Figure 4 shows a schematic of a TSQ Altis Plus MS.

Figure 4. TSQ Altis Plus MS schematic



No.	Description	No.	Description
1	Sweep cone	2	Ion transfer tube
3	RF lens, electrodynamic ion funnel (EDIF) for the TSQ Altis MS and TSQ Altis Plus MS	4	MP00 assembly (MP00 cage, MP00 multipole, exit lens, and L0 lens)
5	Ion beam guide with neutrals blocker	6	Q1 mass analyzer (segmented quadrupoles with a hyperbolic surface)
7	Q2 mass analyzer or active collision cell with axial DC field (The Q2 quadrupole can behave as an ion transmission device or a collision cell with axial DC field.)	8	Q3 mass analyzer (segmented quadrupoles with a hyperbolic surface)
9	Dual-mode electron multiplier detector		

Models in the TSQ Series II product line

The TSQ Series II product line includes the following models listed in order of their release from the first generation to the current generation:

- First generation—Endura and Quantiva
- Second generation—Altis, Quantis, and Fortis
- Third generation—Altis Plus, Quantis Plus, and Fortis Plus

The TSQ Series II instrument control software supports all the TSQ Series II models (General Laboratory Equipment versions).

First generation—Endura and Quantiva

Thermo Fisher Scientific has discontinued the TSQ Quantiva MS and the General Laboratory Use (GLE) version of the TSQ Endura MS. The in vitro diagnostics version of the TSQ Endura MS is still available for shipment to a limited number of countries.

- Both the TSQ Endura MS and the TSQ Quantiva MS shipped with an external syringe pump and an external divert/inject valve (not shown in [Figure 5](#)).
- The TSQ Quantiva MS shipped with the Thermo Scientific Ion Max NG™ API source ([Figure 21](#) on [page 56](#)) and two oil-sealed rotary vane forepumps.
- The TSQ Endura MS shipped with the Thermo Scientific EASY-Max NG™ API source and one oil-sealed rotary vane forepump.

Figure 5. TSQ Quantiva MS and TSQ Endura MS



TSQ Quantiva MS



TSQ Endura MS

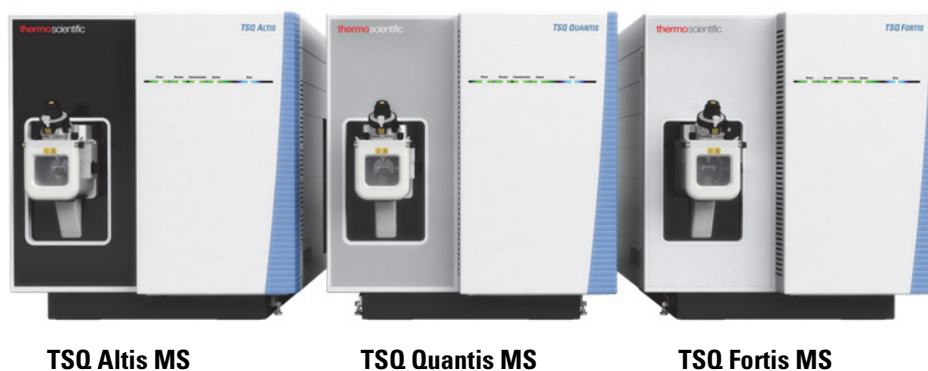
The components of the API source interface for these two mass spectrometers differ as follows:

- The TSQ Quantiva MS has a high-capacity ion transfer tube (HCTT) and an electrodynamic ion funnel (EDIF) RF lens.
- The TSQ Endura MS has a narrow-bore ion transfer tube and a stacked-ring ion guide (SRIG) RF lens.

Second generation—Altis, Quantis, and Fortis

The second generation of TSQ Series II mass spectrometers includes the TSQ Altis MS, TSQ Quantis MS, and TSQ Fortis MS.

Figure 6. TSQ Altis, Quantis, and Fortis models (showing the difference in the front panels)



The primary improvements in these models versus the first generation include the following:

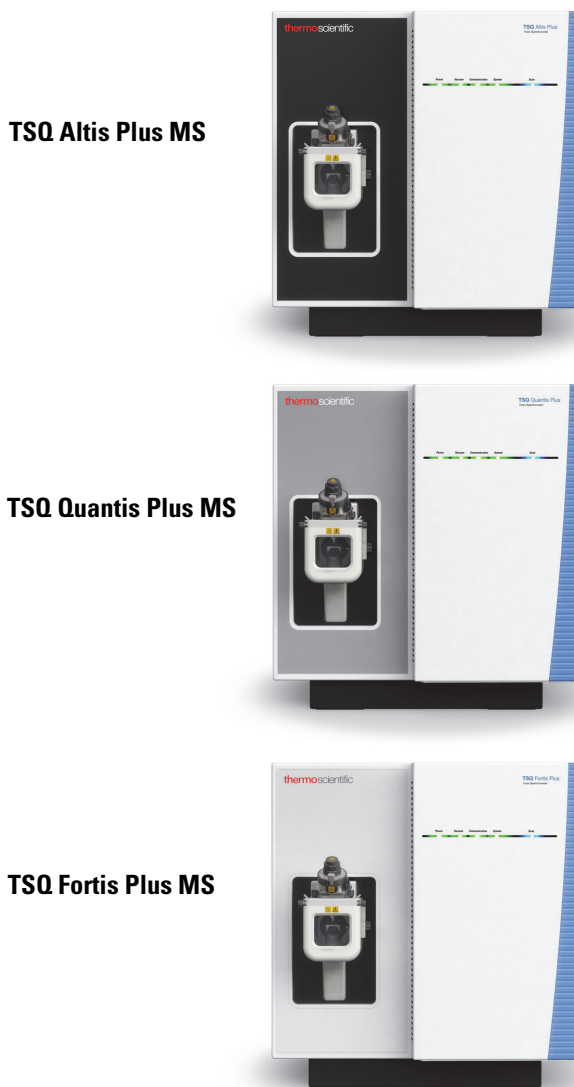
- All three of these models use the OptaMax™ NG API source (Figure 23 on page 58), which is APCI ready. In addition, all three models have segmented quadrupoles with hyperbolic surfaces and an enhanced dual-mode electron multiplier detector.
- The TSQ Altis MS includes a high-capacity ion transfer tube (HCTT) and an electrodynamic ion funnel (EDIF) RF lens, both of which increase the ion flux.
- The TSQ Quantis MS includes a narrow-bore ion transfer tube and a stacked ring ion guide (SRIG) RF lens.
- The TSQ Fortis MS includes a narrow-bore ion transfer tube. Instead of an RF lens, a Matrix Separator Ion Guide (MSIG) focuses the expanding ion plume as it exits the ion transfer tube. The MSIG consists of a skimmer and a tube lens.

Third generation—Altis Plus, Quantis Plus, and Fortis Plus

The primary improvements in the latest generation of mass spectrometers versus the previous generation include the following:

- Lower mass drift in the TSQ Altis Plus model provided by its improved Q-cap quadrupole mass analyzer
- Faster polarity switching for all three Plus models (5 ms)
- Improved turbomolecular pump with increased reliability in all three Plus models
- New collision cell that provides broad m/z transmission in all three Plus models

Figure 7. TSQ Series II Plus models (showing the difference in the front panel colors)



Mass range, speed, and selectivity for each model

Table 1 lists the specifications for the models in the TSQ Series II product line.

Table 1. TSQ Series II specifications by model (using the TSQ Series II version 3.4 instrument control software)

MS model	Relative cost	<i>m/z</i> range in amu	SRM/sec	Selectivity
Third generation				
TSQ Altis Plus	High	2–2010	600	0.2 Da FWHM
TSQ Quantis Plus	Mid-range	2–3000	600	0.4 Da FWHM
TSQ Fortis Plus	Low	2–3000	600	0.4 Da FWHM ^a
Second generation				
TSQ Altis	High	2–2000	600	0.2 Da FWHM
TSQ Quantis	Mid-range	2–3000	600	0.4 Da FWHM
TSQ Fortis	Low	2–3000	600	0.4 Da FWHM ^a
First generation				
TSQ Quantiva	High	2–1800	500	0.2 Da FWHM
TSQ Endura	Low	2–3400	500	0.4 Da FWHM

^a This value applies only to the Q1 quadrupole.

Compatible ion sources

Table 2 lists the ion sources that are compatible with the TSQ Series II mass spectrometers.

Table 2. Compatible ion sources for the TSQ Series II mass spectrometers (Sheet 1 of 2)

Hardware	Flow rate range	Compatible TSQ Series II models
EASY Spray NG	10 to 1000 nL/min	All GLE models
EASY-Max NG API source	H-ESI: 1–1000 μ L/min	TSQ Endura MS
	APCI: 100–2000 μ L/min	
Ion Max NG API source	H-ESI: 1–1000 μ L/min	TSQ Quantiva MS
	APCI: 100–2000 μ L/min	

Table 2. Compatible ion sources for the TSQ Series II mass spectrometers (Sheet 2 of 2)

Hardware	Flow rate range	Compatible TSQ Series II models
OptaMax NG API source	H-ESI: 1–1000 $\mu\text{L}/\text{min}$	<ul style="list-style-type: none"> • TSQ Altis Plus MS
	APCI: 100–2000 $\mu\text{L}/\text{min}$	<ul style="list-style-type: none"> • TSQ Quantis Plus MS • TSQ Fortis Plus MS • TSQ Altis MS • TSQ Quantis MS • TSQ Fortis MS
OptaMax Duet	H-ESI: 1–1000 $\mu\text{L}/\text{min}$	All GLE models
	APCI: 100–2000 $\mu\text{L}/\text{min}$	
VeriSpray PaperSpray ion source	N/A	All GLE models

Compatible FAIMS interfaces

The FAIMS Pro and FAIMS Pro Duo interfaces are compatible with all the TSQ Series II mass spectrometers that are intended for general laboratory use (GLE models) except for the TSQ Fortis and TSQ Fortis Plus mass spectrometers.

Overview of an LC/MS Analysis

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

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

When the system setup includes a syringe pump and divert/inject valve, there are three additional ways to introduce samples into the MS, as described in [Table 3](#).

Table 3. Methods of sample introduction into the MS

Method	Description
Direct infusion	Connect the syringe pump directly to the API source of the MS. See “ H-ESI or low-flow H-ESI direct infusion ” on page 190.
High-flow infusion	Use a union Tee to combine the flow from the syringe pump with the flow from an LC pump. See “ High-flow infusion without an autosampler ” on page 193.
Manual loop injection	Connect a sample loop, a needle port fitting, and an LC pump to the divert/inject valve. After you fill the sample loop with sample, switch the position of the divert/inject valve, which places the contents of the sample loop in the path of the solvent flow produced by the LC pump. See “ Set up loop injections for a flow-injection analysis ” on page 195.

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

Tip For information about setting up the various sample introduction methods, see [Appendix D, “Sample introduction techniques.”](#)

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

Ionization of the sample takes place in the API source. The specific method that you use to ionize the sample is referred to as the ionization technique. The ion optics transmit the ions produced in the API source into the mass analyzer to determine their m/z values. The polarity of the electric potentials applied to the API source and ion optics determines whether positively charged ions or negatively charged ions are transmitted to the mass analyzer. You can set up data acquisition methods for the MS to analyze positively or negatively charged ions or to switch between these polarity modes during a single run. Each sequence of loading a mass analyzer with ions followed by mass analysis of the ions is called a scan.

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

Note For a list of ion sources that are compatible with your TSQ Series II mass spectrometer, see “Compatible ion sources” on page 27.

For information about the heated-electrospray (H-ESI), atmospheric pressure chemical ionization (APCI), and atmospheric pressure photoionization (APPI) techniques, refer to the user guide for your high-flow ion source. For information about the nanoelectrospray ionization (nanoESI or NSI) technique, refer to the user guide for your nanoflow ion source.

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

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

–or–

- The TSQ Series II mass spectrometers operate as tandem MS systems with two stages of mass analysis. The ion source ionizes the sample, and mass filtering of the ions occurs in the first rod assembly (Q1). In this case, however, mass-selected ions exiting the first rod assembly collide with an inert gas in the second rod assembly (Q2) and fragment to produce a set of ions known as product ions. (A chamber called the collision cell surrounds the second rod assembly. The MS pressurizes the collision cell with an inert gas.) The third rod assembly (Q3) performs mass filtering on the product ions to detect selected ions. Two stages of mass analysis yield far greater chemical specificity than a single analysis stage because of the system’s ability to select and determine two discrete but directly related sets of masses.

During a scan, the first stage of mass analysis elucidates the elemental compositions of pure organic compounds and the components within mixtures. Furthermore, in a scan sequence that involves a second stage of mass analysis, the MS can fragment and separate each ionic fragment of a molecule formed in the ion source to elucidate the structure of the molecule.

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

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

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

LED indicators

See [Figure 8](#) for the LED indicators on the front panel of the MS and [Table 4](#) for their descriptions.

Figure 8. LEDs on the front panel of the MS

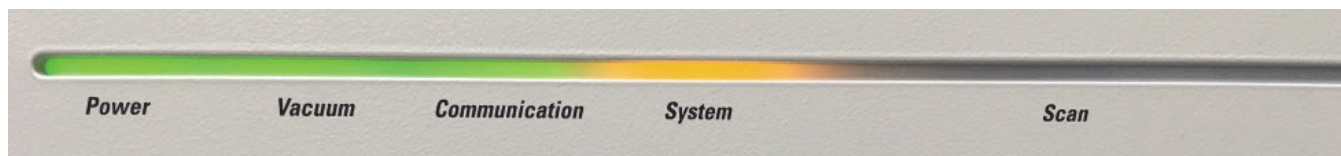


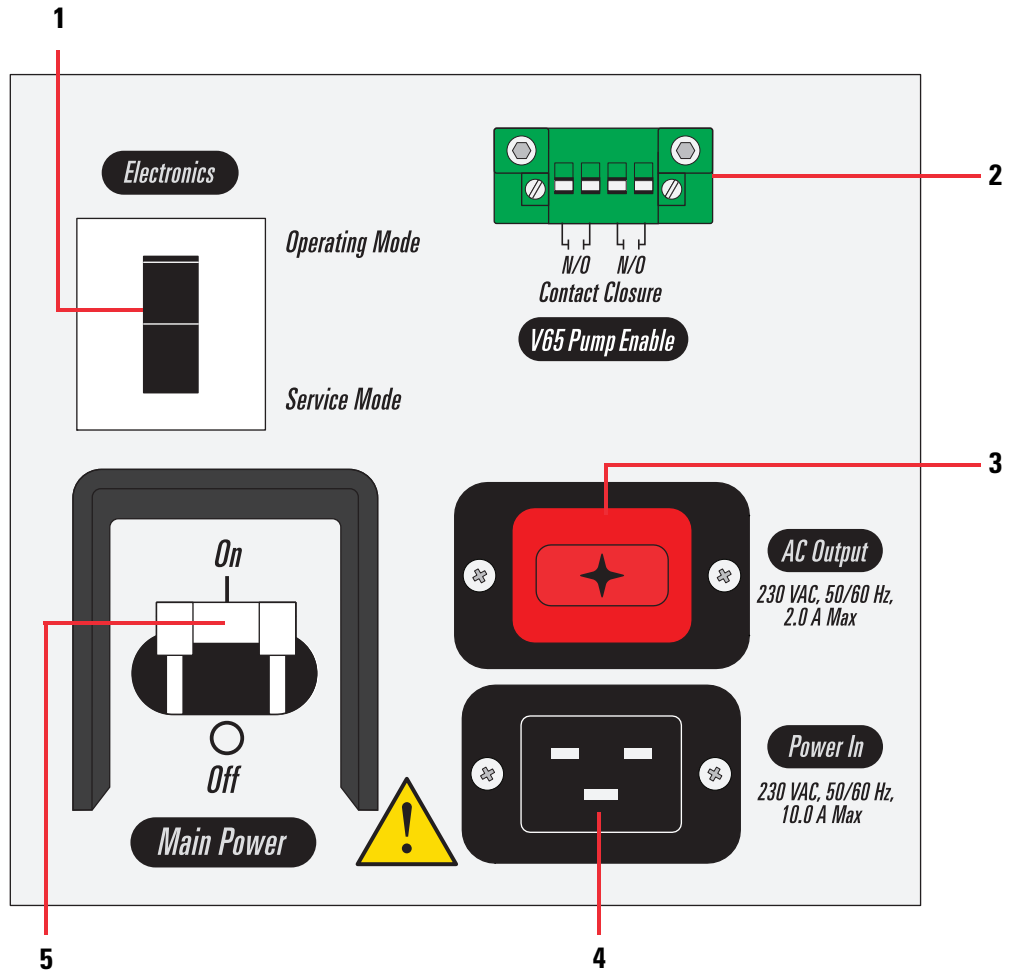
Table 4. Instrument front panel LEDs

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

Power entry module

The MS receives line power at 230 Vac \pm 10%, 5 A, 50/60 Hz through the right-side power entry module (Figure 9).

Figure 9. Power entry module (clockwise 1–5)



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

For more information, see the following topics:

- [Main Power switch](#)
- [Electronics service switch](#)
- [Mechanical pump/forepump enable connector](#)

Main Power switch

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

Placing the Main Power switch in the Off position turns off any forepump connected to the MS through contact closure, but it does not turn off line power to the forepumps, as they connect directly to the laboratory line power.



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

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.

Mechanical pump/forepump enable connector

The MS starts and stops the required forepump or forepumps (depending on the model) by using a relay control cable that connects to the forepump's contact closure connector.

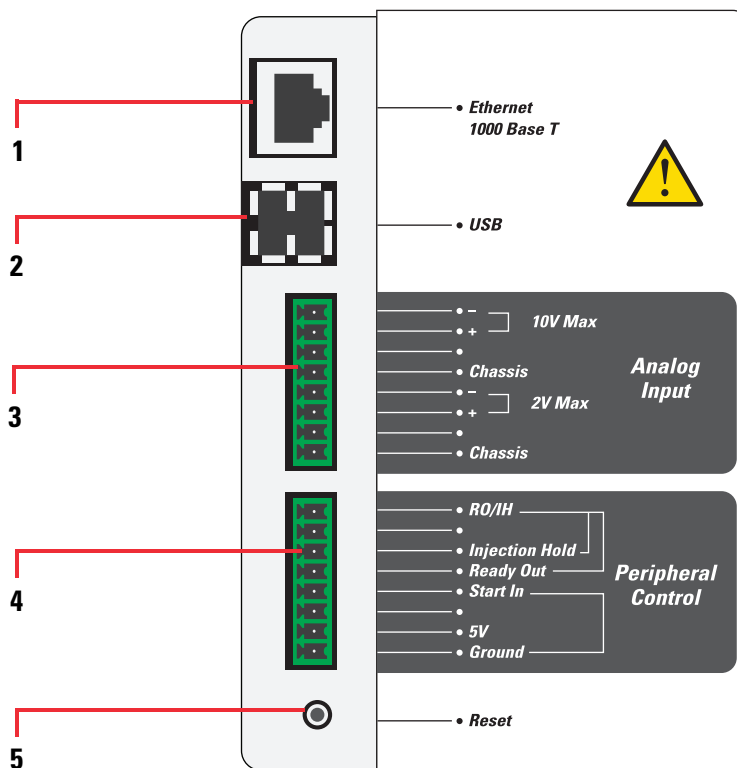
Communications panel

The communications panel, which is located in the recessed area on the right side of the MS, includes 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 computer. For more information about resetting the MS, see [“Reset the MS if it is not communicating with the data system”](#) on [page 92](#).

Figure 10 shows the communication connectors and the reset button.

Figure 10. Communication panel (right side of the MS)

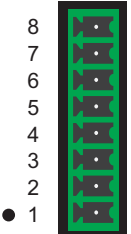



No.	Description
1	Ethernet port—Provides a connection to the Ethernet switch for the LC/MS system. The LC/MS system includes the data system computer, the MS, and the optional LC system.
2	USB ports—Provide a connection for the syringe pump and the divert/inject valve.
3	Analog Input connector—See Table 5 on page 35 .
4	Peripheral Control connector—See Table 6 on page 36 .
5	Reset button—Resets the instrument to a power-up state.

IMPORTANT Because pressing the reset button resets the instrument to the power-up state, press the reset 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.

Table 5 describes the function of the analog input pins.

Table 5. Pin-out descriptions for the analog connector

Pin	Name	Description
Analog Input		
Pin#		

The two analog channels (2V Max and 10V Max) 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)
2	Not used	
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)
6	Not used	
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)

Table 6 describes the function of the peripheral control pins.

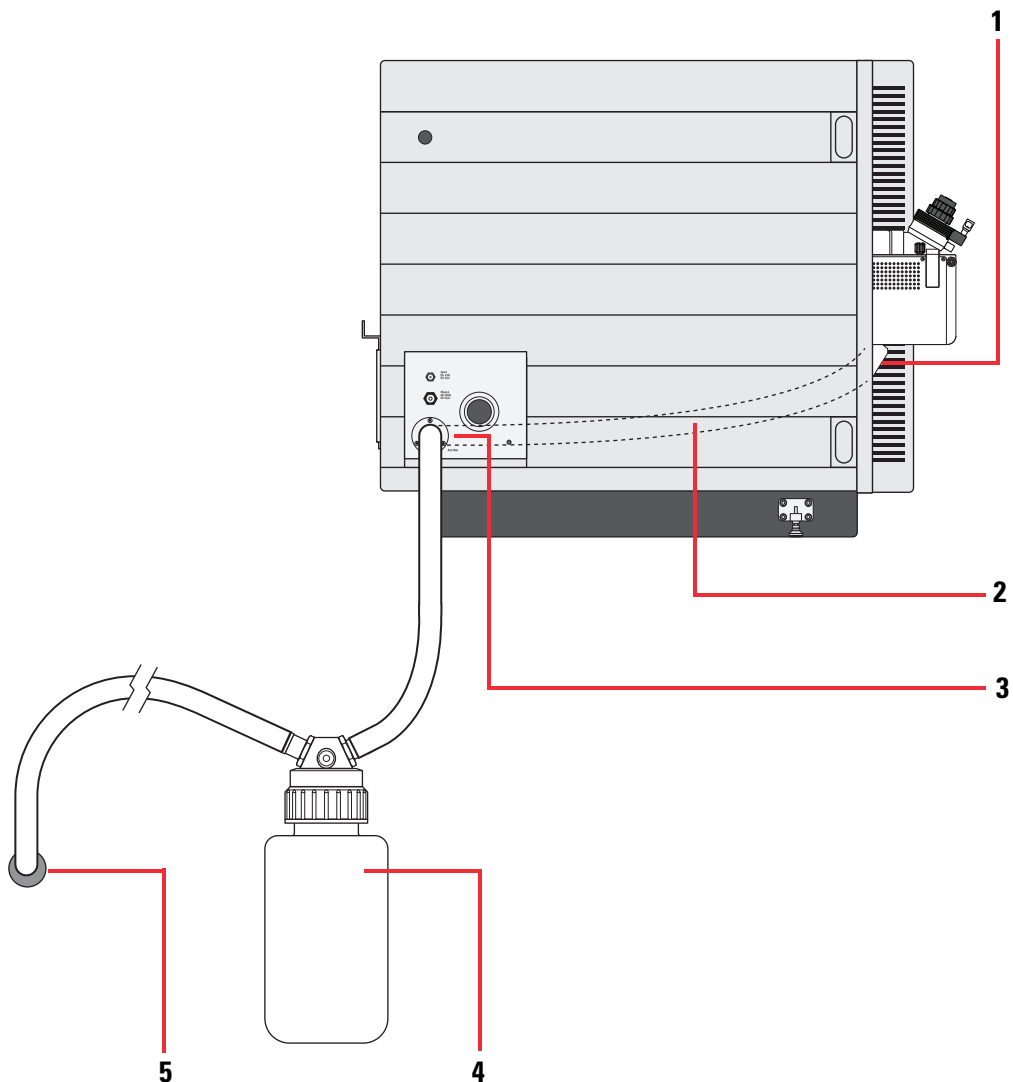
Table 6. Pin-out descriptions for the peripheral control connector

Pin	Name	Description
Peripheral Control		
1	Ground	Earth ground
2	5V	Provides a 5 Vdc, 500 mA output (with pin 1).
3	Not used	
4	Start In	<p>Receives the start signal from the contact closure connection of a connected external device.</p> <p>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.</p> <p>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.</p>
5	Ready Out	<p>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.</p> <p>Output: Maximum 24 Vdc, 3 A</p>
6	Injection Hold	<p>Provides a relay-driven programmable output signal to the connected external device, such as a fraction collector.</p> <p>Output: Maximum 24 Vdc, 3 A</p>
7	Not used	
8	RO/IH	Common (return) connection for the Ready Out and Injection Hold pins.

Drainage system

The drainage system for a TSQ Series II MS begins with the drainage port at the bottom of the API source interface on front panel of the MS and ends with the waste container that connects to the drain port on the left side of the MS. An internal pipeline connects the drainage port at the bottom of the API source interface to the drain port on the left side of the MS.

Figure 11. Drainage system



No.	Description	No.	Description
1	Drainage port below the API source interface	2	Internal drainage tubing
3	Drain/waste port on the left side of the MS	4	Waste container
5	Connection to a laboratory exhaust system		

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.

To ensure proper performance of the cooling system, maintain at least 10 inches of air space between the laboratory wall or other obstructions for the air intake fans on the right side of the MS and the ventilation slots on the back of the MS.

The only user-serviceable part of this cooling system is the air filter behind the front panel and in front of the air intake fans. For the recommended maintenance schedule, see [“Maintain the air filter”](#) on [page 170](#).



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

Scan parameters in the Tune and Method Editor windows

These topics describe some of the scan parameters that you set in the Tune application or the Method Editor.

- [Scan types](#)
- [Profile and centroid data](#)
- [Ion polarity modes](#)

Tip You can access the Tune application from the Windows desktop or Start menu. You can access the Method Editor from the Instrument Setup window of the Xcalibur data system, the Chromeleon chromatography data system, or the TraceFinder application.

Scan types

The TSQ Series II mass spectrometers 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, SIM Q1, and SIM Q3
- MS/MS scan types: Product Ion Scan, Precursor Ion Scan, Neutral Loss Scan, SRM, and QED scan type.

See these topics:

- [Quadrupole modes](#)
- [Summary of the quadrupole modes for the various scan types](#)
- [Full scan Q1 and Q3 scan types](#)
- [Selected ion monitoring scan type](#)
- [Product ion scan type](#)
- [Precursor scan type](#)

- [Neutral loss scan type](#)
- [Selected reaction monitoring scan type](#)
- [Quantitation enhanced data-dependent scan type](#)

Quadrupole modes

The TSQ Series II mass spectrometers have three rod assemblies. The first and third rod assemblies, Q1 and Q3, are hyperbolic quadrupoles. The second rod assembly, Q2, is a square-profile quadrupole.

Rod assemblies can operate in either of two modes:

- 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 the quadrupole modes for the various scan types

Table 7 provides a summary of the quadrupole modes by scan type.

Table 7. Summary of scan types (Sheet 1 of 2)

Scan type	Q1 quadrupole	Q2 collision cell	Q3 quadrupole
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; 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

Table 7. Summary of scan types (Sheet 2 of 2)

Scan type	Q1 quadrupole	Q2 collision cell	Q3 quadrupole
SRM scan	Set	Fragment ions; then pass all fragments.	Set
QED	Set	Fragment ions; then pass all fragments.	Set ^d

^a Scan means the full scan or transmission of a specified range of ions.

^b Pass all ions means pass ions or fragments within a wide range of m/z values without selectivity.

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

^d When the SRM intensity exceeds the user-set threshold, a single Product Ion scan is immediately acquired.

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 first 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 within a user-defined range. 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.)

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

To perform a SIM experiment or an SRM experiment, you must know what ions or reactions you are looking for. Therefore, you must determine the precursor ion for identifying your analytes before you set up a SIM experiment and the precursor and product ions for your analytes before you set up an SRM experiment. Once you determine these m/z values, you can use the SIM or SRM scan types to run routine quantitative analysis experiments on these analytes.

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 specific ions that are known to occur in the mass spectrum of the target analyte.

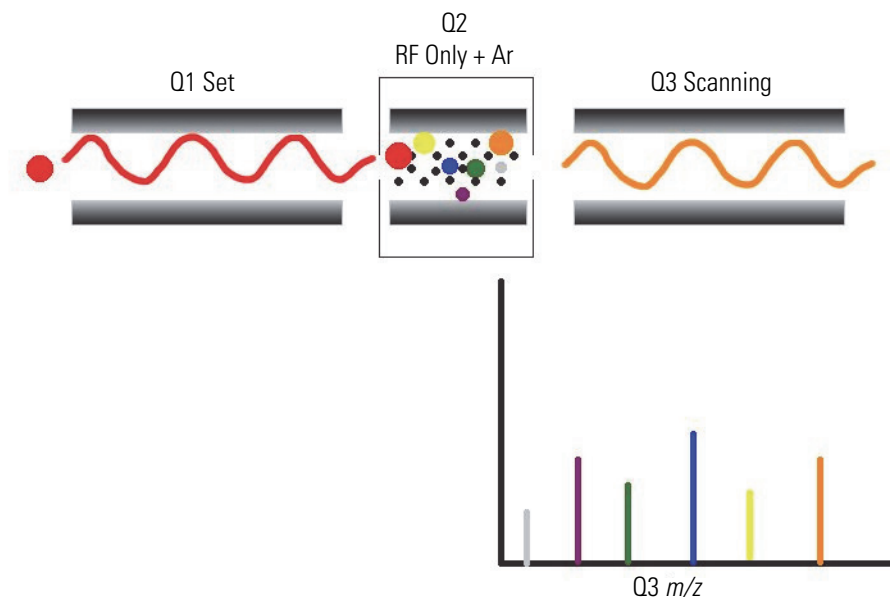
SIM can improve the detection limit and decrease analysis time, but it can also reduce specificity compared to SRM. Because SIM monitors only specific ions, any compound that is isobaric will appear to be the target compound, which can result in a false positive.

Product ion scan type

The product ion scan type performs two stages of analysis (Figure 12). In the first stage, the ion source forms ions that enter Q1, which is set to transmit ions of a specific 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, the collision cell.

In the second stage of analysis, ions in the collision cell can fragment 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.

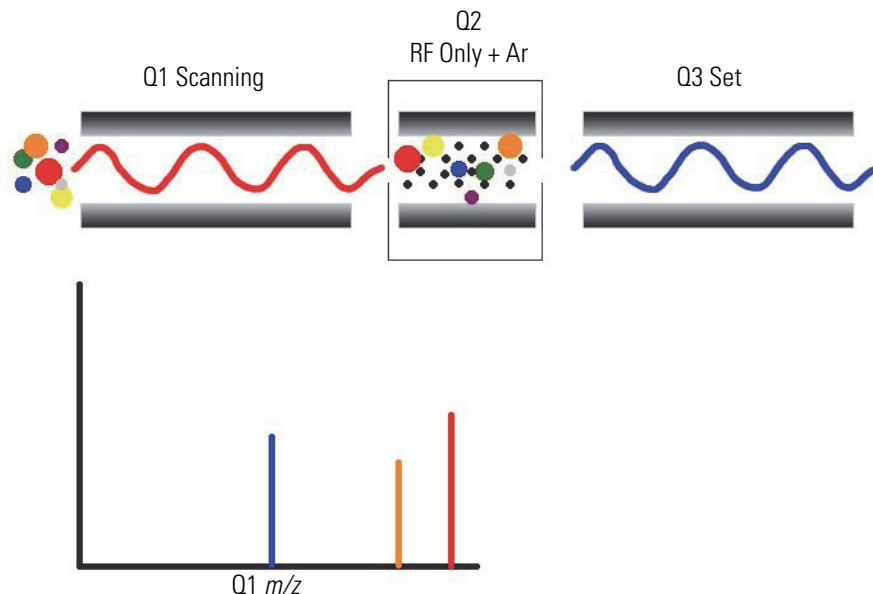
Figure 12. Illustration of the product scan type

Precursor scan type

The precursor scan type also uses two stages of analysis (Figure 13). 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 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 13. 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 14), 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 fragment 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. 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 15 shows an example common fragment ion.)

Figure 14. Illustration of the neutral loss scan type

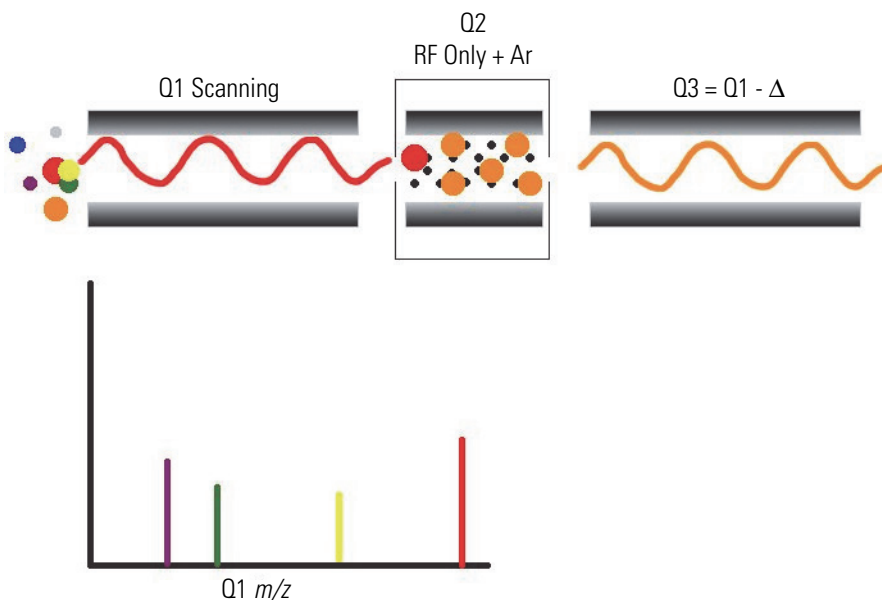
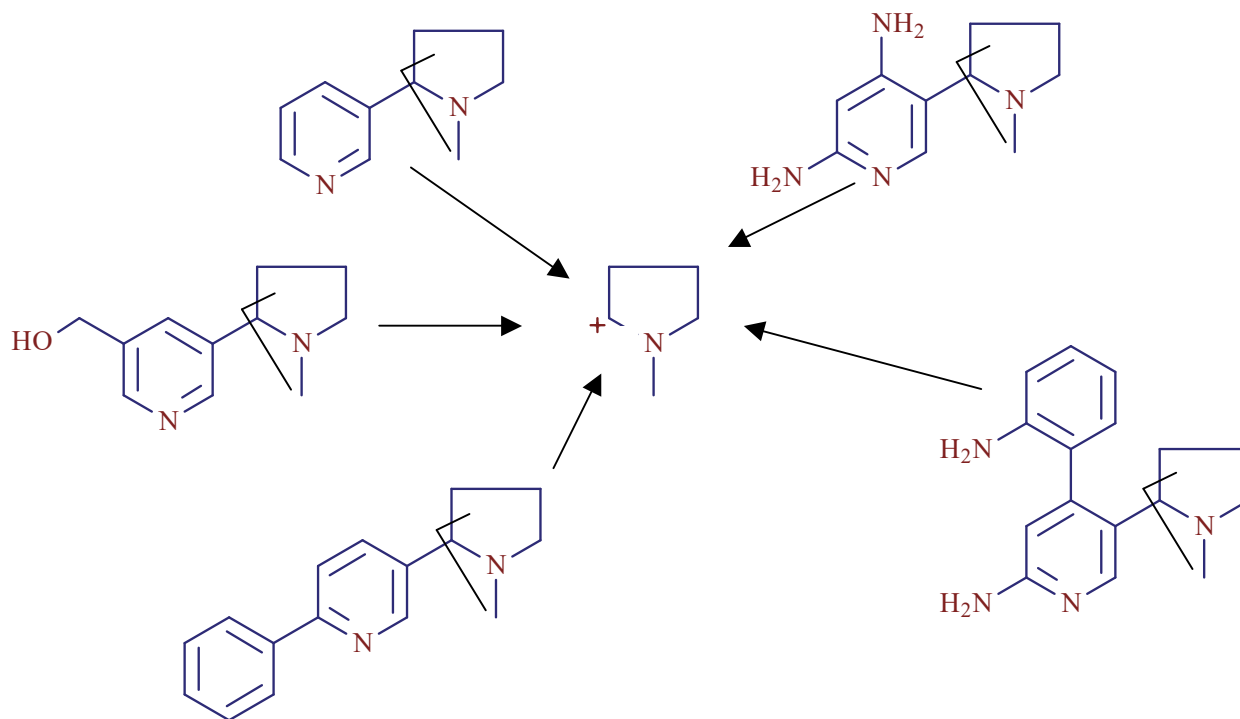


Figure 15. Examples of compounds with a common fragment

Selected reaction monitoring scan type

Selected reaction monitoring (SRM) is synonymous with triple-quadrupole mass spectrometry. SRM is a method where the following processes occur in the order listed:

1. The first quadrupole mass analyzer (Q1) selects and isolates a precursor ion of a specific mass-to-charge (m/z) value.
2. The collision cell (Q2) fragments the precursor ion to produce product ions.
3. The third quadrupole mass analyzer (Q3) sequentially selects and isolates the resulting product ions as they exit the collision cell.
4. The electron multiplier detects the product ions after they exit Q3.

In a similar way to SIM, SRM provides for very rapid analysis of trace components in complex mixtures. Additionally, the SRM provides greater selectivity, which gives greater sensitivity compared to SIM. This is because the SRM monitors a specific product ion from a specific precursor ion, which virtually eliminates any ions, but the specific precursor/product combination being monitored. Any interfering compound would have to form a precursor ion of the same m/z value 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 value as the selected product ion from the target compound.

Quantitation enhanced data-dependent scan type

Quantitation enhanced data-dependent (QED) is a real-time method that triggers a confirmational MS/MS scan near the chromatographic peak apex, which provides rich and high quality product ion spectra for compound confirmation with simultaneous quantitation.

When using QED, a full scan MS/MS mass spectrum is obtained by data-dependent scanning for confirmatory analysis during the SRM experiment that is used for routine quantitation. When a particular SRM transition reaches a user-set intensity threshold, the instrument automatically triggers QED, using an innovative technique called Reversed Energy Ramp (RER), which produces the high sensitivity product ion spectrum. The RER scan generates a highly sensitive, fragment-rich MS/MS spectrum that can be used to positively confirm the identity of a compound by comparing the product ion spectra against a spectral library.

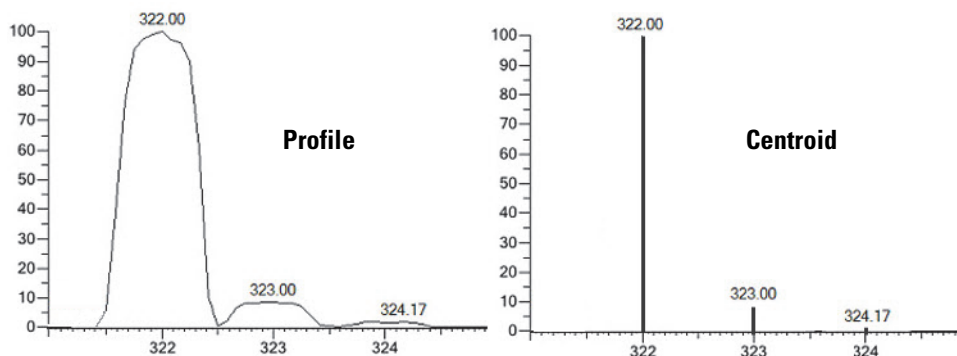
Profile and centroid data

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. 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 is that it requires about one-tenth the computer disk space of profile data. However, with centroid data, you lose information about the fine isotope features and the linearity of the ion signal.

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

Figure 16. Example of profile data on the left and centroid data on the right



Ion polarity modes

The TSQ Series II MSs can operate in either the positive or negative ion polarity mode. You can obtain positive ion scans, negative ion scans, or when using polarity switching, a combination of positive and negative ion scans. 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.

Functional description of the MS components

The following topics describe the principal components of the TSQ Series II mass spectrometers:

- [Vacuum system and inlet gases hardware and N2 gas flow paths](#)
- [Atmospheric pressure ionization source](#)
- [API source interface](#)
- [MP0 ion optics and neutrals blocker](#)
- [Mass analyzers and collision cell](#)
- [Ion detection system](#)

Vacuum system and inlet gases hardware and N2 gas flow paths

The vacuum system evacuates the region around the API source interface, ion optics, mass analyzer, and ion detection system. The inlet gas hardware controls the flow of collision gas, sheath gas, auxiliary gas, and air (during venting) into the MS.

See these topics:

- [Vacuum pumps](#)
- [Vacuum manifold](#)
- [Vacuum gauges](#)
- [Inlet gas supply hardware](#)
- [Sheath gas, auxiliary gas, and sweep gas flow paths](#)

Vacuum pumps

The forepump creates the vacuum necessary to properly operate the turbomolecular pump. It also evacuates the ion transfer tube region of the vacuum manifold. The 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.

Forepump requirements

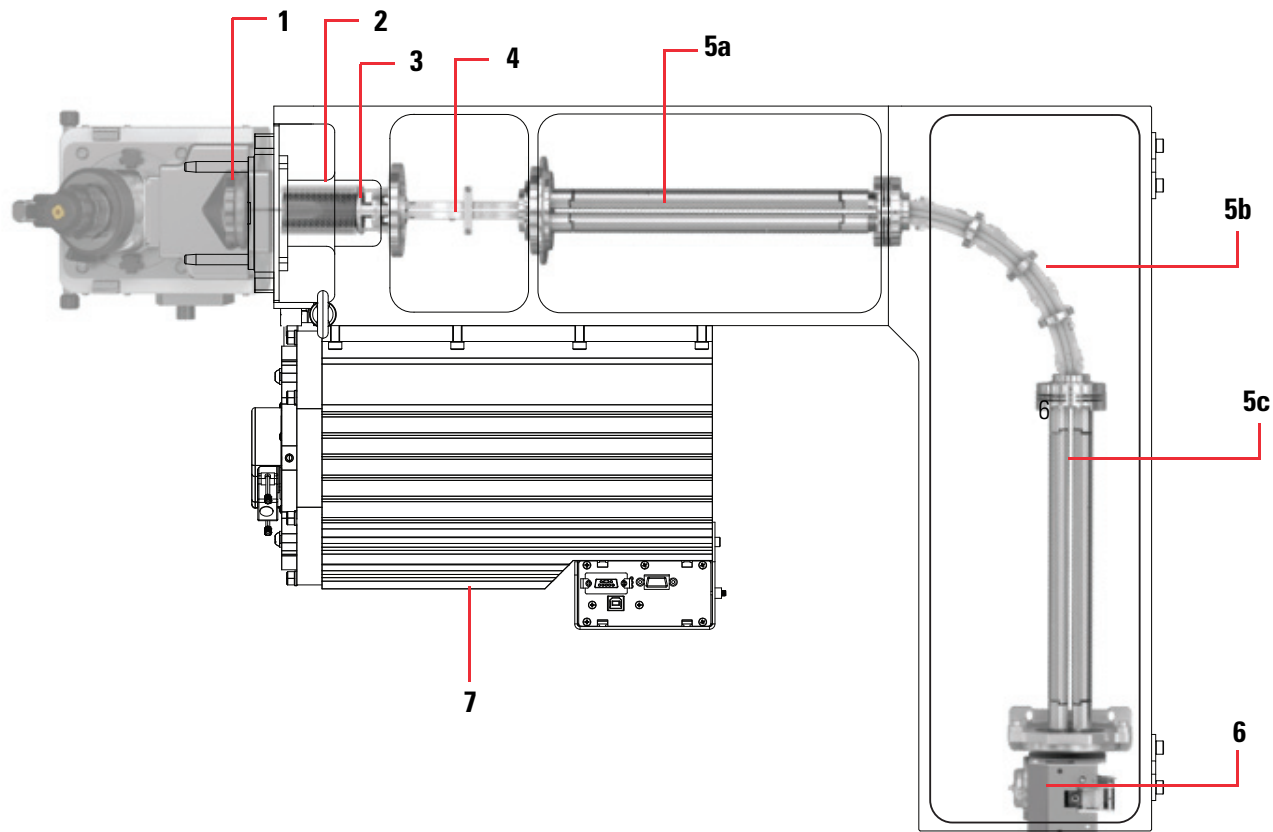
- The following TSQ Series II mass spectrometers (which use a transfer tube with a narrow bore) need one external forepump each:
 - TSQ Endura MS
 - TSQ Fortis Plus MS
 - TSQ Fortis MS
 - TSQ Quantis Plus MS
 - TSQ Quantis MS
- The following TSQ Series II mass spectrometers (which use a high-capacity transfer tube with an elongated bore) need two external oil forepumps or one external dry pump each:
 - TSQ Altis Plus MS
 - TSQ Altis MS
 - TSQ Quantiva MS

Note Dry pumps are an option for the TSQ Series mass spectrometers. The dry pumps are Leybold EcoDry 65 Plus vacuum pumps and Edwards nXL110i vacuum pumps. The oil pumps are Leybold model SV65BIFC vacuum pumps.

Vacuum manifold

Figure 17 shows the vacuum manifold with the top cover plates removed next to the turbomolecular pump. 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 17. Placement of the turbomolecular pump next to the vacuum manifold



No.	Description	No.	Description
1	API source interface	2	RF lens and ion transfer tube chamber
3	MP00 ion optics chamber	4	MP0 ion optics chamber (also known as Q0)
5a	Q1 mass analyzer chamber	5b	Q2 collision cell
5c	Q3 mass analyzer chamber	6	Ion detector
7	Turbomolecular pump		

Table 8 lists the typical pressures in region 2 (which is evacuated by the forepump or forepumps) and region 5 (which is evacuated by the triple-inlet turbomolecular pump).

Table 8. Typical pressures in regions 2 and 5

MS Model	Region 2 Source Pressure readback	Region 5 Analyzer Pressure readback
TSQ Altis Plus	3–4 Torr	$3-7 \times 10^{-6}$ Torr
TSQ Quantis Plus	1–2 Torr	$2-6 \times 10^{-6}$ Torr
TSQ Fortis Plus	1–2 Torr	$1-6 \times 10^{-6}$ Torr
TSQ Altis	3–4 Torr	$3-7 \times 10^{-6}$ Torr
TSQ Quantis	1–2 Torr	$2-6 \times 10^{-6}$ Torr
TSQ Fortis	1–2 Torr	$1-6 \times 10^{-6}$ Torr
TSQ Quantiva	$2-6 \times 10^{-6}$ Torr	$3-7 \times 10^{-6}$ Torr
TSQ Endura	$3-7 \times 10^{-6}$ Torr	$2-6 \times 10^{-6}$ Torr

Vacuum gauges

Two types of vacuum gauges measure the pressure in specific regions of the vacuum manifold.

- Convectron pressure gauge—Measures pressure down to a fraction of a milliTorr (mTorr). The instrument uses two convection gauges:
 - Source pressure gauge—Measures the pressure in the RF lens and ion transfer tube region in the vacuum manifold.
 - Collision gas pressure gauge—Measures the pressure in the collision cell.
- Ionization gauge—Measures the pressure in the analyzer region of the vacuum manifold. To measure the pressure, the ionization gauge produces energetic electrons that cause the ionization of residual molecules. 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.

In the Tune application, you can observe the readback values for the vacuum gauges in the Status pane (under Vacuum) on the By Function page.

Inlet gas supply hardware

The inlet gas hardware includes the following components:

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

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

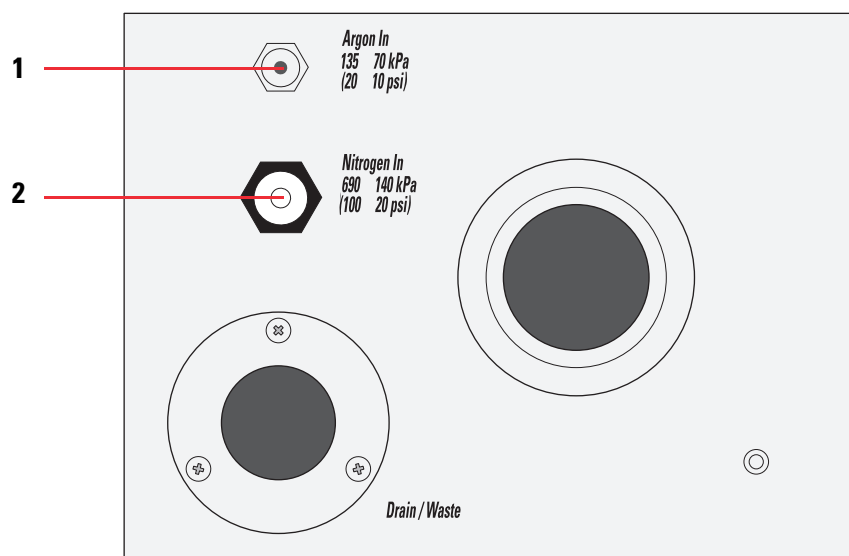
- Nitrogen Gas Valves—The data system controls the valves that regulate the nitrogen pressure. You can set the gas flow rates in the Ion Source pane of the Tune application.

Dry nitrogen gas (690 ± 140 kPa [100 ± 20 psi], 99% purity) enters the left side of the MS through a 1/4 in. port. The valves for the sheath, auxiliary, and sweep gases control the flow of dry nitrogen gas into the API source. For information about the purpose of the three nitrogen gas flows, see “Sheath gas, auxiliary gas, and sweep gas flow paths” on page 53.

- 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.

The external gas line connections are on the left side of the MS.

Figure 18. Gas inlets (on the left side of the MS)



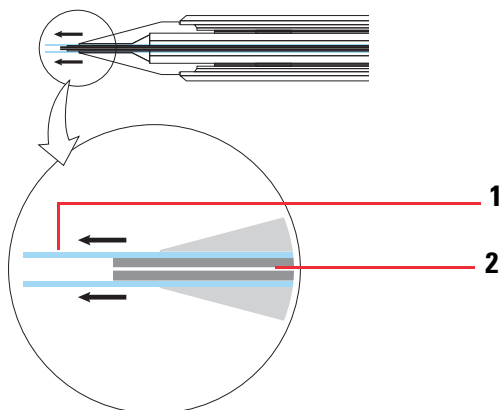
No.	Description	No.	Description
1	Argon gas inlet	2	Nitrogen gas inlet

Sheath gas, auxiliary gas, and sweep gas flow paths

You can apply nitrogen gas at the API source by using any combination of the three gas sources: Sheath gas, Auxiliary gas, and (optional) Sweep gas.

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.

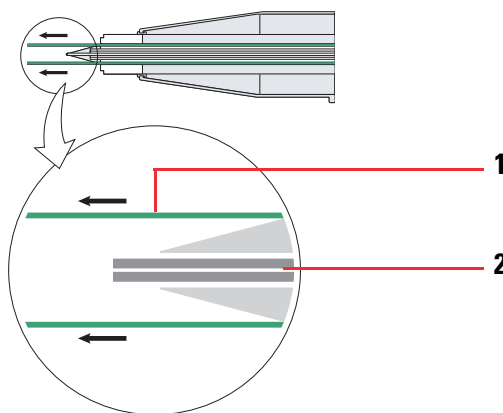
Figure 19. Sheath gas flow for ESI source (blue lines)



No.	Description	No.	Description
1	Sheath gas	2	Electrospray needle

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.

Figure 20. Auxiliary gas flow (green lines)



No.	Description	No.	Description
1	Sheath gas	2	Electrospray needle

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.

All analyses are analyte dependent and require separate optimization with sheath gas, sweep gas, and auxiliary gas to determine which combination yields optimum performance. Optimize with each gas independently before you perform experiments using MSⁿ techniques and before you perform any quantitative analysis experiments.

For higher LC flow rates, apply auxiliary gas to increase the signal intensity.

When you are analyzing complex matrices such as plasma or nonvolatile salt buffers, you must use sweep gas to increase the ruggedness of the system. For full-scan MS or data-dependent scan experiments, apply sweep gas to improve the signal-to-noise ratio.

Atmospheric pressure ionization source

The API source forms gas phase sample ions from sample molecules that are contained in solution. The API source also serves as the interface between the LC and the MS. You can use the ion source that comes with your TSQ Series II mass spectrometer to use the heated electrospray ionization technique (H-ESI).

Note For information about all the compatible ion sources for your instrument, see “Compatible ion sources” on page 27.

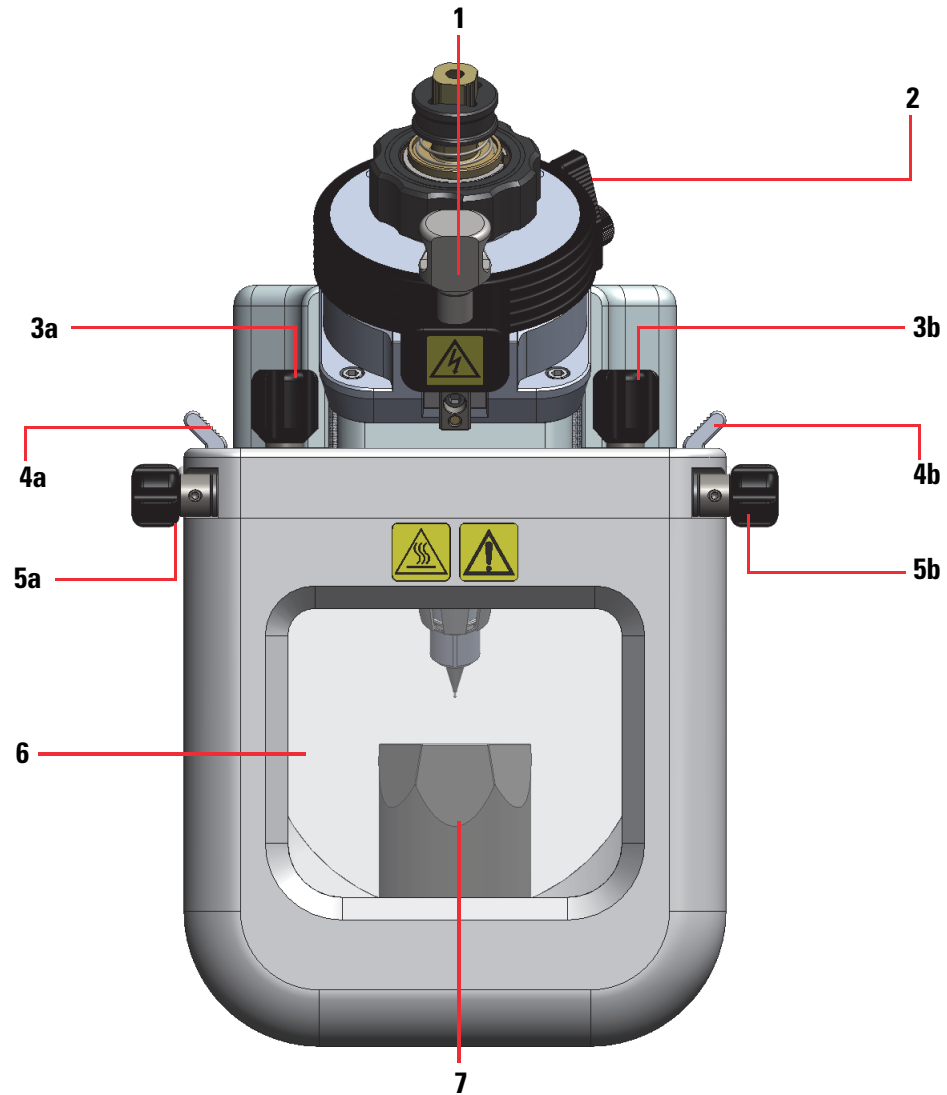
To run the mass spectrometer in the APCI mode or the APPI mode with the OptaMax NG ion source, you must order additional kits. Refer to the *OptaMax NG Ion Source User Guide* for ordering information.

The optional Thermo Scientific VeriSpray PaperSpray ion source that is compatible with the TSQ Series II mass spectrometers does not use an external LC system and autosampler to introduce sample into the ion source.

The MS has a built-in drain at the front of the system that routes the solvent waste from the API source to the solvent waste container connected to the left-side drain/waste port. For information about the solvent waste connection, refer to the getting connected guide for your mass spectrometer.

The TSQ Endura MS shipped with the EASY-Max NG™ ion source, and the TSQ Quantiva MS shipped with the Ion Max NG™ ion source. The Ion Max NG ion source has an additional feature for adjusting the depth of the spray insert that the EASY-Max NG ion source lacks.

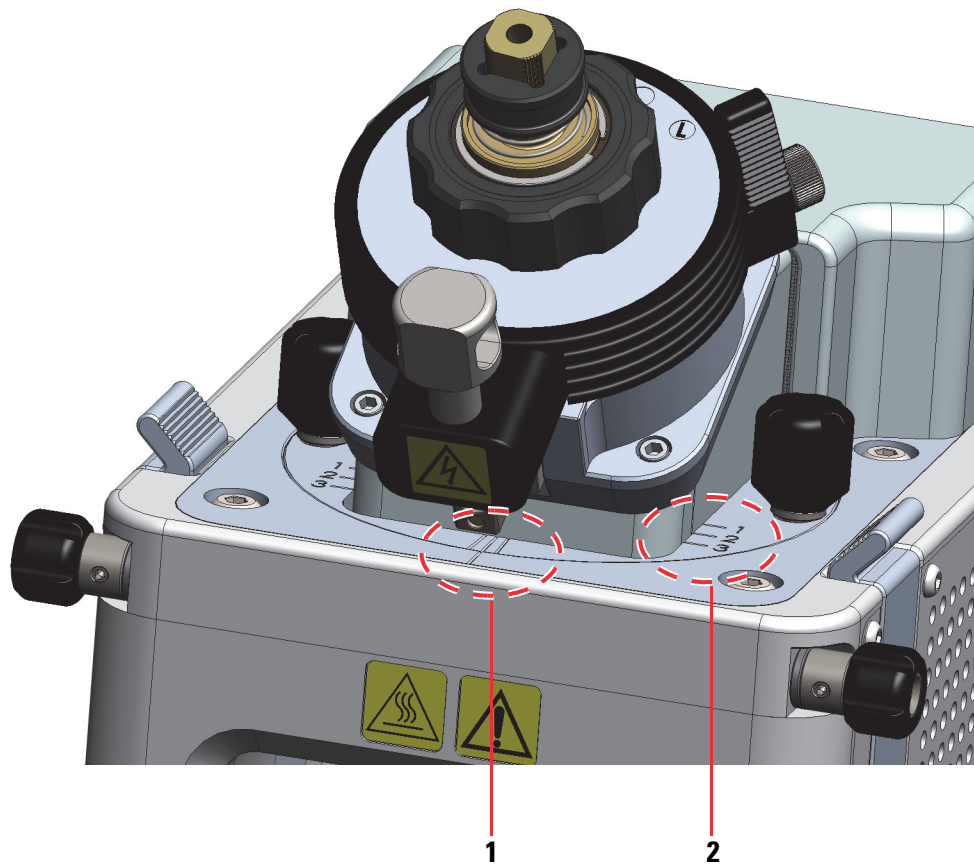
Figure 21. Ion Max NG ion source from the front



No.	Description	No.	Description
1	Grounding union holder	2	API spray insert depth adjustment knob
<p>Note The EASY-Max NG ion source does not have a depth adjustment knob.</p>			
3a	Left retainer knob for the API spray insert and heater assembly	3b	Right retainer knob for the API spray insert and heater assembly
4a	Left locking lever (locked position)	4b	Right locking lever (locked position)
5a	Left-to-right adjustment knob	5b	Right-to-left adjustment knob
6	Window	7	Drain insert

Figure 22 shows the position markers on the Ion Max NG ion source.

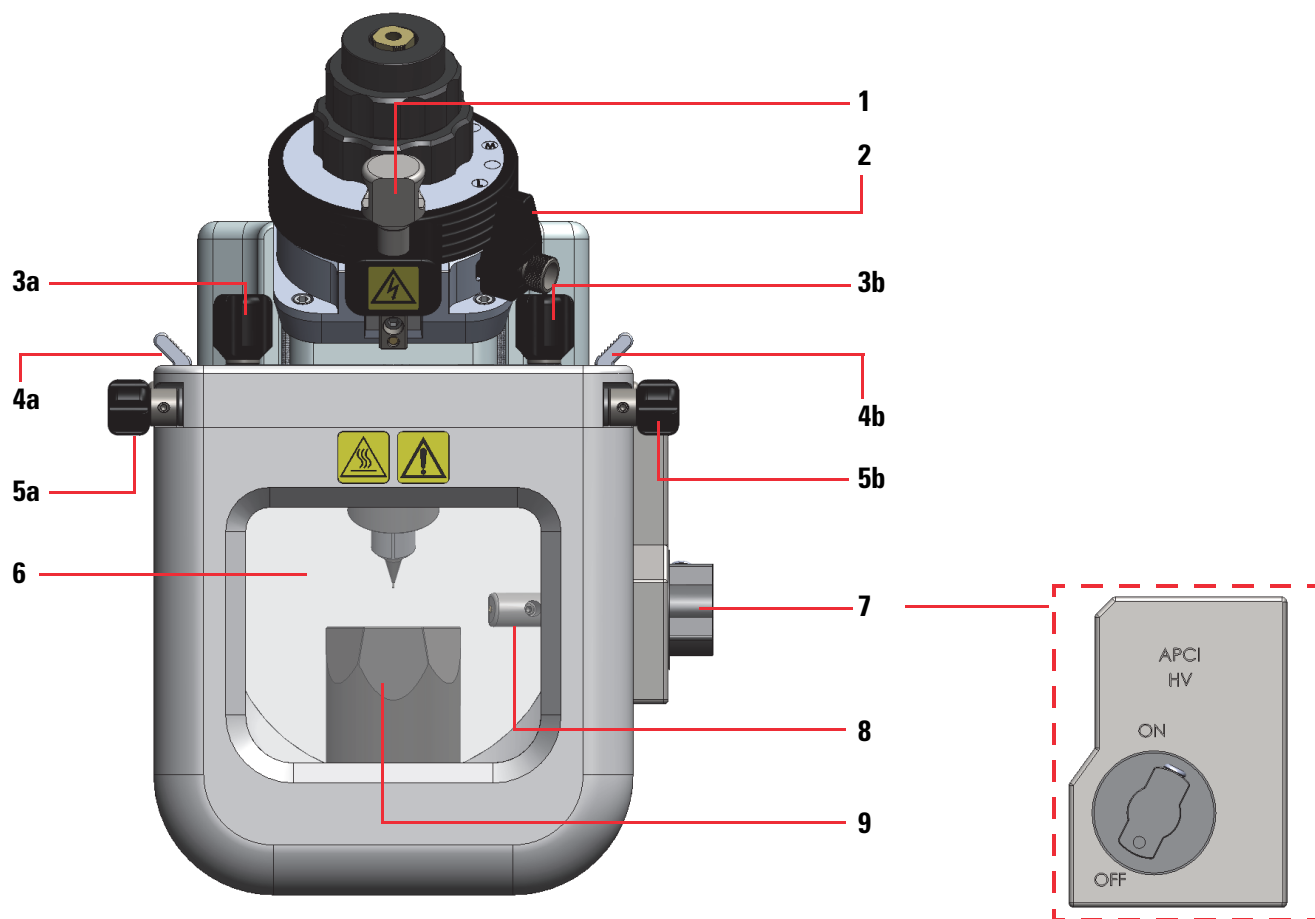
Figure 22. Left-to-right (1) and front-to-back (2) position markers on the Ion Max NG ion source



With the exception of the TSQ Endura MS (which only ships to selected countries), all the models in the TSQ Series II product line that are currently shipping come with the OptaMax NG ion source.

The OptaMax NG ion source is APCI ready; that is, it has a built-in corona discharge needle mount inside the housing and an APCI On/Off control knob on the exterior right side of the housing. See Figure 23.

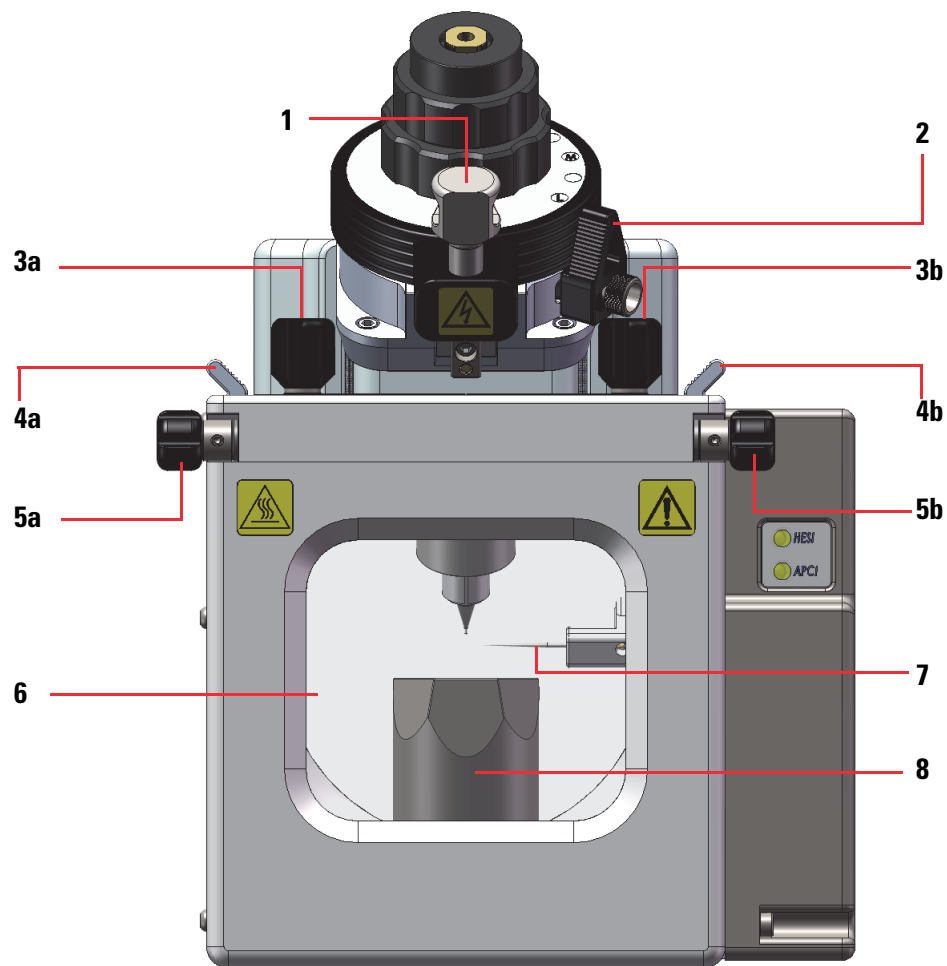
Figure 23. OptaMax NG ion source from the front



No.	Description	No.	Description
1	Grounding union holder	2	API spray insert depth adjustment knob
3a	Left retainer knob for the API spray insert and heater assembly	3b	Right retainer knob for the API spray insert and heater assembly
4a	Left locking lever (locked position)	4b	Right locking lever (locked position)
5a	Left rotational adjustment knob	5b	Right rotational adjustment knob
6	Window	7	APCI On/Off knob
8	APCI needle mount	9	Drain insert

The OptaMax Duet ion source is a separate option that you can purchase from Thermo Fisher Scientific. The OptaMax Duet ion source includes depth and side-to-side adjustment for the API spray insert. It also includes a built-in corona discharge needle that you can turn on or off from the software controls. See [Figure 24](#).

Figure 24. OptaMax Duet NG ion source from the front



No.	Description	No.	Description
1	Grounding union holder	2	API spray insert depth adjustment knob
3a	Left retainer knob for the API spray insert and heater assembly	3b	Right retainer knob for the API spray insert and heater assembly
4a	Left locking lever (locked position)	4b	Right locking lever (locked position)
5a	Left side-to-side adjustment knob	5b	Right side-to-side adjustment knob
6	Window	7	Corona discharge needle for the APCI mode
8	Drain insert		

API source interface

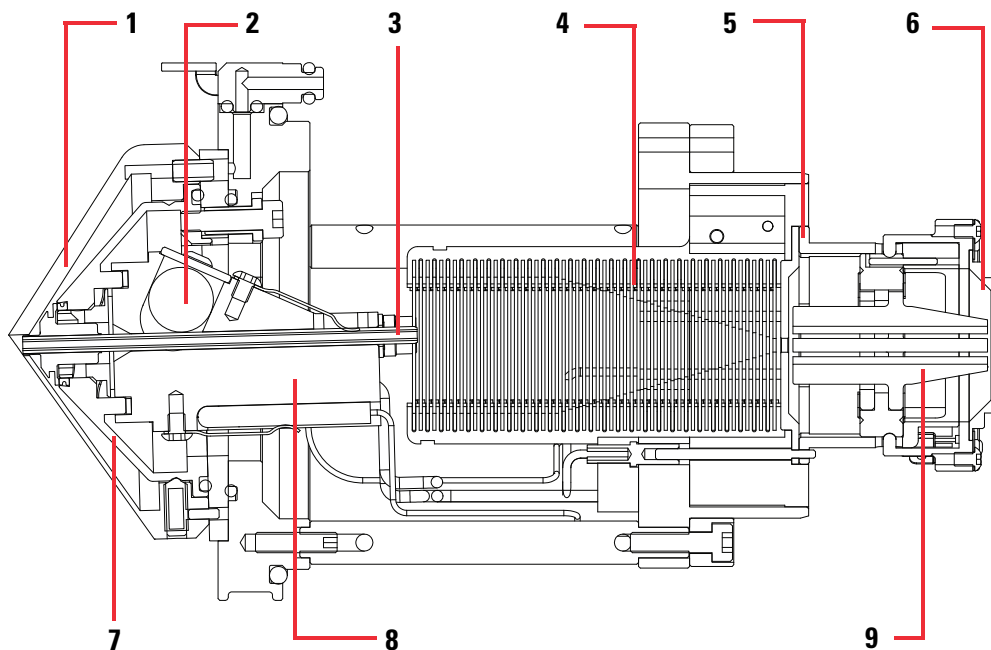
The following topics describe the components of the API source interface:

- Ion sweep cone
- Spray cone
- Ion transfer tube
- Heater block
- Vent prevent ball
- RF lens and exit lens
- Tube lens and skimmer (TSQ Fortis and TSQ Fortis Plus)
- MP00 ion optics – MP00 multipole and L0 lens

Except for the atmospheric pressure side of the spray cone and the nose cone of the ion transfer tube that is within the API source, the API source interface components are located in a vacuum chamber.

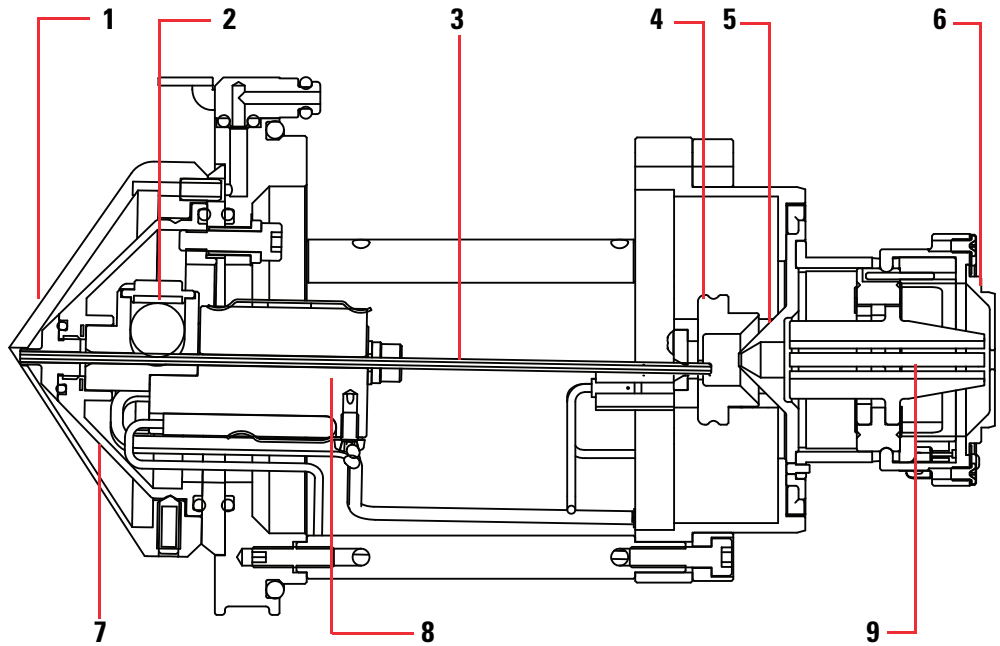
The following figures show cross-section schematics of the API source interface:

- [Figure 25](#) shows the API source interface for the TSQ Altis Plus MS and the TSQ Altis MS. The API source interface for the TSQ Quantiva MS is similar to this source.
- [Figure 26](#) shows the API source interface for the TSQ Fortis Plus MS and the TSQ Fortis MS.
- [Figure 27](#) shows the API source interface for the TSQ Endura MS. The API source interface for the TSQ Quantis Plus MS and the TSQ Quantis MS is similar to this source.

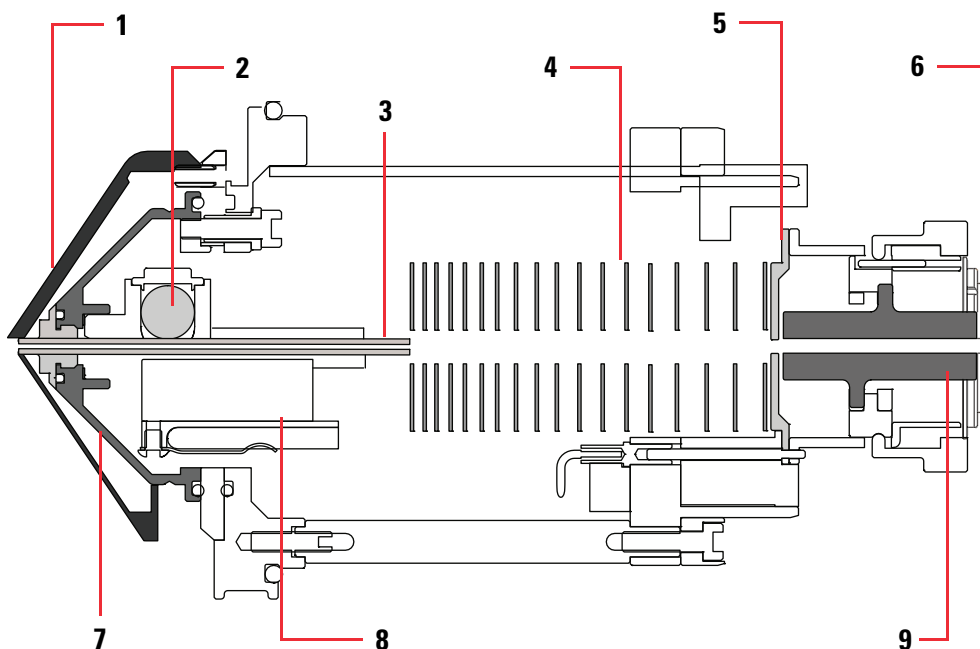
Figure 25. API source interface for the TSQ Altis Plus MS and TSQ Altis MS (cross section)

No.	Description	No.	Description	No.	Description
1	Ion sweep cone	2	Vent prevent ball	3	Ion transfer tube
4	Electrodynamic Ion Funnel (EDIF)	5	Exit lens	6	L0 lens
7	Spray cone	8	Heater block	9	MP00 multipole

Figure 26. API source interface for the TSQ Fortis Plus MS and 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	MP00 multipole

Figure 27. API source interface (TSQ Endura MS cross section)

No.	Description	No.	Description	No.	Description
1	Ion sweep cone	2	Vent prevent ball	3	Ion transfer tube
4	Stacked Ring Ion Guide (SRIG)	5	Exit lens	6	L0 lens
7	Spray cone	8	Heater block	9	MP00 multipole

Ion sweep cone

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 the mass spectrometer (MS) can 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.

IMPORTANT You must remove the ion sweep cone before performing nanospray ionization (NSI) experiments or installing the FAIMS interface.

Spray cone

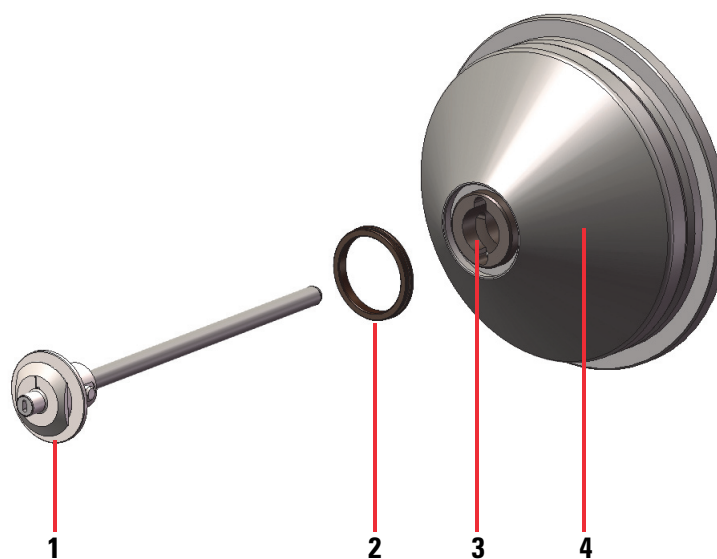
The spray cone is an integral component of the API source interface cage. The ion transfer tube fits through a small orifice in the center of the spray cone. A graphitized Vespel™ seal acts as a seal between the spray cone and the back of the ion transfer tube's nose cone.

The custom tool that you use to remove and install the ion transfer tube depends on whether the ion transfer tube is secured to the spray cone with a quarter-turn pin or a threaded fitting.

The following TSQ Series II mass spectrometers use an ion transfer tube that is secured with a quarter-turn pin:

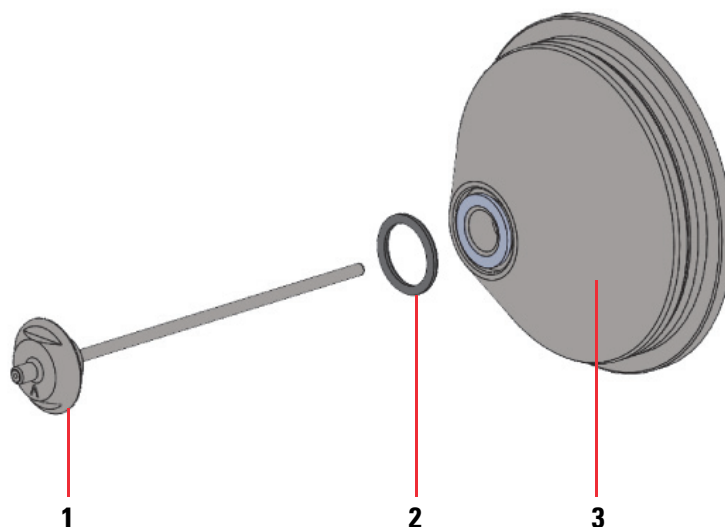
- TSQ Altis Plus
- TSQ Altis
- TSQ Quantiva

Figure 28. Spray cone (with a quarter-turn bushing) with the ion transfer tube and graphitized Vespel O-ring removed



No.	Description	No.	Description
1	High-capacity ion transfer tube for the TSQ Altis Plus MS and the TSQ Altis MS	2	Graphitized Vespel seal
<p>Note The ion transfer tube for the TSQ Quantiva MS is also a high-capacity transfer tube, but its nose cone does not have any etchings. See “Ion transfer tube” on page 65.</p>			
3	Bushing for the quarter-turn ion transfer tube	4	Spray cone

Figure 29. Spray cone with the ion transfer tube and O-ring removed (TSQ Quantis Plus and TSQ Quantis)



No.	Description	No.	Description
1	Ion transfer tube for the TSQ Quantis Plus MS and the TSQ Quantis MS	2	Graphitized Vespel seal
<p>Note The ion transfer tubes for the TSQ Endura MS, TSQ Fortis Plus MS, and TSQ Fortis MS are also secured to the spray cone with a threaded fitting.</p>			
3	Spray cone with a threaded entry port. See Figure 30 on page 68 .		

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 mass spectrometer (MS).

For information about maintaining the ion transfer tube, see [“Maintain the external components of the API source interface.”](#) For information about ordering a new ion transfer tube, see [“API source interface replaceable parts.”](#)

Table 9. Descriptions of the ion transfer tubes in the TSQ Series II mass spectrometers (Sheet 1 of 2)

TSQ Series II model	Ion transfer tube description
TSQ Altis and TSQ Altis Plus	<p>The high-capacity transfer tube (HCTT) for these mass spectrometers is a short tube with a stadium-shaped orifice (1). Its internal bore has a non-circular cross section (1), and its nose cone has the letter L etched into its front face. This etched letter lets you quickly identify the high-capacity transfer tube. A quarter-turn pin (2) behind the nose cone secures the tube to the API source interface.</p>
TSQ Quantiva	<p>The ion transfer tube is a short tube with a stadium-shaped (1) orifice (non-circular bore). A quarter-turn pin (2) behind the nose cone secures the tube to the API source interface.</p>

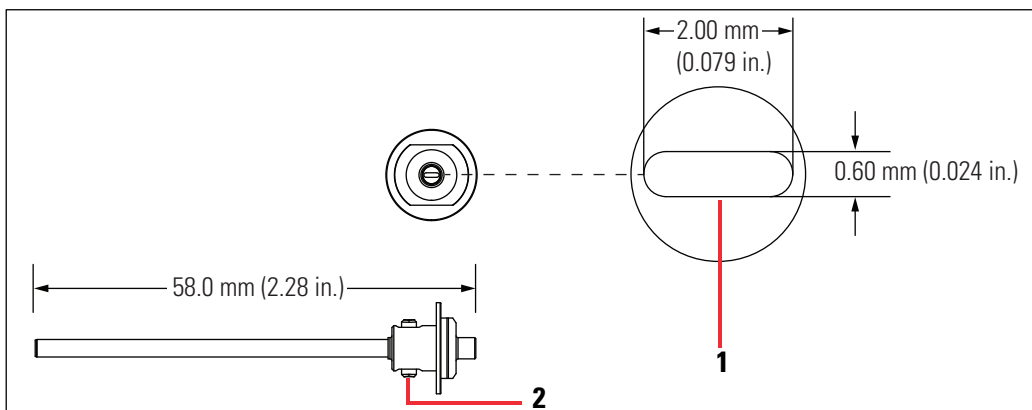
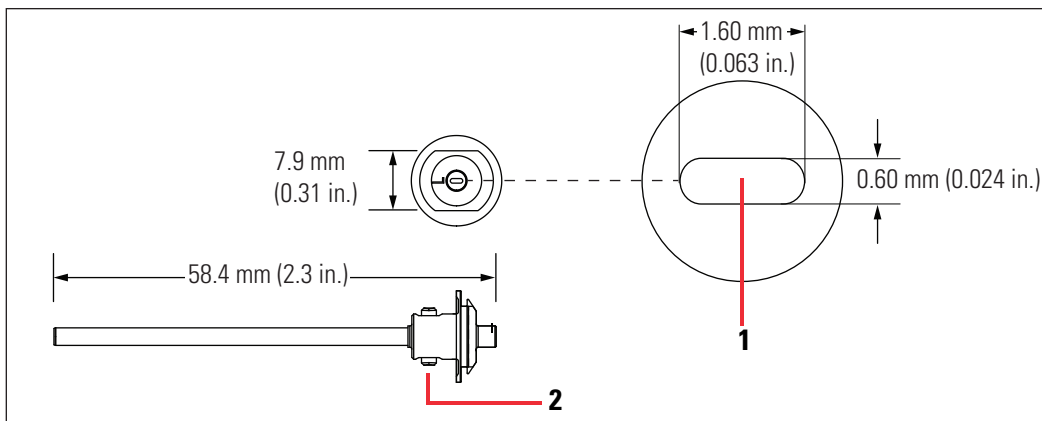
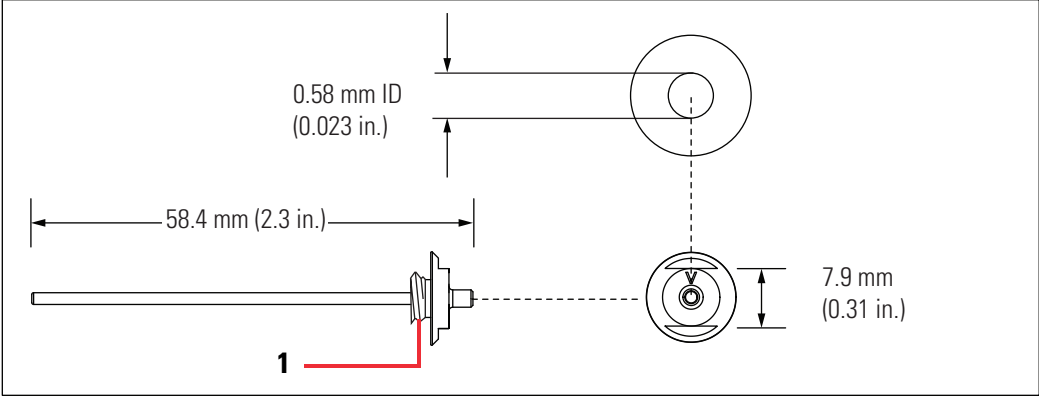
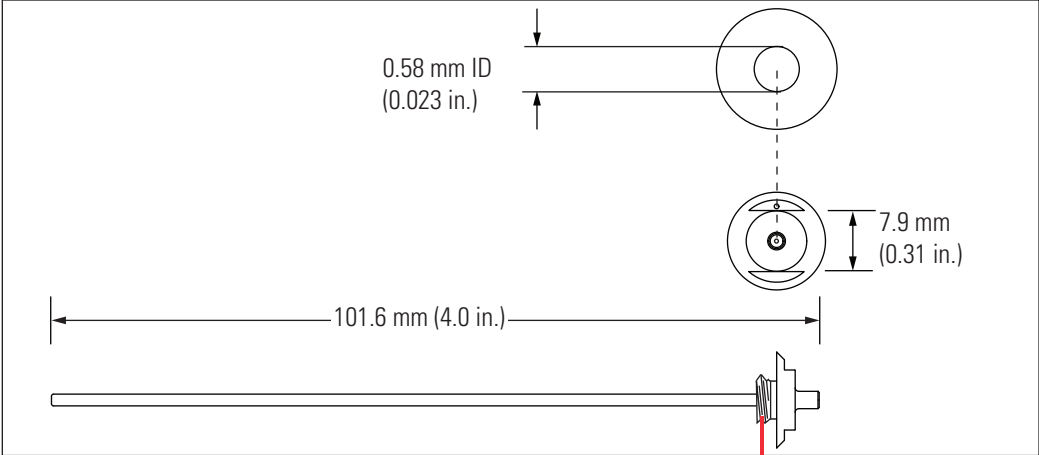


Table 9. Descriptions of the ion transfer tubes in the TSQ Series II mass spectrometers (Sheet 2 of 2)

TSQ Series II model	Ion transfer tube description
TSQ Quantis, TSQ Quantis Plus, and TSQ Endura	<p>The ion transfer tube is a short tube with a cylindrical bore (circular cross section). The nose cone has the letter V etched into its front face. The threading (1) behind the nose cone secures the tube to the API source interface.</p> 
TSQ Fortis and TSQ Fortis Plus	<p>The ion transfer tube is a long tube with a cylindrical bore (circular cross section). The threading (1) behind the nose cone secures the tube to the API source interface.</p> 

Heater block

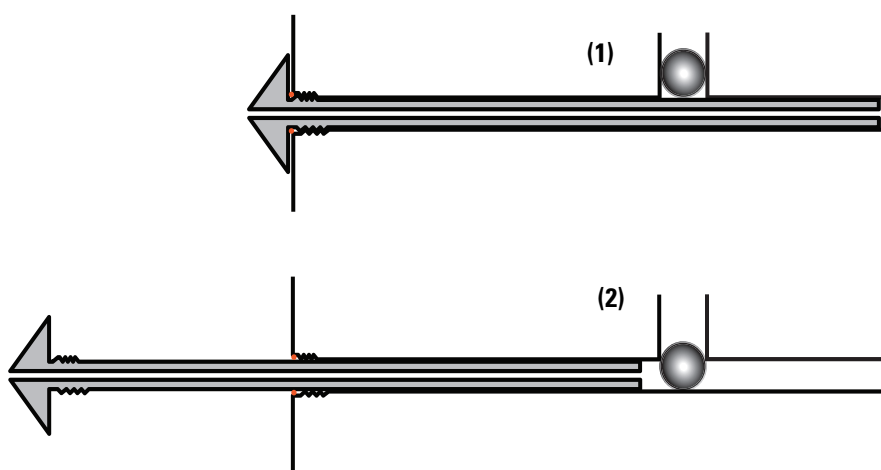
The heater block of the API source interface contains two heater cartridges that surround the ion transfer tube and heat the tube to temperatures up to 400 °C (752 °F). A decreasing pressure gradient draws ions into the ion transfer tube in the atmospheric pressure region.

Vent prevent ball

When you remove the ion transfer tube (after it has cooled to room temperature), the vent prevent ball of the API source interface drops into place to stop air from entering the vacuum manifold. By acting as a barrier, the vent prevent ball lets you remove the ion transfer tube for cleaning or replacement without venting the system.

For information about cleaning or replacing the ion transfer tube, see “[Maintain the external components of the API source interface](#)” on page 144.

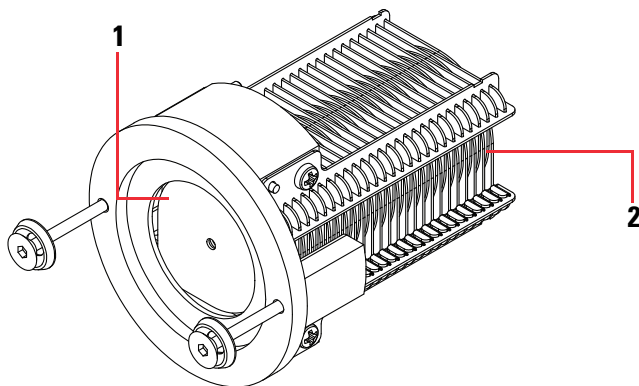
Figure 30. Vent prevent ball positions: (1) installed ion transfer tube and (2) ion transfer tube being removed



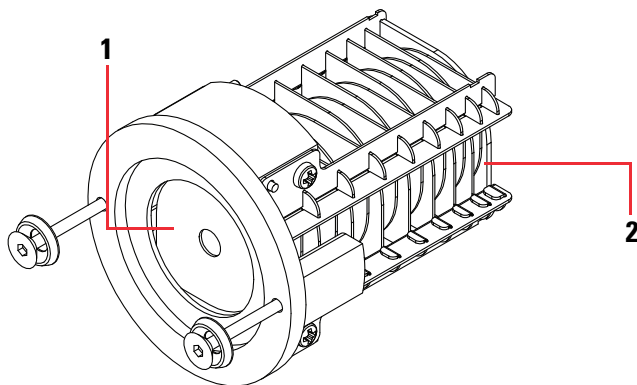
RF lens and exit lens

The API source interface for all the TSQ Series II mass spectrometers except for the TSQ Fortis MS and TSQ Fortis Plus MS includes an RF lens and an exit lens.

Ions from the ion transfer tube pass through the RF lens and then the exit lens (Figure 31 and Figure 32). 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 31. RF lens and exit lens for the TSQ Altis MS, TSQ Altis Plus MS, and TSQ Quantiva MS

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

Figure 32. RF lens and exit lens for the TSQ Quantis MS, TSQ Quantis Plus MS, and TSQ Endura MS

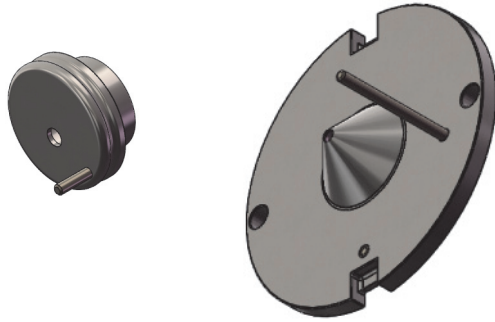
No.	Description	No.	Description
1	Exit lens	2	RF lens [Stacked Ring Ion Guide (SRIG)]

Tube lens and skimmer (TSQ Fortis and TSQ Fortis Plus)

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

[Figure 33](#) shows the tube lens on the left and the skimmer on the right.

Figure 33. Tube lens (left) and skimmer (right)



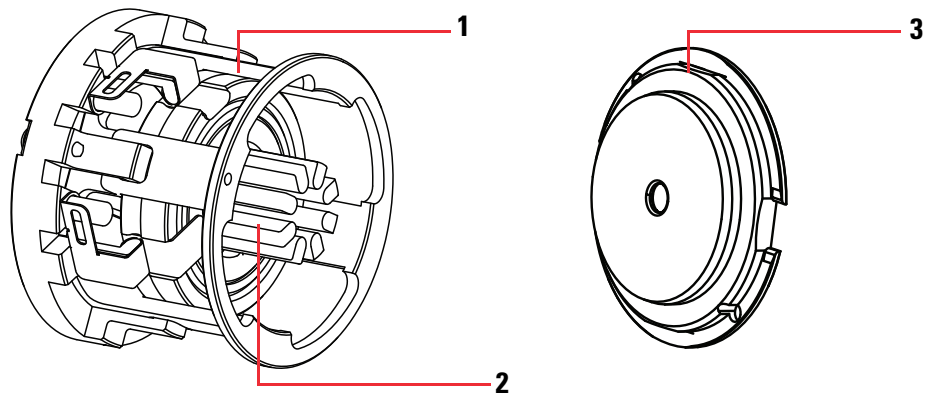
MP00 ion optics – MP00 multipole and L0 lens

The API source interface for all the TSQ Series II mass spectrometers includes an 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 multipole.

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

Figure 34. MP00 assembly (left) and L0 lens (right)



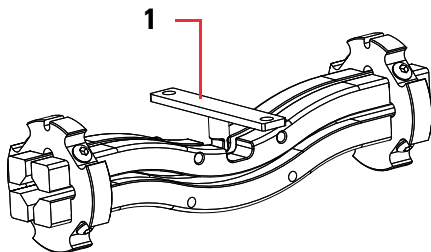
No.	Description	No.	Description
1	MP00 assembly	2	MP00 multipole (array of eight metal elements)
3	L0 lens		

MP0 ion optics and neutrals blocker

The MP0 ion optics (Figure 35) transmits ions from the MP00 ion optics to the first quadrupole (Q1).

The multipole MP0 ion optics includes the multipole MP0 and lenses TK1 and TK2. The neutrals blocker (1 in Figure 35) is attached to the MP0 multipole.

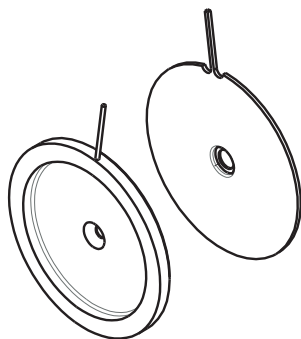
Figure 35. MP0 multipole with neutrals blocker (1)



Multipole MP0 is an array of square-metal rods that transmit ions. The MS applies an RF voltage to the rods to generate an electric field that guides the ions along the axis of the multipole. The MP0 DC offset voltage increases the translational kinetic energy of the ions as they leave MP00. The RF 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 TK1 and the TK2 lenses are metal disks with a circular hole in the center through which the ion beams passes (Figure 36). 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 TK1 and TK2 lenses are also a vacuum baffle between multipole MP0 and quadrupole Q1.

Figure 36. TK1 (left) and TK2 (right) lenses



Mass analyzers and collision cell

The TSQ Series II mass spectrometers are triple-quadrupole mass spectrometers. The first and third quadrupoles operate as mass analyzers, and the second quadrupole serves as a collision cell.

Note For ease of documenting the first, second, and third rod assemblies as separate pieces of hardware, this manual refers to them as Q1, Q2, and Q3, respectively. However, when discussing each rod assembly's function for the scan types, this manual uses the terms *precursor mass analyzer*, *collision cell*, and *product mass analyzer*, respectively.

For details, see these topics:

- [Quadrupole rod assemblies](#)
- [Applied RF and DC fields](#)
- [Mass analysis](#)
- [Collision cell and CID efficiency](#)
- [Quadrupole offset voltage](#)
- [Mass analyzer lenses](#)

Quadrupole rod assemblies

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

See these topics:

- [Quadrupoles Q1 and Q3](#)
- [Q2 quadrupole](#)

Quadrupoles Q1 and Q3

The TSQ Endura MS and the TSQ Quantiva MS were the first generation of TSQ Series II mass spectrometers:

- For the TSQ Endura MS, quadrupoles Q1 and Q3 are square arrays of circular rods ([Figure 37](#)).
- For the TSQ Quantiva MS, quadrupoles Q1 and Q3 are square arrays of precision-machined true hyperbolic rods with larger inter-rod spacing ([Figure 38](#)).
- For both of these first generation models, quartz spacers act as electrical insulators between the rods and the supporting structure.

Figure 37. Quadrupole Q1 or Q3 (TSQ Endura MS)

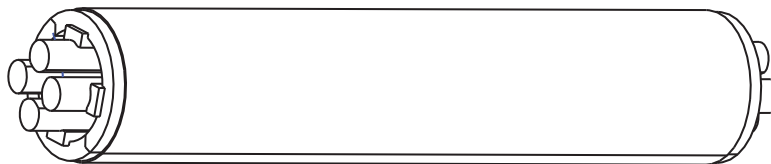
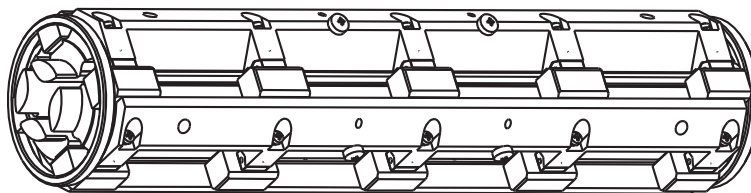


Figure 38. Hyperquad Q1 or Q3 (TSQ Quantiva MS)



Thermo Fisher Scientific made the following improvements to the Q1 and Q3 quadrupoles in the second generation of TSQ Series II mass spectrometers:

- For the TSQ Quantis and TSQ Fortis mass spectrometers, adding a set of pre-filter and post-filter sections that carry only RF voltage improved the ion transmission from that of the first generation models.
- For the TSQ Altis MS, the quadrupoles have a similar geometry to those in the TSQ Quantis and TSQ Fortis mass spectrometers with RF-only sections, but they also have fully hyperbolic surfaces and larger spacing between the rods.

In the current third generation of TSQ Series II mass spectrometers, Thermo Fisher Scientific has improved the accuracy and stability of the Q1 and Q3 quadrupoles in the TSQ Altis Plus MS by modifying their design and dimensions.

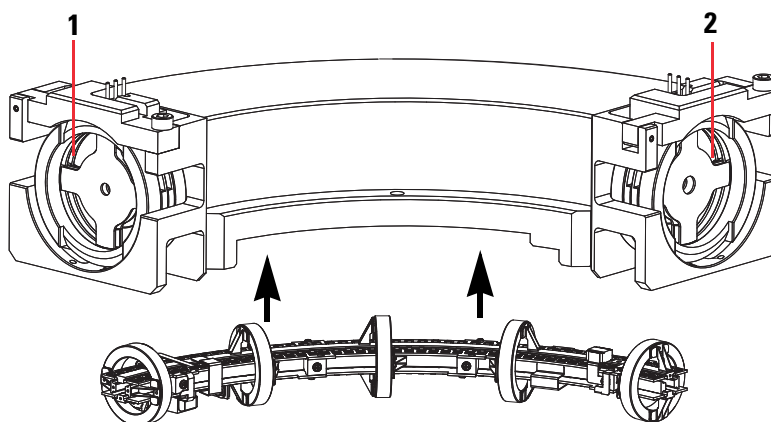
Q2 quadrupole

The Q2 quadrupole in all TSQ Series II mass spectrometers is an active collision cell. Technically, it is a chamber that encloses an RF-only quadrupole ion guide where collision-induced dissociation of ions can take place if argon (or nitrogen) gas is present. The collision cell has an axial field down its length to speed up throughput. This design allows up to 600 SRM transitions per second, with the exception of the TSQ Endura and TSQ Quantiva mass spectrometers.

Note For the TSQ Endura and TSQ Quantiva mass spectrometers, the maximum number of SRM transitions per second is 500.

For the TSQ Quantiva, TSQ Endura, TSQ Altis, TSQ Quantis, and TSQ Fortis mass spectrometers, the Q2 quadrupole is a square-profile quadrupole rod assembly. The rods of the quadrupole assembly are bent into a 90-degree arc, which reduces the footprint of the instrument, prevents the transmission of unwanted neutral species to the detector, and dramatically lowers the noise level in the scan data.

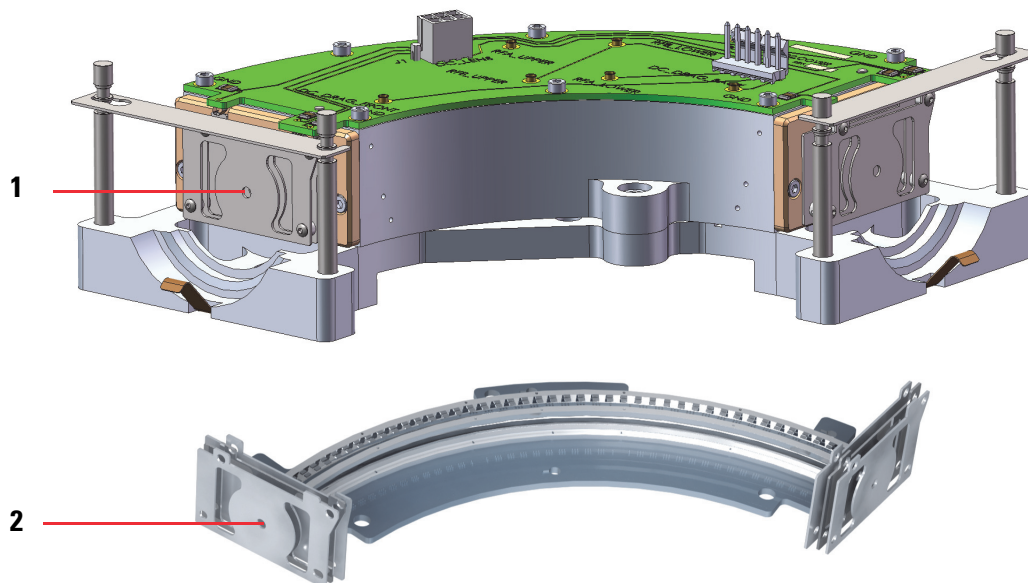
Figure 39. Q2 quadrupole (bottom) separated from the active collision cell housing (top) for the first and second generations of TSQ Series II mass spectrometers



No.	Description	No.	Description
1	EL21, EL22, and EL23 lenses	2	EL31, EL32, and EL33 lenses

The current third generation of TSQ Series II mass spectrometers—the TSQ Altis Plus, TSQ Quantis Plus, and TSQ Fortis Plus—have an updated collision cell. The design of this updated collision cell includes new dimensions, an optimized quadrupole rod geometry and a new PCB support structure that results in better ion transmission efficiency.

Figure 40. Q2 quadrupole for the TSQ Plus mass spectrometers separated from the collision cell housing

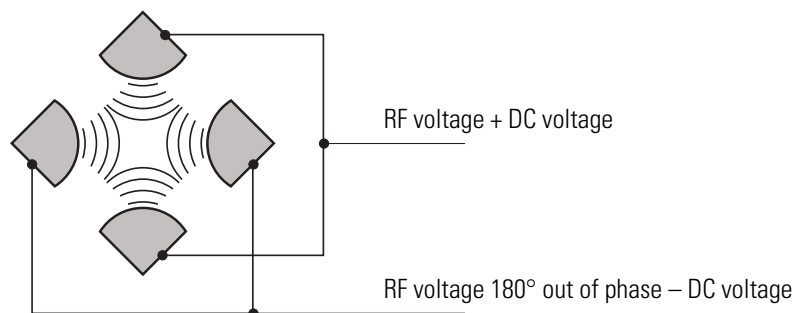


No.	Description	No.	Description
1	Collision cell	2	Quadrupole 2 (Q2) and lenses

Applied RF and DC fields

In a quadrupole rod assembly, because rods opposite each other in the array connect electrically, the four rods are considered two pairs of two rods each. The MS applies RF and DC voltages to the rods. As shown in Figure 41, although the RF voltages applied to the four rods are the same, the two pairs are 180 degrees out of phase (that is, one pair has a positive voltage and the other a negative voltage). The same is true for the applied DC voltages.

Figure 41. Polarity of the RF and DC voltages applied to the Q1 and Q3 mass analyzers



The quadrupole coil module and the rod driver module provide the voltages for operating the quadrupole. The RF voltage applied to the quadrupole rods is of constant frequency.

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

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

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

Mass analysis

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

When the MS applies one particular set of RF and DC voltages to the mass analyzer rods, only ions of one m/z (for example, m/z 180) are maintained within bounded oscillations, as their velocity carries them through the mass analyzer. At the same time, all other ions undergo unbounded oscillations. These ions strike one of the rod surfaces, become neutralized, and are pumped away, or they are ejected from the rod assembly.

Later, both RF and DC voltages change, and ions of a different m/z (for example, m/z 181) are allowed to pass, while all other ions (including m/z 180) become unstable and undergo unbounded oscillations. This process of transmitting ions of one m/z after another continues as the RF and DC voltages change in value.

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

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

Collision cell and CID efficiency

In the MS/MS scan modes, the MS uses the strength of the axial drag field to remove the ions of the previous reaction from the collision cell.

The collision cell surrounds Q2 and is usually pressurized from 0.5×10^{-3} to 4×10^{-3} Torr with argon collision gas. The collision cell is where collision-induced dissociation (CID) takes place.

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

Quadrupole offset voltage

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

In MS modes of operation, the instrument uses a fixed or slowly varying voltage offset between Q1 and Q3. However, in MS/MS experiments, the quadrupole offset voltage applied to Q2 and Q3 usually varies as acquisition proceeds. The MS automatically computes the necessary Q3 quadrupole offset voltage and then varies the voltage, as appropriate, as each scan proceeds.

The offset voltage applied to Q2 (which contains the collision cell) is responsible for the collision energy. The collision energy is the difference in potential between the region where ions start being governed mostly by the electric forces (in the vicinity of Q0, which is also known as MP0) and Q2 (where they collide with collision gas). As the offset voltage on Q2

increases, so does the kinetic energy of the precursor ions. As a result, the energy of ion/Ar (or ion/N) collisions also increases. You can set the collision energy from 0 to ± 65 V in the first two generations of TSQ Series II mass spectrometers and from 0 to ± 120 V in the current generation of TSQ Series II mass spectrometers.

During tuning, the MS determines the optimum mass-dependent quadrupole offset voltage for Q1 and for Q3.

Mass analyzer lenses

The quadrupole region (Q1, Q2, and Q3 chambers) has three lens sets:

- The lenses between Q1 and Q2 are designated as EL21, EL22, and EL23.
- The lenses between Q2 and Q3 are designated as EL31, EL32, and EL33
- The lens between Q3 and the ion detection system is designated as EL4.

Circular holes in the center of the lenses allow the ion beam to pass through.

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

The EL2x lens set (between quadrupoles Q1 and Q2) and the EL3x lens set (between quadrupoles Q2 and Q3) serve the following functions:

- To minimize the amount of collision gas that enters the main quadrupole chamber (Q1 and Q3) from the collision cell (Q2).
- To shield Q1 from the RF voltage applied to Q2 and vice versa (EL2x lens set) and to shield Q3 from the RF voltage applied to Q2 and vice versa (EL3x lens set).
- To focus the ion beam: The three lenses between Q1 and Q2 (and those between Q2 and Q3) together form a three-element aperture lens.

Lens EL4 is located between Q3 and the ion detection system. Lens EL4 has its own wire in the system and is at ground potential. Its purpose is to shield Q3 from the high voltage applied to the ion detection system and to shield the ion detection system from the high RF voltages applied to Q3.

Ion detection system

The ion detection system includes a high-energy conversion dynode, a discrete dynode electron multiplier, and an electrometer circuit board. The electron multiplier is set to a gain of about 1×10^5 (that is, for each ion or electron that enters, 1×10^5 electrons exit) in MS mode and 1×10^6 in MS/MS mode. The electrometer circuit board converts the current that leaves the electron multiplier through the anode to a voltage, and the data system converts the voltage into the ions per second value.

Maintain the MS on a daily basis

To reduce downtime, these topics describe the tasks that you can do before and after you operate the MS:

- [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:

- [Check the vacuum pressure levels](#)
- [Find and fix air leaks](#)
- [Check the argon and nitrogen gas supplies](#)


Check the vacuum pressure levels

You can check the current pressure values in the ion transfer tube-RF lens, and the foreline region (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.

❖ To check the vacuum pressure levels

1. Open the Tune window.
2. Click the **Status** tab and click the **Expand** icon, , next to Vacuum.

- Compare the current values of the pressures in the vacuum manifold with the values listed in [Table 10](#) for the TSQ Altis and Altis Plus models, [Table 11](#) for the TSQ Quantis and Quantis Plus models, and [Table 12](#) for the TSQ Fortis and TSQ Fortis Plus models.

If the values are higher than normal, you might have an air leak.

Table 10. TSQ Altis Plus MS and TSQ Altis typical pressure readings

Conditions	Pressure (Torr)	
	Source pressure ^a (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	<0.5	Less than 6×10^{-6}
Collision gas off, ion transfer tube orifice open	<3.5	Less than 9×10^{-6}
Collision gas set to 1.5 mTorr, ion transfer tube orifice open	<3.5	Approximately 3×10^{-5}

^a When the ion transfer tube is set to a temperature of 325 °C

Table 11. TSQ Quantis Plus MS and TSQ Quantis MS typical pressure readings

Conditions	Pressure (Torr)	
	Source pressure ^a (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	<0.5	Less than 6×10^{-6}
Collision gas off, ion transfer tube orifice open	<2.0	Less than 9×10^{-6}
Collision gas set to 1.5 mTorr, ion transfer tube orifice open	<2.0	Approximately 3×10^{-5}

^a When the ion transfer tube is set to a temperature of 325 °C

Table 12. TSQ Fortis MS and TSQ Fortis Plus typical pressure readings

Conditions	Pressure (Torr)	
	Source pressure ^a (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	<0.5	Less than 6×10^{-6}
Collision gas off, ion transfer tube orifice open	<2.0	Less than 9×10^{-6}
Collision gas set to 1.5 mTorr, ion transfer tube orifice open	<2.0	Approximately 3×10^{-5}

^a When the ion transfer tube is set to a temperature of 300 °C

Table 13. Typical pressure readings for the TSQ Quantiva MS

Conditions	Source pressure ^a (foreline, ion transfer tube, RF lens region)	Analyzer pressure (analyzer region)
Collision gas off, ion transfer tube orifice sealed	<0.5 Torr	Less than 6×10^{-6} Torr (after pumping for at least 12 hours)
Collision gas off, ion transfer tube orifice open	3.8–4.2 Torr	Less than 9×10^{-6} Torr
Collision gas set to 1.5 mTorr, ion transfer tube orifice open	3.8–4.2 Torr	Approximately 3×10^{-5} Torr

^a When the ion transfer tube is set to a temperature of 350 °C

Table 14. Typical pressure readings for the TSQ Endura MS

Conditions	Source pressure ^a (foreline, ion transfer tube, S lens region)	Analyzer pressure (analyzer region)
Collision gas off, ion transfer tube orifice sealed	<0.5 Torr	Less than 6×10^{-6} Torr (after pumping for at least 12 hours)
Collision gas off, ion transfer tube orifice open	<2.0 Torr	Less than 9×10^{-6} Torr
Collision gas set to 1.5 mTorr, ion transfer tube orifice open	<2.0 Torr	Approximately 3×10^{-5} Torr

^a When the ion transfer tube is set to a temperature of 350 °C

- After powering up the system, monitor the vacuum readings and confirm they are decreasing with time. Wait until the readings are within typical pressure ranges for your MS. If the pressure remains high, contact your Thermo Fisher Scientific representative for assistance.

Find and fix air leaks

A major air leak can prevent the pressure levels from being low enough to turn on the system. Possible causes of a major leak might be a loose or disconnected fitting, an improperly positioned O-ring, or an open valve.

❖ To find and fix air leaks

- 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](#).
- Shut down the MS for service. See “[Shut down the MS system completely for planned service or storage](#)” on [page 88](#).
- Visually inspect the vacuum system and vacuum lines for leaks.
- 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.

Check the argon and nitrogen gas supplies

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

Table 15. Procedures for checking the argon and nitrogen gas supplies

Gas	Procedure
Argon	<ol style="list-style-type: none">1. Check the regulator to make sure there is sufficient gas. Replace the tank when the tank pressure falls below 500 psi.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	<ol style="list-style-type: none">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 ($100 \text{ ft}^3/\text{day}$). 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 Do not operate the MS without nitrogen flow as this can damage the source and front end optics due to particulate matter in the atmosphere. Before you operate the MS, verify that there is sufficient nitrogen for the API source.



If the system runs out of nitrogen while you are acquiring scans in the Tune application, a prompt appears with a warning that the nitrogen supply is probably empty. If you are running an acquisition sequence, the data system completes the current run. The system does not proceed to the next sample because the MS cannot return to the Ready state when the nitrogen set point cannot be reached. Meanwhile, the MS continues scanning.

For more information about gas requirements, refer to the preinstallation requirements guide for your MS.

After operating the mass spectrometer

Follow these tasks after operating the MS:

- Flush the inlet components
- Purge the oil in the forepump
- Empty the solvent waste container
- Place the system in Standby mode

Flush the inlet components

Flush the spray insert after running samples, if the system will be idle afterwards. You can use the syringe pump or an LC pump to flush a 50:50 methanol/water solution through the spray insert at a flow rate of 200 to 400 $\mu\text{L}/\text{min}$ for approximately 15 minutes.

Note If you have just run the mass calibration procedure with the EMRS, flush the inlet components with a 50:50 acetonitrile/water solution.

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



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

❖ To flush the inlet components

1. Turn off the liquid flow from the syringe pump.
2. Place the MS in **Standby** mode.
3. Remove the syringe from the syringe pump as follows:
 - a. Lift the syringe holder off of the syringe.
 - b. Press the pusher block's release button and slide the block to the left.
 - c. Remove the syringe from the holder.
 - d. Carefully remove the syringe needle from the Teflon™ tube on the syringe adapter assembly.

4. Rinse the syringe with a solution of 50:50 methanol/water.
5. Flush the sample transfer line, sample tube, and spray insert as follows:
 - a. Load the clean syringe with a solution of 0.1% formic acid in 50:50 methanol/water (or another appropriate solvent, such as a solution of 0.1% formic acid in 50:50 acetonitrile/water).
 - 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.

Purge the oil in the forepump

If your MS system includes oil-sealed rotary vane forepumps, you must routinely purge (ballast) volatile solvents and water vapor from the oil.

The best time to ballast the oil is at the end of the workday 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 for instructions and recommendations about ballasting. Make sure to close the ballast valve before continuing normal operation.



CAUTION Make sure the pump is properly vented during balast; otherwise harmful chemicals can release into the lab.

Empty 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 regional regulations.

Place the system in Standby mode

After you complete the daily maintenance procedures, place the MS in Standby mode if you have not already done so. See [“Place the MS in Standby mode for short periods between use”](#) on [page 86](#).

System startup, shutdown, and reset

The following topics describe how to start up or shut down the MS and how to work with the various power modes—On, Off, and Standby—that are available from the Tune window or data system:

- Place the MS in On mode for operation
- Place the MS in Standby mode for short periods between use
- Shut down the MS system completely in an emergency
- Shut down the MS system completely for planned service or storage
- Restart the MS system after a complete shutdown
- Reset the MS if it is not communicating with the data system
- MS components On/Off status

Place the MS in On mode for operation

In the On mode, the MS is ready for operation.


To turn on the MS when it is in the off state or Standby mode, do one of the following:


- Turn on the MS from the Tune window
- Turn on the MS from the data system


Turn on the MS from the Tune window

The MS is connected to the data system computer, the data system computer is turned on, and the MS is in the off state or Standby mode.

❖ To turn on the MS from the Tune window

1. Open the Tune application by clicking the **Tune** icon, , on the data system computer's desktop.

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

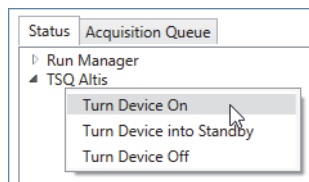
The triangle turns from white to green, , and the System LED on the front panel of the MS turns green.

Turn on the MS from the data system

The MS is connected to the data system computer, the data system computer is turned on, and the MS is in the off state or Standby mode.

❖ To turn on the MS from the Xcalibur data system

- Open the Xcalibur data system.
- Right-click *MS model* on the Status page and choose **Turn Device On**.





The System LED on the front panel of the MS turns green.

Place the MS in Standby mode for short periods between use

If you are not going to use the MS for short periods of time, place it in Standby mode.

❖ To place the MS in Standby mode

- Open the Tune application by doing one of the following:
 - From the Windows taskbar, click the **Start** icon, , and then choose **Thermo Instruments > model x.x > model Tune**.
 - On the desktop, click the **Tune** icon, .
- If your LC/MS system includes a liquid chromatograph, turn off the mobile phase flow to the API source.

For instructions, refer to the liquid chromatograph (LC) manual.

- In the Tune window, click the **System Standby** icon, , to place the MS in Standby mode.

The two bars in the System Standby icon change from white to green, and the System LED on the front panel of the MS 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, see “MS components On/Off status” on page 94.

Shut down the MS system completely in an emergency



CAUTION This is an emergency shut down procedure. Do not shut down the MS for routine maintenance of the API source interface components.

If you must shut down the MS in an emergency, follow this procedure.

❖ To shut down the LC/MS system in an emergency

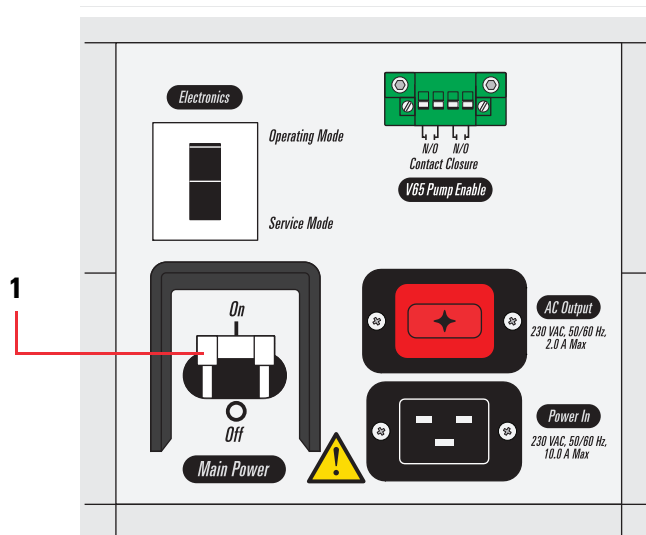
1. To shut down the MS in an emergency, place the Main Power switch in the Off position.

The power switch is located on the power panel on the right-side of the MS (1 in Figure 42).

This switch turns off all power to the MS and any forepumps connected through contact closure, without harming any components within the instrument.

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

Figure 42. Main power switch on the MS power module in the On position



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

Shut down the MS system completely for planned service or storage

Field service engineers must shut down the MS to service components under vacuum.

Thermo Fisher Scientific recommends that you keep the system under vacuum even during long periods when it is not in use—however, although Thermo Fisher Scientific does not recommend it, you can shut down the MS when you are not planning to use it for an extended period of time.

For short periods between use, place the MS in Standby mode.

IMPORTANT Do not shut down the MS for short periods between use, as pumping down the system takes many hours.

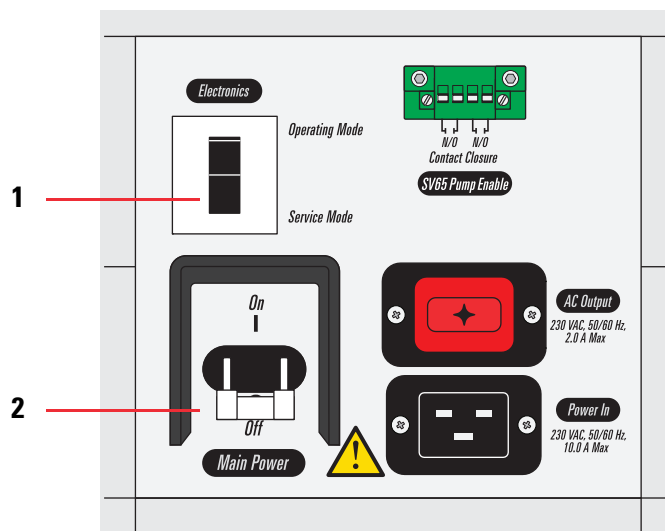
❖ To shut down the mass spectrometer completely

1. Follow the procedure in “Place the MS in Standby mode for short periods between use” on page 86.
2. Place the Electronics service switch in the Service Mode (down) position (1 in Figure 43).

Placing the Electronics service switch in the Service Mode turns off all LEDs on the front panel and the power to the nonvacuum system electronics.

3. Turn off the Main Power switch.

Figure 43. Electronics switch in the Service Mode position (1) and Main Power switch in the Off position (2)



The following occur:

- All power to the MS, including the turbomolecular pumps, turns off. In addition, the forepumps turn off.
 - After approximately 60 seconds, power to the vent valve solenoid shuts off, the vent valve opens, and the vacuum manifold vents with filtered air. You might hear a hissing sound.
 - After about 5 minutes, the vacuum manifold is at atmospheric pressure.
4. Unplug the mass spectrometer'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, or autosampler.

5. If you plan to leave the system off for an extended period of time, Thermo Fisher Scientific recommends that you also turn off the LC, the autosampler, the data system computer, and the gases, as follows:
- a. Turn off the optional LC system and autosampler as described in their manuals. Then, shut down the data system computer and turn off the monitor.
 - b. Close the argon and nitrogen gas supplies at their tanks.

Restart the MS system after a complete shutdown

When you restart the MS system after a complete shutdown, follow these steps to restart the system.

1. [Restart the data system computer](#)
2. [Pump down and restart the MS after a complete shutdown](#)



Restart the data system computer

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

Note After you restart the data system computer, 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, see [“Reset the MS if it is not communicating with the data system”](#) on page 92.

❖ To restart the data system computer

Do one of the following:

- Press CTRL+ALT+DELETE on the keyboard. Then, click the **Power** icon, , at the lower right of the monitor screen and choose **Restart**.
- From the Windows taskbar, click the **Start** icon, . Then, choose **Power > Restart**.
- Press the data system computer's power button. Wait at least 20 seconds. Press the power button again.

Pump down and restart the MS after a complete shutdown

Before you can operate the MS, you must pump down the system. Make sure that the data system is running before you turn on the MS.

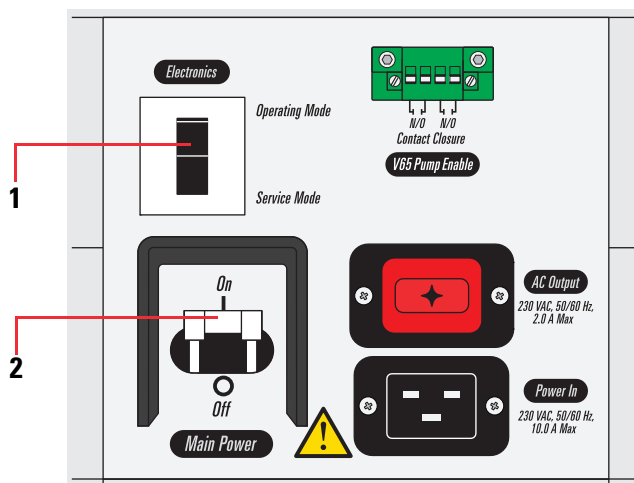
❖ To restart the MS system pump

1. Open the argon and nitrogen gas lines at the tanks if they are closed. Then, check the gas supplies. See [“Check the argon and nitrogen gas supplies”](#) on page 82.
2. Ensure that the Main Power switch is off and that the Electronics service switch is in the Service Mode position.
3. If you disconnected the MS from line power, reconnect it to line power. If you disconnected a forepump for the MS from line power, reconnect it.
4. Turn on the Main Power switch.

Placing the Main Power switch in the On position turns on the turbomolecular pumps and any forepump that is connected to the MS (through the Pump Enable connector). All LEDs on the front panel of the MS remain off.

5. Wait 15 minutes before you place the Electronics service switch in the Operating Mode (up) position.
6. Wait at least 15 hours for the forepumps and the turbomolecular pumps to create sufficient vacuum.

Figure 44. Electronics 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	Off
	• Communication	
MS startup completed	• Vacuum	Green
	• Communication	Yellow
	• System	

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.


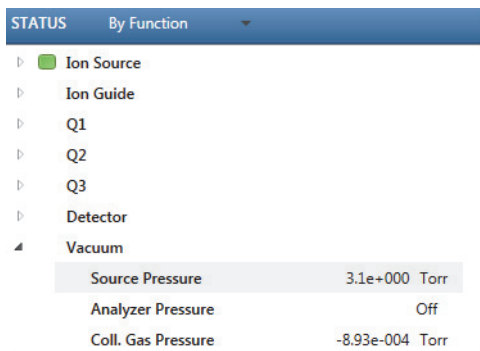
- Open the Tune application by double-clicking the **Tune** icon, , on the desktop. Then, open the Status pane and double-click **Vacuum**.

Figure 45 shows the Status pane in the Tune window.

Figure 45. Status pane in the Tune window

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

Table 16. Threshold limits for the vacuum pressure gauges

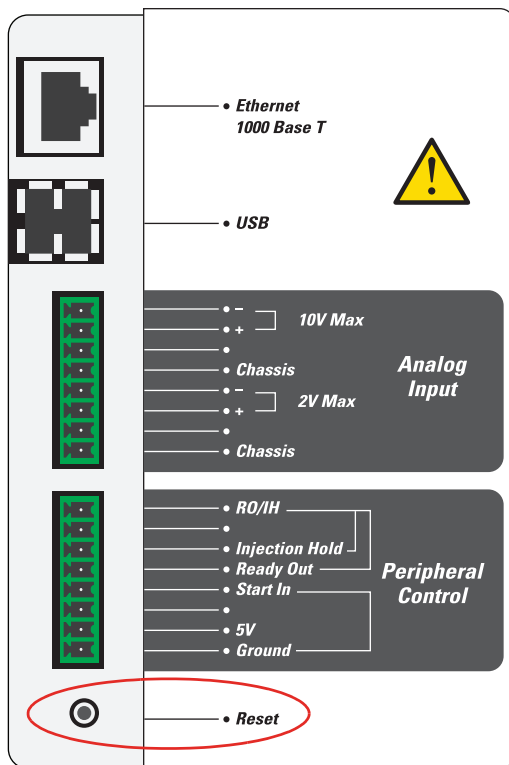
MS model	Source pressure	Analyzer pressure
TSQ Altis Plus and TSQ Altis	4.5 Torr	
TSQ Quantis Plus and TSQ Quantis	3 Torr	$<9.0 \times 10^{-6}$ Torr
TSQ Fortis Plus and TSQ Fortis	3 Torr	
TSQ Quantiva	4.5 Torr	$<9 \times 10^{-6}$ Torr
TSQ Endura	3.0 Torr	$<9 \times 10^{-6}$ Torr

Reset the MS if it is not communicating with the data system

In the unlikely event that communication is lost between the MS and the data system computer, you can reset the MS by using the reset button (1 in [Figure 46](#)) located on the right-side communications panel.

❖ To reset the MS

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 46. Reset button on the communication panel

The following sequence of events 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.

MS components On/Off status

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

- Place the mass spectrometer in Standby mode. Standby is the normal condition to leave the mass spectrometer in when it is not in use.
- Place the mass spectrometer in Off mode. Off mode is similar to standby, except all high voltage components of the mass spectrometer and the ion gauge are turned off.
- Turn on the mass spectrometer by placing it in On mode.
- Place the Electronics service switch in the Service Mode position. The Electronics service switch turns off all components in the mass spectrometer other than the +24 V power supply, forepump, turbomolecular pump, and fans.
- Place the Main Power circuit breaker switch in the Off (O) position. Placing the Main Power circuit breaker switch in the Off (O) position removes all power to the mass spectrometer, including the vacuum system.

Table 17 summarizes the on/off status of MS components, voltages, and API gas flows.

Table 17. On/Off status of MS components, voltages, and API gas flows (Sheet 1 of 2)







Mass spectrometer component	On mode 	Standby mode 	Off ^a mode 	Electronics service switch, Service Mode position	Main Power switch, Off (O) position
Vent valve	Closed	Closed	Closed	Closed	Open
APCI corona discharge needle	On	Off	Off	Off	Off
Conversion dynode	On	Off	Off	Off	Off
Electron multiplier	On	Off	Off	Off	Off
ESI needle spray voltage	On	Off	Off	Off	Off
Gas, argon (collision [CID gas]) ^b	On	Off	Off	Off	Off
Power supply, electron multiplier and conversion dynode	On	Off	Off	Off	Off
Vaporizer temperature ^a	On	Off	Off	Off	Off
Ion transfer tube DC offset	On	On	Off	Off	Off
Ion transfer tube temperature control	On	On	Off	Off	Off
Mass analyzer, DC offset voltage	On	On	Off	Off	Off
Mass analyzer, RF voltage	On	On	Off	Off	Off

Table 17. On/Off status of MS components, voltages, and API gas flows (Sheet 2 of 2)

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

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

^b You can control this setting in your instrument 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. The DC and RF voltages are on at a reduced level to maintain the system stability.

Connect the sample flow to the API source

To connect the sample flow to the H-ESI source or the APCI source, follow the appropriate topic:

- [Connect the sample flow to the H-ESI source](#)
- [Connect the sample flow to the APCI source](#)

Note Use the fittings (PEEK or Viper™) that are appropriate for your application. The illustrations in [Figure 47](#) and [Figure 48](#) are examples only.

Connect the sample flow to the H-ESI source

❖ To connect the sample flow to the H-ESI source

1. Use the appropriate fitting to connect the solvent line from the LC system or the syringe pump to the grounding union.
2. After you connect the solvent line to the grounding union, check for leaks at each of the tubing connections before you place the system in On mode.

Note Refer to the ion source user guide for more information.

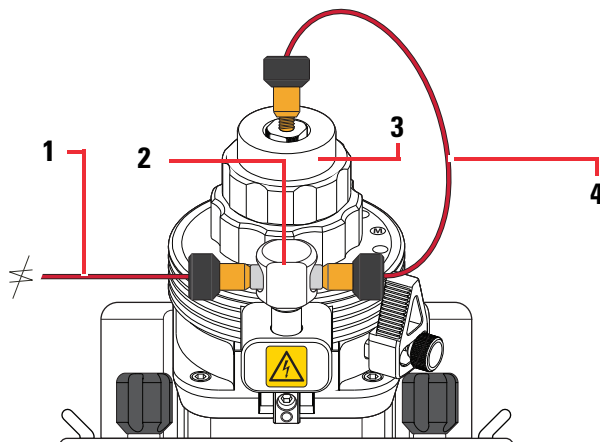


CAUTION If liquid is leaking out of a tube or a fitting, the components and liquid might be electrically conductive and could cause an electric shock when touched.

Turn off the voltages to the ion source housing by setting the instrument to Standby mode before wiping up a small leak from the plumbing connections to the ion source.



CAUTION Never bypass the grounding union when connecting the LC system to the ion source. Bypassing the grounding union creates an electric shock hazard to the user and other connected devices.

Figure 47. Connection to the H-ESI or the low-flow H-ESI source

No.	Description
1	<p>Connection between the LC system or the syringe and the H-ESI or low-flow H-ESI source</p> <p>For standard flow applications, use a Viper capillary or a length of Red PEEK tubing and two natural PEEK fingertight fittings to connect the LC system or the syringe to the grounding union.</p> <p>For nanoflow applications, use a nanoViper capillary.</p> <p>The TSQ Source Installation Kit includes Viper capillaries.</p>
2	Grounding union holder
3	H-ESI or low-flow H-ESI spray insert
4	A PEEK Viper capillary connects the H-ESI spray insert to the grounding union

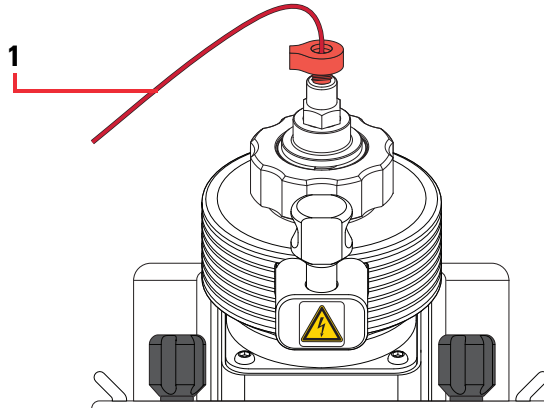
Connect the sample flow to the APCI source

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.

❖ To connect the sample flow to the APCI source

Use tubing (red PEEK or natural PEEK) with a fingertight fitting to connect the sample flow to the sample inlet of the APCI spray insert (Figure 48).

Figure 48. Connection to the APCI spray insert



No.	Description
1	Tubing from sample line (red PEEK or natural PEEK)

Calibrate the MS

The following topics describe how to set up the MS system for the automated System Check and System Calibration processes and how to interpret the results:

- [Prepare the MS system for calibration](#)
- [Run the automated System Calibration routine](#)
- [Run the automated System Check routine](#)
- [Tune and calibration parameters](#)
- [Calibration solution peak values](#)

Read the following caution statement before you operate the instrument.



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 and do not touch the ion source housing or the tubing that connects the grounding union to the spray insert.

Prepare the MS system for calibration

The Tune application includes built-in instructions for preparing the MS system for the automated System Check and System Calibration processes.

The following topics in this section provide supplemental information for the built-in instructions.

Follow the topics in the order listed.

1. (Optional) [Access the system preparation instructions from the Calibration pane](#)
2. [Set up the syringe pump with the calibration solution](#)
3. [Position the H-ESI probe or the calibration probe for the calibration process](#)
4. [Apply the favorites settings for the calibration process](#)
5. [Start the flow of calibration solution to the ion source](#)

6. Check the full scan for missing or interfering peaks
7. Evaluate the spray stability

Access the system preparation instructions from the Calibration pane

The Tune application includes embedded instructions for preparing the MS system for calibration.

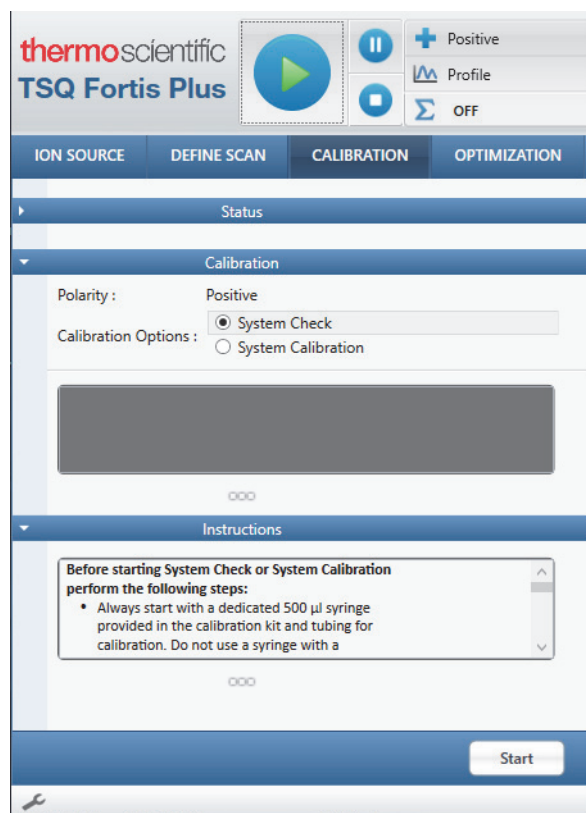
❖ To access the instructions for preparing the MS system for calibration

1. Open the Tune application.
2. Click the **Calibration** tab.

The Calibration pane opens to the left of the graphs.

3. Click the **Calibration** bar to expand the Calibration section.
4. Click the **Instructions** bar to expand the Instructions section (Figure 49).

Figure 49. Instructions pane on the Calibration page of the Tune application



5. Use the scroll bar to display the instructions. Then, if you are not familiar with the calibration setup, go to the next topic for more details, [“Set up the syringe pump with the calibration solution.”](#)

Set up the syringe pump with the calibration solution

The TSQ Series II mass spectrometers use extended mass range solution (EMRS) for the automated System Calibration process.

IMPORTANT Use only the dedicated 500 µL syringe and tubing provided in the calibration kit.

❖ To set up the syringe pump for the calibration process

1. Fill the syringe with a sufficient amount of fresh calibration solution and verify that the calibration solution flows through the tubing and H-ESI needle without resistance.

The System Calibration process takes 30 to 50 minutes with the syringe pump set to a flow rate from 3 to 5 µL/min.

IMPORTANT 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.

Consider wearing other chemically resistant gloves when working with the EMRS.

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

- Do not return any EMRS back to the original vial.
- Do not store the EMRS in a glass syringe. Discard unused the 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 the EMRS and reserpine solutions:

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

2. If the calibration solution does not flow through the tubing and needle without resistance, do the following:

- Make new clean cuts at both ends of the PEEK tubing.
- Inspect the tip of the needle insert (preferably under a microscope) for dirt or damage.
- If necessary, replace the H-ESI needle insert. Use the tool to ensure correct needle protrusion.

For information about setting up the syringe and connecting it to the sample transfer line, see [Appendix B, “Set up the syringe and the syringe pump.”](#)

3. When you connect the sample transfer line to the ion source housing's grounding union make sure that the union is made of stainless steel, as solvent leaks between the sample transfer line and the union can create an electric shock hazard if the union is not properly grounded.



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.

Go to the next topic for information on how to “[Position the H-ESI probe or the calibration probe for the calibration process.](#)”

Position the H-ESI probe or the calibration probe for the calibration process

The calibration probe is an option that ships with the TSQ Series II Plus models. If you have a second generation TSQ Series II mass spectrometer, you can order the calibration probe from Thermo Fisher Scientific.

Note The calibration probe is not compatible with the EASY-Max NG API source or the Ion Max NG API source.

If you have a calibration probe, Thermo Fisher Scientific recommends that you use it instead of the H-ESI probe when you calibrate the MS, as the calibration probe is specifically designed for this purpose. After you run the calibration routine, uninstall the calibration probe and reinstall the H-ESI probe.

The installation procedure for the calibration probe is the same as the installation procedure for the H-ESI probe.

❖ To position the H-ESI probe or the calibration probe for the calibration process

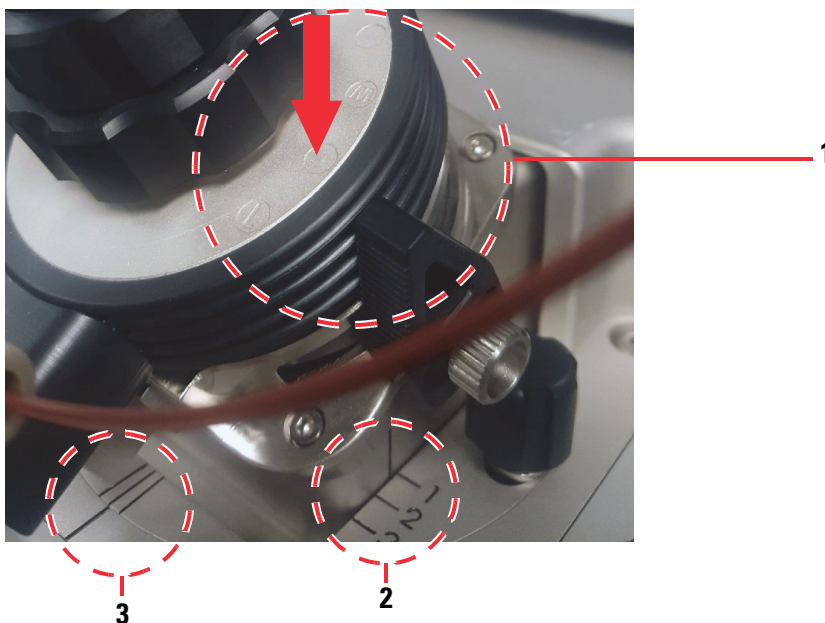
- Adjust the probe height between L and M, except for the TSQ Endura MS.

Note The TSQ Endura MS uses the EASY-Max NG API source, which does not provide any height adjustment for the probe.

- Adjust the front-to-back position of the probe (typically near position 1 and 1.5 for a syringe flow rate from 2 to 5 $\mu\text{L}/\text{min}$).
- Center the left-to-right position of the probe.

Figure 50 shows the probe position for the calibration process.

Figure 50. Probe position for the calibration process




No.	Description	No.	Description
1	Depth position (z axis) between M and L	2	Front-to-back position (y axis) at a position slightly >1
3	Left-to-right position (x axis) at the center position		

Go to the next topic for information about how to “[Apply the favorites settings for the calibration process.](#)”

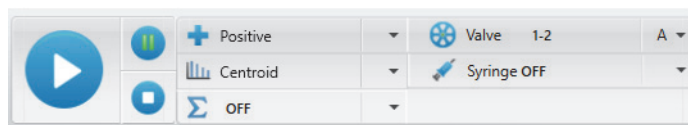
Apply the favorites settings for the calibration process

The Tune application includes favorites settings for calibrating the MS with EMRS.

❖ To apply the favorites settings for the calibration process

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

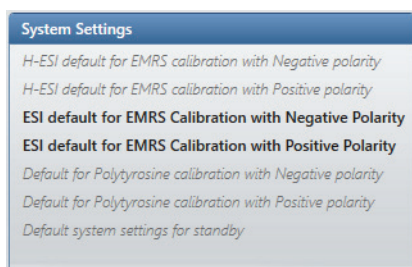
Placing the MS in Standby mode prevents the ion transfer tube from heating to a temperature setting that is too high for the calibration procedure.



2. In the data type list, and select the **Profile** data type.
3. Click the **Define Scan** tab.

4. In the Define Scan pane, select the **Full Scan** mode.
5. Under System Settings in the Favorites pane, do one of the following:
 - To calibrate the MS in the positive ion mode with the calibration probe, right-click **ESI Default for EMRS Calibration with Positive Polarity** and choose **Apply**.
 - To calibrate the MS in the negative ion mode with the calibration probe, right-click **ESI Default for EMRS Calibration with Negative Polarity** and choose **Apply**.
 - To calibrate the MS in the positive ion mode with the H-ESI probe, right-click **H-ESI Default for EMRS Calibration with Positive Polarity** and choose **Apply**.
 - To calibrate the MS in the negative ion mode with the H-ESI probe, right-click **H-ESI Default for EMRS Calibration with Negative Polarity** and choose **Apply**.

Figure 51. System Settings menu with the available favorites for the calibration probe



The default parameter settings appear at the top of the Favorites pane (Figure 52).

Figure 52. Default parameter settings for the calibration with the EMRS in the positive polarity mode for the H-ESI probe

FAVORITES		STATUS
Scan Type	Full Scan (Q1)	
Scan Range (m/z)	50-1650	
Q1 Resolution (FWHM)	0.7	
Scan Rate (Da/sec)	1000	
Ion Source Type	Heated ESI	
Pos Ion Spray Voltage (V)	3500	
Sheath Gas (Arb)	4	
Aux Gas (Arb)	0	
Sweep Gas (Arb)	0	
Ion Transfer Tube Temp (°C)	300	
Vaporizer Temp (°C)	0	
Polarity	Positive	

Table 18 lists the source settings for the calibration probe.

Table 18. Source settings for the EMRS using the calibration probe (Sheet 1 of 2)

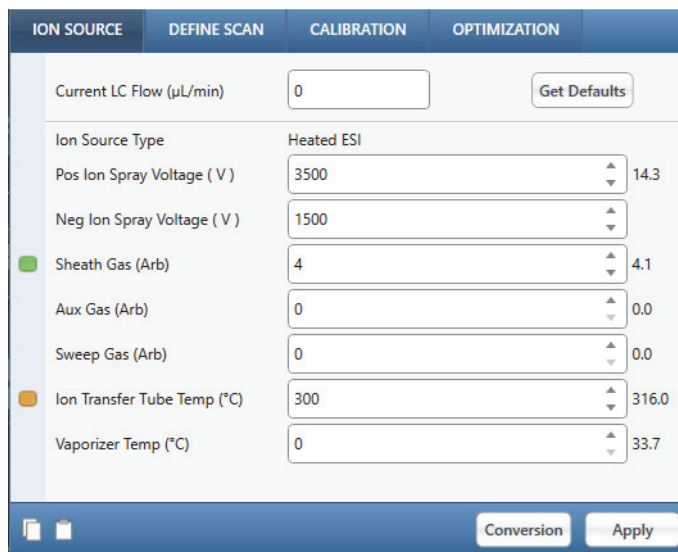
Parameter	Positive polarity mode	Negative polarity mode
Spray Voltage (V)	3500	3200
Sheath Gas (Arb)	0	0

Table 18. Source settings for the EMRS using the calibration probe (Sheet 2 of 2)

Parameter	Positive polarity mode	Negative polarity mode
Aux Gas (Arb)	0	0
Sweep Gas (Arb)	0	0
Ion Transfer Tube Temp (°C)	325 (300 for TSQ Quantis and TSQ Fortis)	325 (300 for TSQ Quantis and TSQ Fortis)
Vaporizer Temperature (°C)	Parameter not available with ESI	Parameter not available with ESI
Source Fragmentation (V)	30 (20 for TSQ Fortis)	30 For all
Syringe pump flow rate (µL/min)	2 to 5	2 to 5

- In the Tune window, click the **Ion Source** tab. Then, check the settings in the Ion Source pane (Figure 53).

Figure 53. Default ion source settings for the H-ESI probe



Go to the next topic for information about how to “[Start the flow of calibration solution to the ion source.](#)”

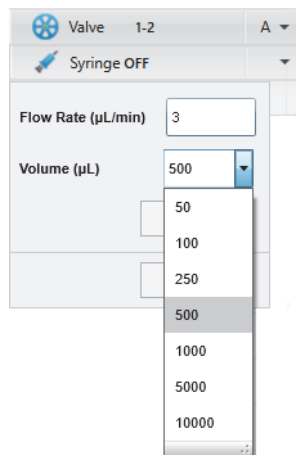
Start the flow of calibration solution to the ion source

For the System Calibration process, infuse the EMRS into the ion source by using the syringe pump.

❖ To start the syringe pump

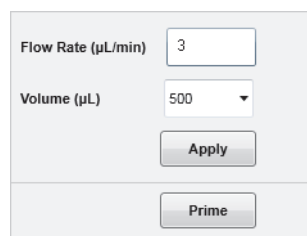
- In the Tune application toolbar, click the down arrow at the right of the Syringe On/Off control. Then, do the following:
 - In the Volume (µL) list, select **500**.


Figure 54. Syringe size list



- In the Flow Rate ($\mu\text{L}/\text{min}$) box, type a value from 2 to 5.

Figure 55. Syringe pump settings box



2. Click **Syringe Off** to turn on the syringe pump.
The button name changes to Syringe On.
3. Click **Apply**.
4. With the calibration solution flowing through the solvent line, do the following:
 - a. Verify that the inlet plumbing connections do not leak.
 - b. If necessary due to air in the sample transfer line, open the syringe pump settings again. Press and hold **Prime** to prime the syringe at 100 $\mu\text{L}/\text{min}$. Continue to press Prime until the signal from the EMRS appears in the spectrum view, which typically takes 3 to 5 seconds.
 - c. Verify that the system readback is normal, .
 - d. Let the system equilibrate for 15 minutes.

Check the full scan for missing or interfering peaks

After you start the flow of the calibration solution to the ion source, monitor the full scan spectrum of the calibration solution.

❖ **To check for missing or interfering peaks**

1. If you have not already applied the favorites setting for the polarity mode you are calibrating, apply it now.

The favorites setting for the positive polarity mode sets the scan mode to Full Scan (Q1) with a mass range from 50 to 1650 m/z .

2. Inspect the spectrum in the spectrum view of the Tune window.
 - For the positive mode, check the peaks at the following m/z values: 69, 102, 215, 622, 922, and 1522.
 - For the negative mode, check the peaks at the following m/z values: 69, 113, 302, 602, 1034, and 1634.
3. For each of the expected peaks, check that the peak is the most abundant peak within ± 10 amu of the expected m/z value.
4. If necessary, adjust the gas settings in the Ion Source pane, especially the Aux Gas parameter setting or the Sweep Gas parameter setting.
5. Check for the following interfering or missing m/z values:
 - For the positive mode, check for contaminating peaks at m/z 100 and m/z 212. Possible sources of the m/z 100 contaminant include the nitrogen line or the ion source housing. The contaminant at m/z 212 is probably caused by wearing nitrile gloves while working with the EMRS.
 - For the negative mode, check for a missing or small peak at m/z 302. The peak at m/z 302 disappears as the EMRS degrades. If the peak is too small or missing, fill the syringe with fresh solution.

Go to the next topic for information about how to [“Evaluate the spray stability.”](#)

Evaluate the spray stability

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

Before you evaluate the spray stability, verify that the syringe contains the appropriate calibration solution and the ion source parameters pane displays the appropriate settings. Also, make sure that the calibration solution has warmed to room temperature, which takes about 30 minutes after you remove it from refrigeration.

Parameter	Setting
Syringe pump settings box	2 to 5 $\mu\text{L}/\text{min}$ flow rate and a syringe volume that matches the size of the syringe installed on the syringe pump
Ion polarity mode	Positive or Negative
Data type	Profile

❖ **To evaluate the spray stability**

1. Click the **Define Scan** tab. Then, in the Define Scan pane, set the following parameters:

- Scan Type: **SIM (Q1)**
- Precursor (m/z): **622 (602 in Negative Mode)**
- Source Fragmentation (V): Depends on the MS model

MS model	Voltage (V)	
	Positive mode	Negative mode
All TSQ Series II mass spectrometers, except for the TSQ Fortis and TSQ Fortis Plus	30	30
Only the TSQ Fortis and TSQ Fortis Plus	20	30

Figure 56. Scan parameters for a TSQ Series II MS (except for a TSQ Fortis model) in positive mode



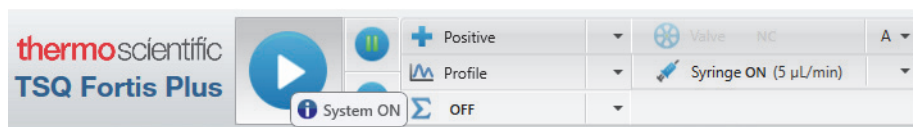
Figure 57. Scan parameters for a TSQ Fortis or TSQ Fortis Plus model in positive mode

ION SOURCE	DEFINE SCAN	CALIBRATION	OPERATION
Scan Type	SIM Scan (Q1)		
Q1 Resolution (FWHM)	0.7		
Scan Option	<input checked="" type="radio"/> Scan Rate <input type="radio"/> Dwell Time		
Scan Rate (Da/sec)	250		
Scan Width (m/z)	10		
CID Gas (mTorr)	0		
Use Calibrated Tube Lens	<input checked="" type="checkbox"/>		
Source Fragmentation	20		
Q1 SIM Scan Table			
ADD DELETE IMPORT EXPORT			
	Compound	Precursor (m/z)	
1	compound	622	

Figure 58. Scan parameters for a TSQ Fortis or TSQ Fortis Plus Series II MS in negative mode

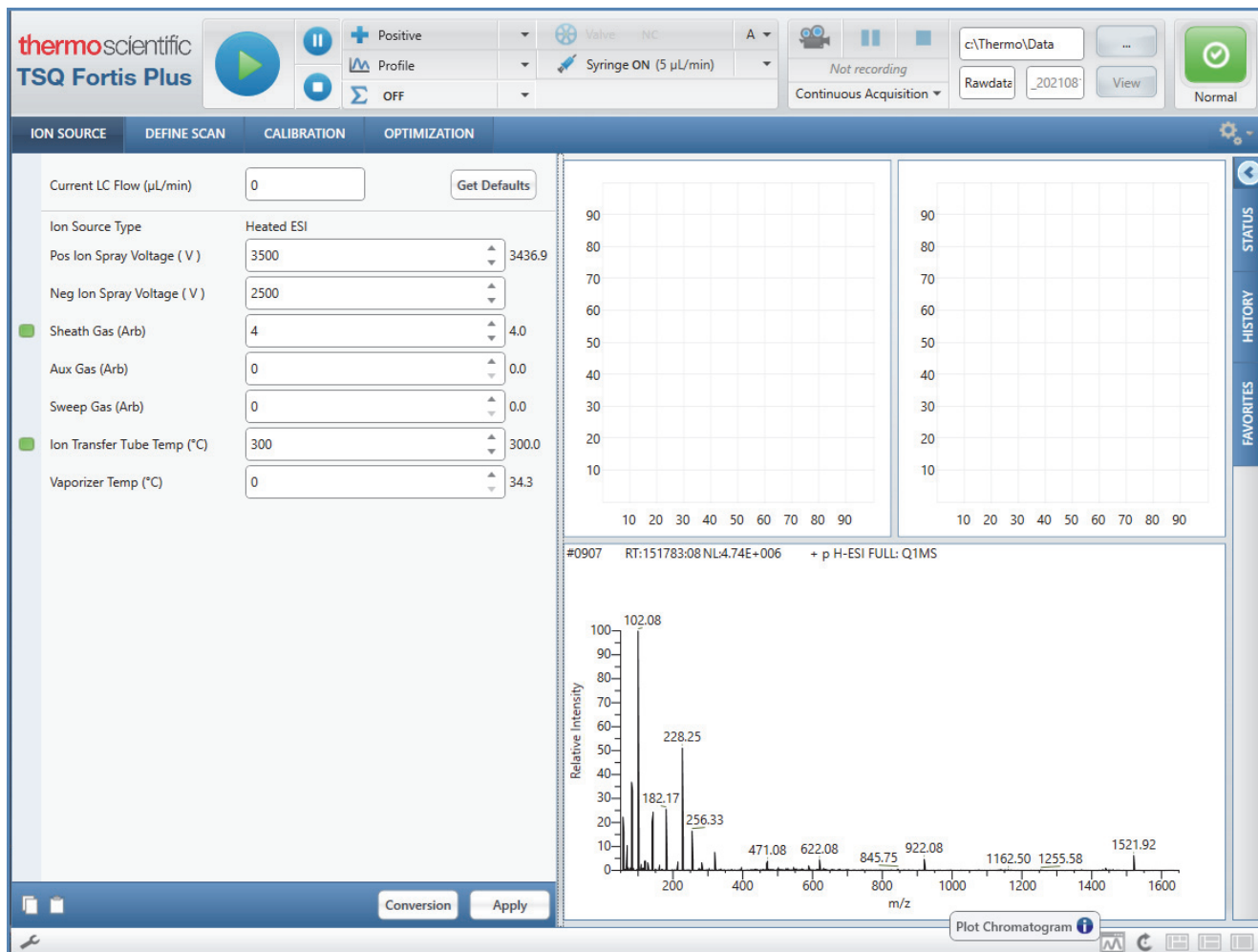
ION SOURCE	DEFINE SCAN	CALIBRATION	OPERATION
Scan Type	SIM Scan (Q1)		
Q1 Resolution (FWHM)	0.7		
Scan Option	<input checked="" type="radio"/> Scan Rate <input type="radio"/> Dwell Time		
Scan Rate (Da/sec)	250		
Scan Width (m/z)	10		
CID Gas (mTorr)	0		
Use Calibrated Tube Lens	<input checked="" type="checkbox"/>		
Source Fragmentation	30		
Q1 SIM Scan Table			
ADD DELETE IMPORT EXPORT			
	Compound	Precursor (m/z)	
1	compound	602	

- Click the **System On** icon to 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.

Figure 59. Real-time mass spectrum in the spectrum view

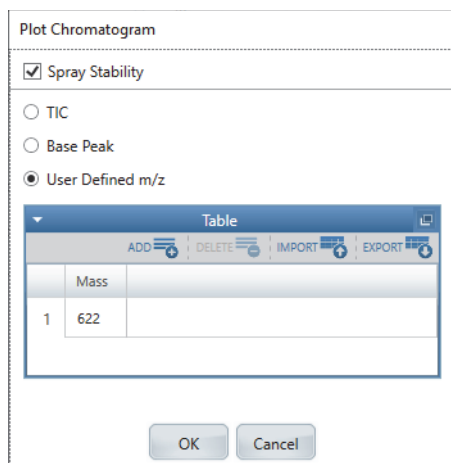


3. Click the **Plot Chromatogram** icon, , at the lower right of the Tune window.

The Plot Chromatogram dialog box opens.

4. In the Plot Chromatogram dialog box, do the following:
 - a. Select the **Spray Stability** check box and the **User Defined m/z** option.
 - b. In the mass table, type **622** in the Mass column of row 1.

Figure 60. Plot Chromatogram dialog box with a user defined m/z value



5. Click **OK**.

The Spray Stability check begins.

You can observe the signal stability and the effects of changes to various parameters in the chromatogram and spectrum plots. You can also observe a real-time graph of the RSD for a 10 Da-selected ion monitoring (SIM) scan that is centered around the masses that you defined in the Plot Chromatogram dialog box.

When the check finishes, the %RSD plot displays the calculated results.

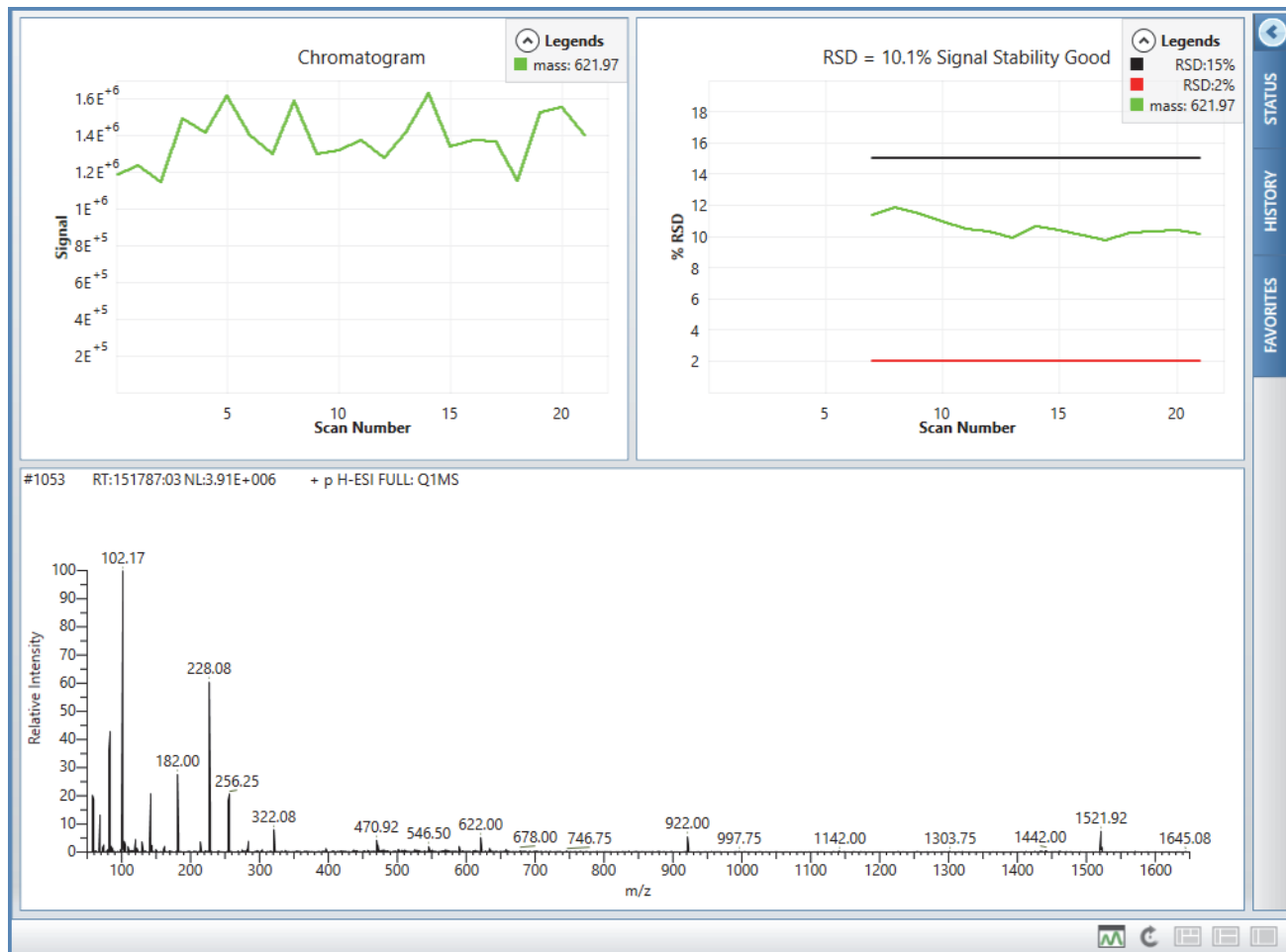
6. Observe the RSD graph, and review the signal stability rating and %RSD value.

Table 19 lists the criteria for a stable spray in either positive or negative ion polarity mode.

Table 19. Recommended %RSD values and ratings for the calibration solutions

Ion polarity mode	Acceptable signal stability rating	Maximum %RSD (threshold)
Positive	Excellent or Good	10
Negative	Excellent or Good	10

Figure 61. Spray Stability check results



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

- a. Ensure the proper installation of the sweep cone.
- b. Make slight adjustments to the forward/backward position of the API probe.
- c. Change the API depth position from L/M to M.
- d. Optimize the spray voltage, starting with 3.5 kV and increasing or decreasing to achieve the maximum stable signal.

The spray voltage must *not* exceed 3.6 kV.

- e. Adjust the sheath gas:
 - For the positive mode, set the sheath gas to 0 or 4.
 - For the negative mode, adjust the sheath gas plus or minus 1 unit. The optimal value for the negative mode can vary from 0 to 5, but it is usually either 0 or between 4 and 5.

- f. Adjust the flow rate. For example, if you started at 5 $\mu\text{L}/\text{min}$, lower the flow rate by 1 $\mu\text{L}/\text{min}$. If you started at 3 $\mu\text{L}/\text{min}$, increase the flow rate by 1 $\mu\text{L}/\text{min}$.
8. Once the spray stability is achieved, select **Full Scan** mode to start the system check or the system calibration.

Run the automated System Calibration routine

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

IMPORTANT Do not operate the system if it fails the calibration routine, as the quality of your data is based on the mass accuracy and resolution of the MS. Contact your regional technical support office.

IMPORTANT

- 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.

The System Calibration routine performs the following steps:

1. Checks the spray stability. If the spray stability check passes, the routine performs the remaining tuning and calibration steps.
2. Calibrates the EM Gain.
3. Tunes Q1 and Q3.
4. Calibrates the mass analyzers by using the mass position and resolution of the peaks in the EMRS spectrum.

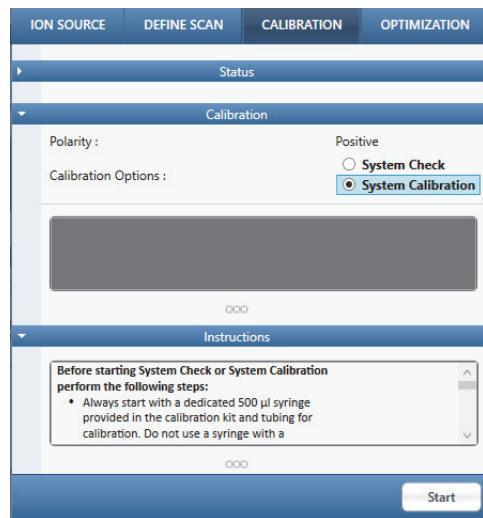
❖ **To run the System Calibration routine**

1. Prepare the MS for calibration. See “[Prepare the MS system for calibration](#)” on [page 99](#).

Note If the calibration has expired, the System Check option is not available.

2. Click the **Calibration** tab.
3. In the Calibration pane, select the **System Calibration** option.

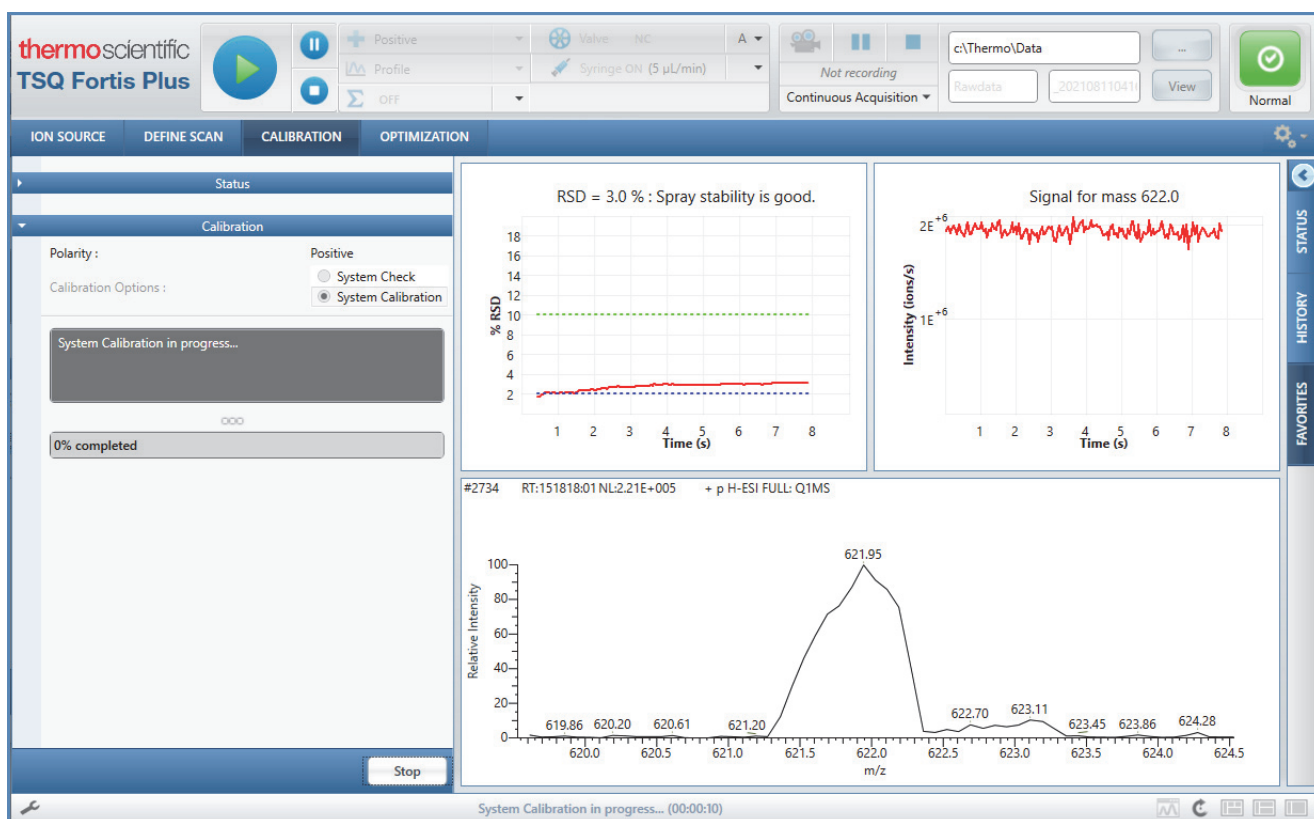
Figure 62. Calibration pane, showing the selection of the System Calibration option



4. Click **Start**.

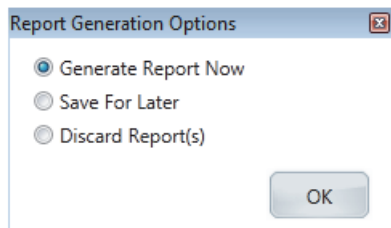
The Stop button replaces the Start button and the System Calibration routine begins with a Spray Stability check.

Figure 63. Beginning of the System Calibration routine



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

Figure 64. Report Generation Options



5. At the prompt, select an option and click **OK**.
6. After the MS completes the calibration procedure in positive mode, run the calibration routine in negative ion mode.

Run the automated System Check routine

The System Check option is not available if the Calibration is expired.

The System Check routine does the following:

1. Checks the spray stability. If the spray stability check passes, the routine runs the next check.
2. Checks the EM Gain calibration.
3. Checks the mass position and resolution calibration by using the measured EMRS spectrum.

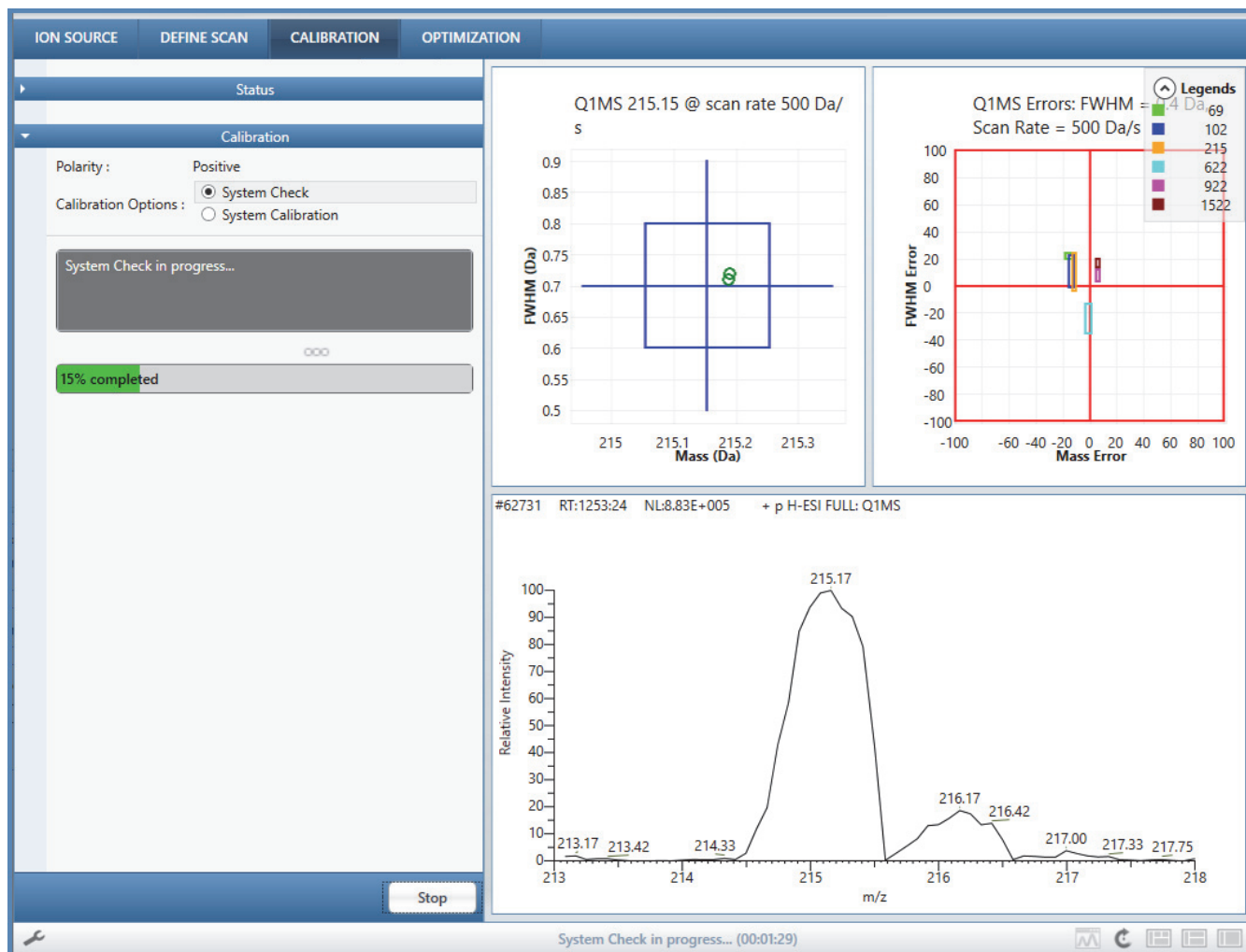
If any check fails, the System Check routine automatically reruns the calibration process for the failed check.

❖ To run the System Check routine

1. Prepare the MS for calibration. See [“Prepare the MS system for calibration.”](#)
2. Click the **Calibration** tab.
3. In the Calibration pane, select the **System Check** option.
4. Click **Start**.

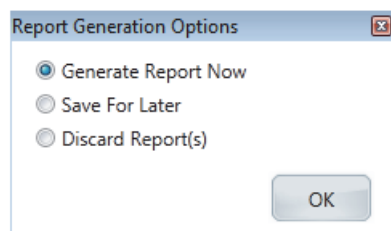
The Stop button replaces the Start button and the routine begins.

Figure 65. System Check routine in progress



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

Figure 66. Report Generation Options



5. At the prompt, select an option and click **OK**.

Tune and 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 voltages of L0 lens, Turner-Kruger Lens 1 (TK1), and the DC offset voltages of the 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. The instrument control software does not optimize the compound-dependent parameters during an EMRS calibration. For information about optimizing the signal for your analytes, see [Chapter 9, “Optimize the compound signal.”](#)

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.

Calibration solution peak values

The mass spectra of the EMRS in positive and negative ion polarity modes ([Figure 67](#) and [Figure 68](#), respectively) have peaks at m/z values close to the theoretical values in [Table 20](#) and [Table 21](#).

IMPORTANT If you observe interfering peaks in the EMRS spectrum that are within ± 10 Da of any of these calibration masses, follow the procedure “[Flush the inlet components,](#)” on [page 83](#). Ensure that the interfering masses show less than 25 percent of the intensity of the calibrant ions.

Table 20. 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) naphthalene	215.15
Hexakis(2,2-difluoroethoxy)phosphazene	622.03

Table 20. Mass spectral peaks $[M+H]^+$ for EMRS in the positive ion polarity mode

Component	Positive mode (m/z)
Hexakis(2,2,3,3-tetrafluoropropoxy) phosphazene	922.01
Hexakis(1h,1h,5h-octafluoropentoxy) phosphazene	1521.97

Figure 67. Mass spectrum of EMRS in positive ion mode

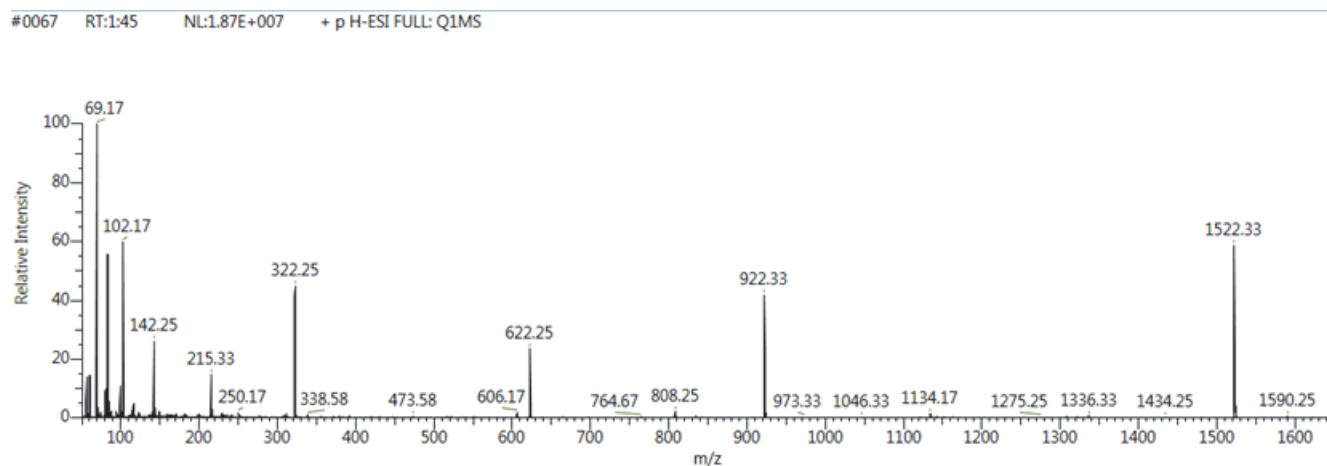


Table 21. Mass spectral peaks for EMRS in the negative ion polarity mode

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

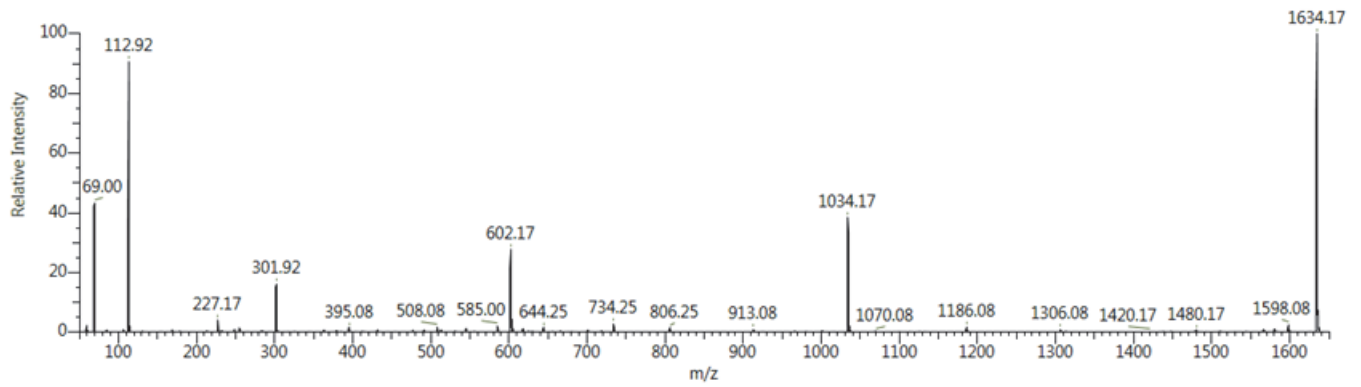
^a $[M-H]^-$

^b $[M+OH]^-$

^c $[M+TFA]^-$

Figure 68. Mass spectrum of EMRS in negative ion mode

#0278 RT:7:24 NL:3.86E+007 -p H-ESI FULL: Q1MS



Starting source conditions for various LC flow rates


The following topics describe the recommended source settings when operating your system in H-ESI, APCI, or NSI mode.

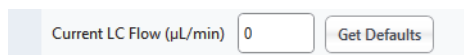
- [Check the recommended ion source settings for the LC flow rate](#)
- [Recommended H-ESI source settings for various LC flow rates](#)
- [Recommended LC/APCI/MS parameters](#)
- [Recommended LC/NSI/MS parameters](#)

Check the recommended ion source settings for the LC flow rate

You can check the recommended ion source settings for various LC flow rates from the Method Editor or the Tune window.

❖ To check the recommended ion source settings for your LC/MS system

1. Do one of the following:
 - Open the Method Editor from the data system or the instrument control application. Then, click the **Global Parameters** tab.
 - Open the Tune window by double-clicking the **Tune** icon,  , on the desktop. Then, click the **Ion Source** tab.
2. In the Ion Source pane of the Tune window or the Ion Source Properties pane of the Method Editor, type the LC flow rate in the Current LC Flow (µL/min) box. Then, click **Get Defaults**.



Current LC Flow (µL/min)

Recommended H-ESI source settings for various LC flow rates

As you increase the liquid flow rate from the LC system, Thermo Fisher Scientific recommends that you increase the gas flow to the ion source and the temperature of the ion transfer tube heater and the vaporizer to avoid excess fluid buildup in the ion source housing.

The recommended starting settings for the spray voltage are independent of the LC flow rate:

- Positive polarity mode: 3500 V
- Negative polarity mode: 2500 V

The recommended starting temperature for the ion transfer tube heater depends on whether the mass spectrometer's ion transfer tube has an elongated bore or a narrow bore.

Table 22. Recommended starting settings for the H-ESI source at various LC flow rates

LC Flow Rates ($\mu\text{L}/\text{min}$)	≤ 14.99	15 – 99.99	100 – 199.99	200 – 499.99	500 – 999.99	1000 – 3000
Sheath gas (arb)	5	25	35	50	60	75
Aux gas (arb)	2	5	7	10	15	25
Sweep gas (arb)	0	0	0	1	2	2
Vaporizer temp ($^{\circ}\text{C}$)	20	75	275	350	350	400
Nitrogen consumption (L/min)	3.5	8	10.5	15	20	25
Ion transfer tube temp ($^{\circ}\text{C}$)						
Altis Plus, Altis, and Quantiva	325	325	325	325	380	380
Quantis Plus, Quantis, and Endura	300	300	300	325	350	375
Fortis Plus and Fortis	275	275	300	325	325	350

Recommended LC/APCI/MS parameters

For the APCI ion source, the recommended setting for the Corona Discharge Voltage depends on the polarity:

- Positive ion discharge current: 4 μA
- Negative ion discharge current: 10 μA

Table 23. Recommended starting settings for the APCI source at various LC flow rates

LC Flow Rates ($\mu\text{L}/\text{min}$)	≤ 14.99	15 – 99.99	100 – 199.99	200 – 499.99	500 – 999.99	1000 – 3000
Sheath gas (arb)	10	15	25	45	45	45
Aux gas (arb)	2	5	5	5	10	10
Sweep gas (arb)	0	0	0	1	2	2
Vaporizer temp ($^{\circ}\text{C}$)	0	275	325	350	400	400
Nitrogen consumption (L/min)	4	7	8	12	16	16
Ion transfer tube temp ($^{\circ}\text{C}$)						
Altis Plus, Altis, and Quantiva	300	300	300	325	375	375
Quantis Plus, Quantis, and Endura	275	275	275	300	325	350
Fortis Plus and Fortis	250	250	250	275	300	325

Recommended LC/NSI/MS parameters

The LC flow rate range for nanospray ionization is 10 to 1000 nL/min.

Spray voltage (V)	Sweep gas (arb units)	Ion transfer tube temp ($^{\circ}\text{C}$)
Positive mode: 1200	0	325
Negative mode: 600		

Optimize 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.

For information, see these topics:

- [View the Performing Compound Optimization animation](#)
- [Set up the MS system for compound optimization](#)
- [Optimize the source parameters in the Optimization pane](#)

View the Performing Compound Optimization animation

You can find animations for various procedures on the product page for your TSQ Series II mass spectrometer.

❖ To view the animation that describes compound optimization

1. To view the animation, go to thermofisher.com.
2. Go to the product page. For example, type the product name in the search box and press ENTER.
3. In the search results list, select the product of interest.
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** in the animations list.

Set up the MS system for compound optimization

❖ To set up the MS and the syringe pump for compound optimization

1. Set up the system to infuse the target compound by high-flow infusion as follows:
 - a. Fill the syringe with a solution of the target compound at a concentration of 100 to 1000 ng/mL.

- b. Plumb the system as follows:
 - Connect the sample line from the syringe to a union Tee.
 - Connect the solvent flow from the LC system to the union Tee.
 - Connect the third leg of the union Tee to the grounding union on the ion source housing.
2. In the Tune window, set the syringe pump to infuse the sample at an initial flow rate of 5 $\mu\text{L}/\text{min}$. Then, increase the flow rate as necessary based on the peak intensity of the sample you are infusing.
3. Set the LC pump to deliver mobile phase at the analytical flow rate specified in the instrument method and the solvent composition at which the target compound elutes from the LC column.

For plumbing instructions see “[High-flow infusion without an autosampler](#),” in [Appendix D](#), “[Sample introduction techniques](#).”

Optimize the source parameters in the Optimization pane

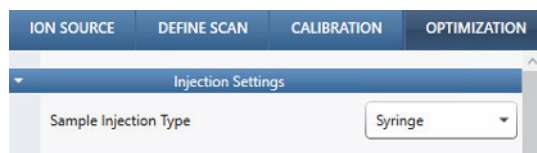
IMPORTANT Thermo Fisher Scientific recommends that you optimize source parameters if the analyte response is low or if you observe high injection-to-injection variability, which might indicate unstable spray stability.

❖ To optimize the parameter settings for compounds of interest

1. Make sure that the syringe has enough of the sample solution.
2. Plumb the system for high-flow infusion. See “[Set up the MS system for compound optimization](#)” on [page 123](#).
3. Place the system in **On** mode.
4. In the Tune window, click the **Ion Source** tab to display the Ion Source pane. Then, enter the source conditions provided by the Set Default feature for the flow rate that you are using.
5. Set the mobile phase from the LC system to the flow rate and solvent composition in the instrument method.
6. In the Tune window, click **Syringe Off** to turn on the syringe pump.
The button name changes to Syringe On.

7. Click the **Optimization** tab. Then, do the following in the Optimization pane:

a. Under Injection Settings, select **Syringe** in the Sample Injection Type list.



b. In the Mass List Type list, select **Precursor** or **Formula**.

- For the Formula mass list type, select one or both ion polarity modes from the Polarity list. Then, specify the adducts to include.
- For the Precursor mass list type, select the **Positive** polarity mode or the **Negative** polarity mode.


IMPORTANT Thermo Fisher Scientific recommends using the theoretical masses for the precursor masses. Enter that mass into the table.

c. In the Source Optimization list, select **On** and then select the **Spray Voltage** check boxes.

d. For a SIM scan, select the **Source Fragmentation** check box and, depending on MS, the **RF Lens** check box or the **Tube Lens** check box. For an SRM scan, also select **On** in the Product Ion Optimization list.

Note Other than the number of product ions, the default values are sufficient for most experiments:

- Product Ion Type: Unknown
- Number of Product Ions: 1 (Modify this setting as appropriate.)
- Exclude Loss Mass (m/z): None
- Low Mass Exclusion (m/z): 10

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 as an additional column in the Optimization Table.

Figure 69. Optimizing the source parameters in the Optimization pane

The screenshot displays the Optimization pane with the following settings:

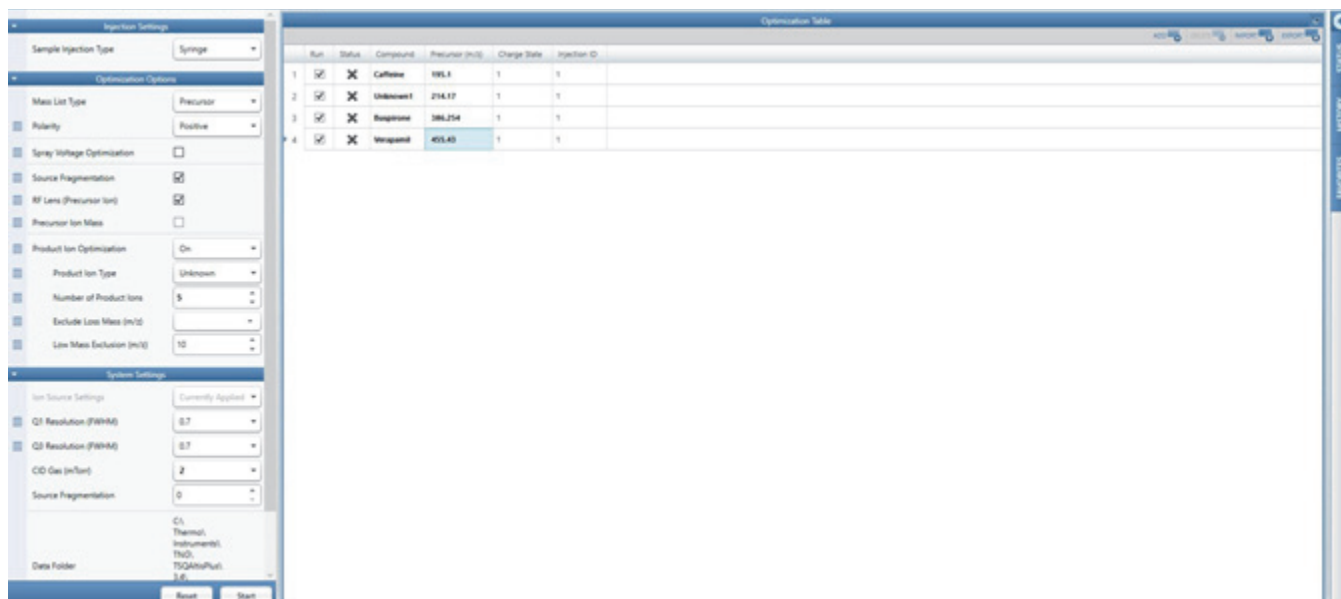
- Sample Injection Type: Syringe
- Optimization Options:
 - Mass List Type: Precursor
 - Polarity: Positive
 - Spray Voltage Optimization:
 - Adjust Start Voltage:
 - Start Voltage: 1500
 - Source Fragmentation:
 - RF Lens (Precursor Ion):
 - Precursor Ion Mass:
 - Product Ion Optimization: On
 - Product Ion Type: Unknown
 - Number of Product Ions: 4
 - Exclude Loss Mass (m/z):
 - Low Mass Exclusion (m/z): 10
- System Settings:
 - Ion Source Settings: Currently Applied
 - Q1 Resolution (FWHM): 0.7
 - Q3 Resolution (FWHM): 0.7
 - CID Gas (mTorr): 1.5
 - Source Fragmentation: 0

Buttons: Reset, Start

8. 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.

Figure 70. Adding the Optimization Table



9. Click **Start**.

After the optimization is complete, the Acquisition Table appears (Figure 71.) (The values for Sheath Gas, Auxiliary Gas, and Sweep Gas in the Tune window source conditions are included in the Source Optimization Results table.)

This table 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 for each compound. You can copy these values to the Method Editor to create an Instrument Method.

Figure 71. Results for source optimization plus compound optimization

The screenshot displays the Thermo Scientific TSQ Altis Plus software interface. The top navigation bar includes sections for ION SOURCE, DEFINE SCAN, CALIBRATION, and OPTIMIZATION. The OPTIMIZATION pane is active, showing two tables: 'Optimization Results' and 'Source Optimization Results'.

Optimization Results Table:

Select	Run ID	Compound	Polarity	Precursor (m/z)	Product (m/z)	Collision Energy (V)	Intensity	Source Fragmentation	RF Lens (V)
<input checked="" type="checkbox"/>	1	Caffeine	Positive	194.971	137.967	20.83	391916.5	26.531	71
<input checked="" type="checkbox"/>	1	Caffeine	Positive	194.971	109.967	25.27	77045.1	26.531	71
<input checked="" type="checkbox"/>	1	Lidocaine	Positive	235.063	85.967	19.61	285531.07	24.49	54
<input checked="" type="checkbox"/>	1	Lidocaine	Positive	235.063	57.967	33.72	29674.51	24.49	54
<input checked="" type="checkbox"/>	1	Buspirone	Positive	386.138	121.967	33.29	43649.4	0	95
<input checked="" type="checkbox"/>	1	Buspirone	Positive	386.138	265.05	29.13	2339.99	0	95
<input checked="" type="checkbox"/>	1	Verapamil	Positive	455.257	164.967	29.99	179231.16	0	94
<input checked="" type="checkbox"/>	1	Verapamil	Positive	455.257	303.05	27.34	41486.14	0	94

Source Optimization Results Table:

Select	Run ID	Compound	Polarity	Spray Current (µA)	Sheath Gas (Arb)	Aux Gas (Arb)	Sweep Gas (Arb)
<input type="radio"/>	1	Caffeine	Positive	1.11	5	1	0
<input type="radio"/>	1	Lidocaine	Positive	1.11	5	1	0
<input type="radio"/>	1	Buspirone	Positive	1.11	5	1	0
<input type="radio"/>	1	Verapamil	Positive	1.11	5	1	0

The interface also includes a left sidebar with 'Open All Raw Files', 'Create Method', 'Copy to Define Scan', and 'Copy to Ion Source' buttons. The bottom status bar shows 'Back to Setup' and 'Clear' buttons.

Acquire sample data

To manually acquire sample data, use either the Tune application, the Xcalibur data system, or equivalent data acquisition software.

Note Before you begin, check the following:

- In the Calibration pane, ensure that all calibrations are up to date.
- Refer to the getting connected guide for your mass spectrometer.

See the following topics:

- [View an animation about creating an SRM method](#)
- [Use the Tune application to acquire sample data](#)
- [Use the Xcalibur data system to acquire sample data](#)
- [Use the templates in the Method Editor to set up the MS experiment](#)

View an animation about creating an SRM method

❖ **To view an animation about creating an SRM method**

1. Go to thermofisher.com.
2. Go to the product page. For example, type the product name in the search box and press **ENTER**.
3. In the search results list, select the product of interest.
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**.

Use the Tune application to acquire sample data

You can acquire sample data with the Tune application by setting the data acquisition parameters in the Tune window or by loading the parameter settings from an instrument method.

❖ To acquire sample data by using the Tune application

1. Open the Tune application.
2. Do one of the following:
 - Click the **Ion Source** tab and specify the ion source settings in the Ion Source pane. Then, click the **Define Scan** tab and specify the scan settings in the Define Scan pane.

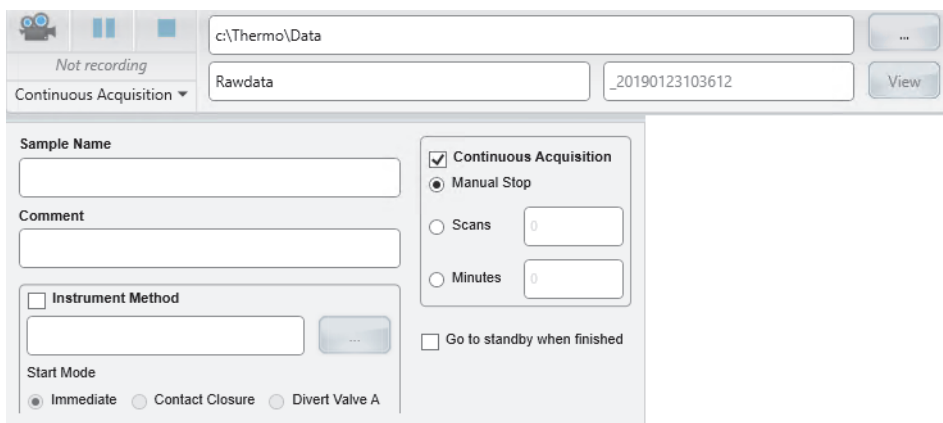
–or–

- Define the ion source and scan settings by selecting an instrument method in [step 5](#).
3. Place the MS in **On** mode.
 4. Click **Continuous Acquisition** to open the dropdown acquisition options pane.

By default, the Continuous Acquisition check box is selected and the Instrument Method check box is clear. In addition, the Manual Stop option is selected for the Continuous Acquisition mode.


Selecting the Instrument Method check box clears the Continuous Acquisition check box and changes the text on the Continuous Acquisition button to Instrument Method.

Figure 72. Data acquisition pane



5. Do one of the following:

- Keep the default setup for data acquisition.

With the default data acquisition settings, you must click the **Stop** icon, , to stop data acquisition.

- Modify the setup for the Continuous Acquisition mode by selecting the **Scans** option or the **Minutes** option. Then in the box at the right, type the number of scans to acquire or the number of minutes to acquire scan data, respectively.

When you select the Scans option or the Minutes option, data acquisition automatically stops after the MS acquires the specified number of scans or the specified time elapses, respectively.

- Select the **Instrument Method** check box. Browse to and select an instrument method. Then, select the Start Mode—**Immediate**, **Contact Closure**, or **Divert Valve**.

When you select the Instrument Method mode, data acquisition automatically stops at the end of the method.

6. (Optional) Select a different destination folder, specify a custom file name for the raw data file, and add more information to the raw data file as follows:

- To change the destination folder for the raw data file, click the **Browse** icon. Then, browse to the destination folder where you want to store the raw data files.

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

- In the File Name box, type a custom file name for the raw data file.

The default file name is Rawdata with an appended time stamp.

Rawdata	_20190123103612
---------	-----------------


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

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

10 Acquire sample data

Use the Tune application to acquire sample data

7. For the Continuous Acquisition mode, click the **Record** icon, , to start data acquisition.

After the Tune parameters reach their specified settings, the data acquisition process begins and the following text appears below the Record icon—Recording in Progress.

8. When you are ready, click the **Stop** icon, , to stop data acquisition.

For information about reviewing the acquired data, refer to the FreeStyle Help.

Use the Xcalibur data system to acquire sample data

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

- If the data system 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.

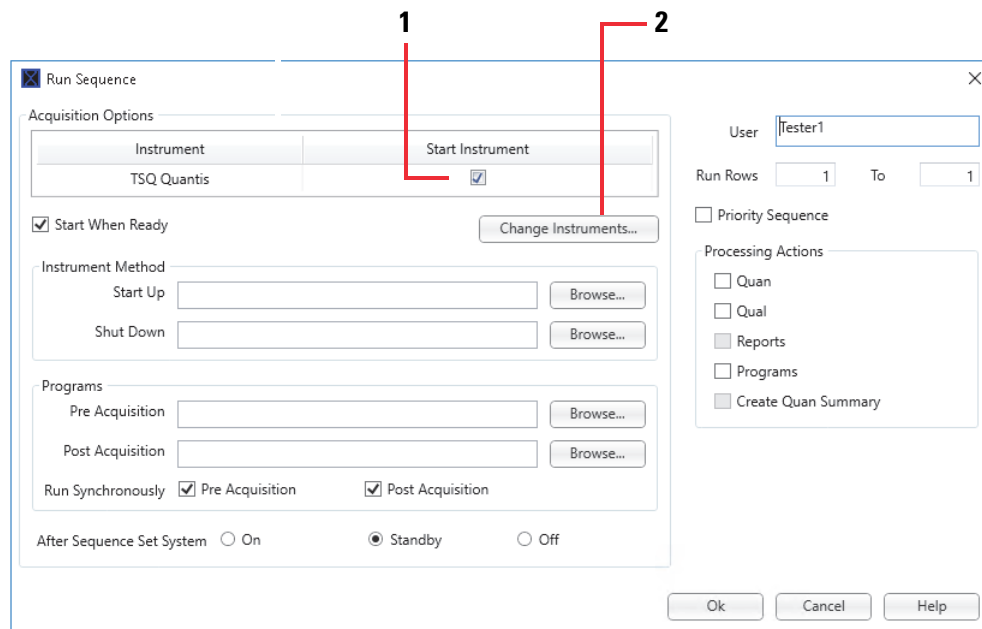
Note For example, for a TSQ Series II MS with a PaperSpray ion source, the Xcalibur data system selects the MS as the start instrument. To run the sequence, you must make sure that no instrument is selected as the start instrument.

❖ To select the 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 73).

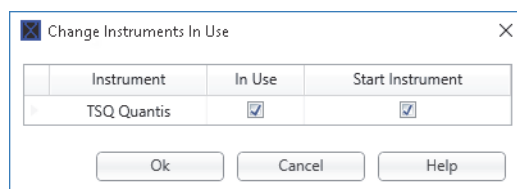
The check mark in the Start Instrument column indicates the default start instrument for the sequence run.

In Figure 73, the TSQ Quantis MS is incorrectly set as the start instrument, possibly because the data system does not control the external autosampler, the autosampler has not been added to the instrument configuration, or the PaperSpray ion source is installed.

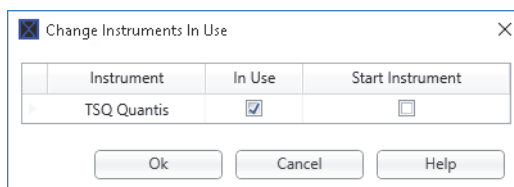
Figure 73. Run Sequence dialog box (partial) showing the selected start instrument

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

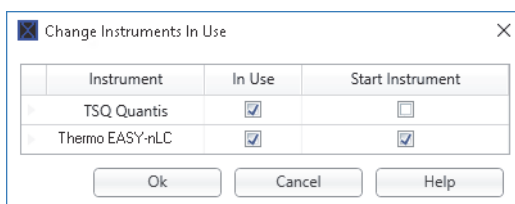
4. If the correct instrument is not selected as the start instrument, do the following:
- Click **Change Instruments** to open the Change Instruments In Use dialog box (Figure 74).

Figure 74. Change Instrument in Use dialog box with the MS incorrectly selected as the start instrument

- 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.



- If the system includes an autosampler that the data system controls, make sure that it is selected as the Start Instrument.



Tip If the system includes an autosampler that the data system controls, troubleshoot why it is not listed as an instrument in use. Fix the error. Then, reopen the Run Sequence dialog box.

- c. Click **OK**.

Note If you do not submit the sequence to the acquisition queue, the data system does not store any changes you make in the Change Instruments in Use dialog box.

5. In the Run Sequence dialog box, complete the remaining selections.
6. Click **OK**.

Use the templates in the Method Editor to set up the MS experiment

The Method Editor in the Xcalibur Instrument Setup window (Figure 75) has templates for different experiment types, including environmental and food safety (EFS) and peptide analysis (PA), for example.

From the Xcalibur Instrument Setup window, you can use the Method Editor to specify the data acquisition settings for your MS 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).

Note An Xcalibur instrument method includes the chromatographic conditions for the liquid chromatograph, the injection settings for the autosampler, and the data acquisition settings for the MS.

For additional information, refer to the Help.

Figure 75. Templates in the Method Editor

The screenshot displays the Method Editor interface with two panels. Panel 1 (left) shows the 'System Templates' section with a grid of buttons for various experiment types: Clinical Research, Environmental, Food Safety Analysis (with sub-buttons for Pesticides and Vet Medicines), Forensic Toxicology, Peptide Analysis, Pharma, Survey & Target, Custom Templates, and My Experiments. Panel 2 (right) shows the 'Scan Parameters' section with a table of scan types and a graph of 'Dwell Time per Tra' vs 'Time (min)'. The table lists various scan types like SRM, Full Scan Q1, and Product Ion Scan, along with their retention times and other parameters. The graph shows dwell time values for different scan types over a 10-minute period.

Compound	Retention Time (min)	RT Window (min)	Polarity	Precursor (m/z)	Product (m/z)	Collision Energy (V)	
878	Difenacoum	9.874	0.5	Positive	445.18	291.054	18.34
879	Fenpyroximat	9.885	0.5	Positive	422.207	215.111	25.42
880	Fenpyroximat	9.885	0.5	Positive	422.207	231.111	24.56
881	Fenpyroximat	9.885	0.5	Positive	422.207	366.183	14.9
882	Abamectin-b1a+	9.952	0.5	Positive	890.526	305.111	24.11
883	Abamectin-b1a+	9.952	0.5	Positive	890.526	307.169	19.56
884	Abamectin-b1a+	9.952	0.5	Positive	890.526	567.262	12.83
885	Resmethrin	10.034	0.5	Positive	339.195	128	42.76
886	Resmethrin	10.034	0.5	Positive	339.195	143.054	24.76
887	Resmethrin	10.034	0.5	Positive	339.195	171.125	14.9
888	Resmethrin	10.034	0.5	Positive	339.195	293.111	14.25
889	Resmethrin NH4	10.036	0.5	Positive	356.222	128.05	41
890	Resmethrin NH4	10.036	0.5	Positive	356.222	143.06	26
891	Resmethrin NH4	10.036	0.5	Positive	356.222	171.07	16
892	Brodifacoum	10.16	0.5	Positive	523.09	178.054	33.71
893	Brodifacoum	10.16	0.5	Positive	523.09	256.111	34.02
894	Brodifacoum	10.16	0.5	Positive	523.09	335	21.48
895	Etofenprox-NH4	10.245	0.5	Positive	394.238	106.982	39.83
896	Etofenprox-NH4	10.245	0.5	Positive	394.238	177.04	14.25
897	Etofenprox-NH4	10.245	0.5	Positive	394.238	359.165	10.25
898	Fenazacuin	10.294	0.5	Positive	307.18	56.889	23.2
899	Fenazacuin	10.294	0.5	Positive	307.18	147.054	20.47
900	Fenazacuin	10.294	0.5	Positive	307.18	161.183	17.79

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

Maintenance

The following topics describe the routine maintenance procedures you must perform to maintain the optimum performance of your TSQ Series II MS.

Note For information about removing and installing the API source housing, refer to its user guide.

- [Maintenance schedule](#)
- [Guidelines for performing maintenance](#)
- [Maintenance animations on the Thermo Fisher Scientific website](#)
- [Tools and supplies for routine maintenance procedures](#)
- [Maintain the API source housing](#)
- [Maintain the external components of the API source interface](#)
- [Maintain the internal components of the API source interface](#)
- [Maintain the forepumps](#)
- [Maintain the air filter](#)

Maintenance schedule

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



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 mass spectrometer (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.

Table 24 lists the maintenance procedures and their recommended frequency.

For instructions about maintaining any of the LC modules, refer to the manual for that instrument.

Table 24. Mass spectrometer maintenance procedures and frequency (Sheet 1 of 2)

MS component	Procedure	Recommended frequency	Reference topic
API source (external)	Flush (clean) the sample transfer line, sample tube, and spray insert.	After acquiring samples	“Flush the inlet components” on page 83
	Clean the API source housing.	As needed	“Maintain the API source housing” on page 142
	Clean the APPI fan filter.	As needed	Refer to the ion source guide.
	Replace the APPI lamp.	As needed	
	Replace the H-ESI needle insert.	When the metal needle is obstructed	
Replace the APCI fused-silica tubing.	When the tubing is obstructed		
API source interface	Clean the ion sweep cone and the spray cone.	Weekly or more often depending on the analytical conditions	“Clean the ion sweep cone and the ion transfer tube” on page 150 “Clean the spray cone” on page 149
	Remove and clean the ion transfer tube.	Weekly or when the ion transfer tube bore becomes contaminated or obstructed	“Remove the ion transfer tube” on page 146 “Clean the ion sweep cone and the ion transfer tube” on page 150
	Replace the ion transfer tube.	If the bore becomes corroded or blocked	“Remove the ion transfer tube” on page 146
	Clean the exit lens or the RF lens.	As needed, depending on analytical conditions	“Clean the lenses” on page 163
	Clean the MP00 multipole and L0 lens.	As needed, depending on the analytical conditions	“Clean the MP00 multipole” on page 165

Table 24. Mass spectrometer maintenance procedures and frequency (Sheet 2 of 2)

MS component	Procedure	Recommended frequency	Reference topic
Forepump (each)	Purge (ballast) the oil of volatile solvents and check for leaks.	Weekly	Manufacturer's manual
	Add oil.	As needed, based on the oil level	
	Change the oil.	Every 12 months of typical use, or when the oil becomes cloudy or discolored	
Cooling fans	Clean the air filter.	Every 4 months	"Maintain the air filter" on page 170

Guidelines for performing maintenance

Follow these guidelines:

- 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 might recontaminate the clean parts.
- Always place the components on a clean, lint-free work surface.
- Gather the necessary tools, supplies, and replacement parts (when applicable) before you begin the maintenance procedure.
- Never overtighten the screws, and avoid excessive force when you reassemble components.

IMPORTANT Make sure that you do not introduce any scratches or surface abrasions while handling the 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" on page 16.



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

Maintenance animations on the Thermo Fisher Scientific website

You can view maintenance animations for the TSQ Series II mass spectrometers that are currently shipping worldwide from their respective product pages on the Thermo Fisher Scientific website.

Note Thermo Fisher Scientific has discontinued the TSQ Endura and TSQ Quantiva mass spectrometers.

❖ To view the animations

1. Go to thermofisher.com.
2. Open the product page for your MS as follows:
 - a. In the Search All field, type the *model*, for example, **TSQ Altis Plus**.
 - 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 The *Removing and Cleaning the Ion Transfer Tube* video shows you how to remove, clean, and reinstall the ion transfer tube.

Tools and supplies for routine maintenance procedures

The MS requires few tools to perform routine maintenance procedures. You can remove and disassemble many of the components by hand. [Table 25](#) lists the necessary chemicals, tools, and equipment for maintaining the instrument.

The TSQ Source Installation Kit includes the custom tools that you use to remove and install the ion transfer tube and L0 lens.

**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 25. Chemicals, tools, and equipment (Sheet 1 of 2)

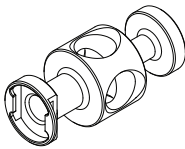
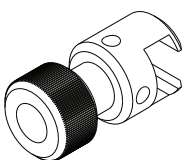
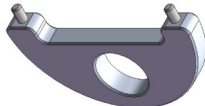
Description	Part number
Chemicals	
Detergent (for example, Liquinox™)	(Liquinox) Fisher Scientific™ <ul style="list-style-type: none"> • 16-000-125 (1 quart) • 16-000-126 (1 gallon)
Methanol, UHPLC/MS-grade	Fisher Scientific A458-1
Nitrogen gas, clean and dry	–
Water, UHPLC/MS-grade	Fisher Scientific W8-1
Tools	
Ion transfer tube removal tools for the following models:	(in the TSQ Source Installation Kit)
<ul style="list-style-type: none"> • In these models, the ion transfer tube is secured with a quarter-turn pin behind its nose cone: <ul style="list-style-type: none"> – TSQ Altis MS and TSQ Altis Plus MS – TSQ Quantiva MS 	70005-20972 
<ul style="list-style-type: none"> • In these models the ion transfer tube is secured with a threaded nose cone. <ul style="list-style-type: none"> – TSQ Quantis MS and TSQ Quantis Plus MS – TSQ Fortis MS and TSQ Fortis Plus MS – TSQ Endura MS 	70111-20258 

Table 25. Chemicals, tools, and equipment (Sheet 2 of 2)

Description	Part number
L0 lens removal tool	70005-20900
	
Screwdriver, Phillips #2 (M3)	—
(Optional) Toothbrush, soft (or similar tool)	—
(Optional) Tweezers, plastic (or similar tool)	—
Equipment	
Beaker or graduated cylinder (for use with methanol)	—
Chamois-tipped swabs	00725-01-00028
Gloves, lint-free and powder-free	Fisher Scientific 19-120-2947
	Unity Lab Services: <ul style="list-style-type: none"> • 23827-0008 (size medium) • 23827-0009 (size large)
Industrial tissues, lint-free	—
Magnification device	—
MICRO-MESH™ polishing swabs, 6000 grit (light purple color), 2.25 in. long	Purchase these swabs from a third-party vendor.
Sonicator	—

Maintain the API source housing


Clean the API source housing as necessary. Follow all safety precautions in the ion source guide. For any additional service, contact your local service engineer.

See these topics:

- [Remove the API source housing from the MS](#)
- [Clean the API source housing](#)

Remove the API source housing from the MS


❖ To remove the API source housing from the MS

1. Turn off the liquid flow from the syringe pump or the liquid chromatograph, as applicable.
2. In the Tune application, click the **System Standby** icon, , to place the MS in Standby mode.



CAUTION Hot surface. The external surface of the housing can be hot enough to burn your skin. Allow the housing to cool to room temperature (approximately 20 minutes) before you touch it.

3. In the Ion Source pane, set the Ion Transfer Tube Temperature and Vaporizer Temperature to 50 °C or less and observe the readback temperatures.
4. After the source cools to room temperature, remove the source housing. Refer to the ion source user guide for information about removing and installing the ion source.

Tip To access the ion source user guides that are available from the Tune window, click the settings icon, . Then, from the dropdown menu, choose **Instrument Manuals**, select the PDF that you want to view, and click **Open**.

Clean the API source housing

❖ To clean the API source housing after you remove it from the MS

1. Make sure that the source housing is cooled to room temperature. Then, remove the API source housing as described in “[Remove the API source housing from the MS.](#)”
2. Put on appropriate personal protective equipment, in particular safety glasses and chemical-resistant gloves.
3. Under an appropriate fume hood, wipe down the interior of the housing with lint-free tissues sprayed with UHPLC/MS-grade methanol.
4. Allow the housing to dry before you reinstall it on the MS.

IMPORTANT When you are not using the MS for short periods of time, keep the MS in Standby mode. In Standby mode, a constant stream of nitrogen exits the API source interface, keeping particulate matter from entering the MS.

Maintain the external components of the API source interface

Because buffer salts and high concentration samples can cause blockages, you must clean the ion sweep cone, the ion transfer tube, and the spray cone on a regular basis.

If the pressure in the ion transfer tube and RF lens region (as measured by the Source Pressure gauge) drops below the pressure listed in Table 26, the ion transfer tube is probably blocked, and you might need to replace it.

Table 26. Source Pressure gauge reading that indicates the ion transfer tube might be blocked

TSQ Series II model	Pressure reading
TSQ Altis MS, TSQ Altis Plus MS, and TSQ Quantiva MS	<2 Torr
All the other models in the TSQ Series II product line	<1 Torr

Clean the following external components of the API source interface at the same time:

- Ion sweep cone
- External surface of the spray cone
- Ion transfer tube

Replace the ion transfer tube if the cleaning procedure does not remove the blockage.



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 sweep cone or ion transfer tube. You do not need to remove the spray cone to clean its external surface.

To maintain the ion sweep cone, the ion transfer tube, and the spray cone, follow these steps:

1. “Remove the ion sweep cone” on page 145
2. “Remove the ion transfer tube” on page 146
3. Clean the following components:
 - “Clean the spray cone” on page 149
 - “Clean the ion sweep cone and the ion transfer tube” on page 150
4. “Reinstall the ion transfer tube” on page 151
5. “Reinstall the ion sweep cone” on page 152
6. “Verify the cleaning process for the external components of the API source” on page 153

Remove the ion sweep cone

The ion sweep cone fits snugly over the spray cone. To clean the inner and outer surfaces of the ion sweep cone, you must remove it from the MS.

❖ To remove the ion sweep cone

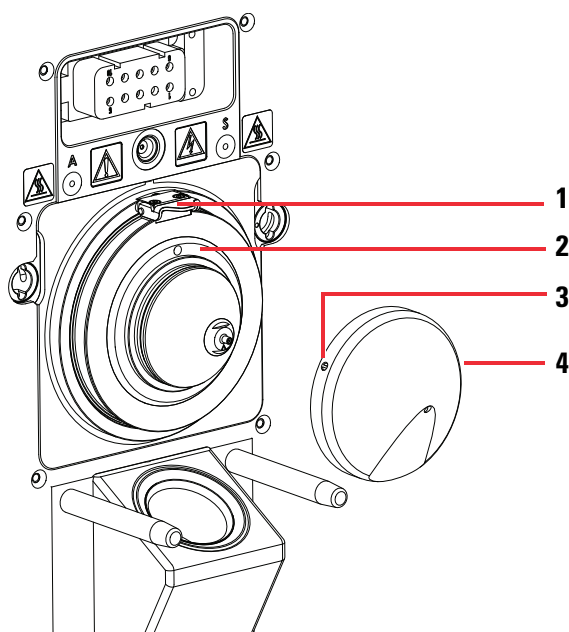
1. Remove the API source housing as described in “Maintain the API source housing” on page 142.
2. Grasp the outer ridges of the sweep cone and pull it off the API source interface (Figure 76). If necessary, loosen the screws on the ion sweep cone with a flat-head screwdriver.



CAUTION

- Make sure that you do not accidentally lift the release lever that is located above the sweep cone, as releasing the lever will vent the MS.
- To avoid contaminating the ion transfer tube, do not touch its exposed entrance.

Figure 76. 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

Remove the ion transfer tube

Removing or installing the ion transfer tube requires the custom tool that is provided in the TSQ Source Installation Kit. This kit includes two ion transfer tube removal tools. The tool you need depends on whether the ion transfer tube is secured by a quarter-turn pin or a threaded fitting.

Table 27. TSQ Series II models categorized by how the transfer tube is secured to the source

MS model	Attachment type
<ul style="list-style-type: none"> • TSQ Altis Plus • TSQ Altis Plus • TSQ Quantiva 	Quarter-turn pin
<ul style="list-style-type: none"> • TSQ Quantis Plus • TSQ Quantis • TSQ Fortis Plus • TSQ Fortis • TSQ Endura 	Threaded fitting

Follow the appropriate procedure for your TSQ Series II MS:

- [Remove an ion transfer tube that is secured with a quarter-turn pin](#)
- [Remove an ion transfer tube that is secured with a threaded fitting](#)

Remove an ion transfer tube that is secured with a quarter-turn pin

This procedure describes how to remove the ion transfer tube from the following models:

- TSQ Altis Plus MS
- TSQ Altis MS
- TSQ Quantiva MS

❖ To remove the ion transfer tube

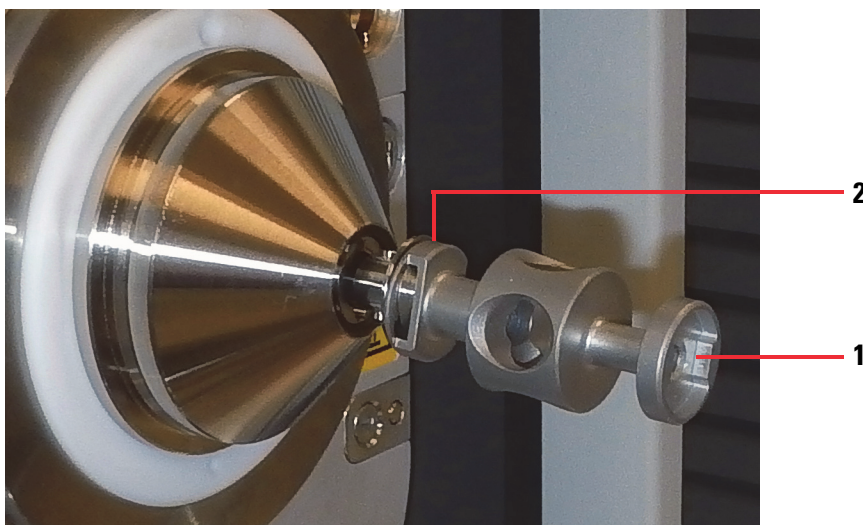
1. Remove the API source housing. See [“Maintain the API source housing”](#) on page 142.
2. Remove the ion sweep cone by grasping its outer ridges and pulling it away from API source interface. See [“Remove the ion sweep cone”](#) on page 145.
3. Align the flat end of the 1/4 turn ion transfer tube removal tool with the flat edges on the ion transfer tube’s nose cone.
 - a. 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 77. Turning the nose cone counterclockwise by a quarter turn



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

Figure 78. Pulling the transfer tube out of the API source interface



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 78).

To clean the ion transfer tube, go to [“Clean the ion sweep cone and the ion transfer tube”](#) on [page 150](#).

Remove an ion transfer tube that is secured with a threaded fitting

This procedure describes how to remove the ion transfer tube from the following models:

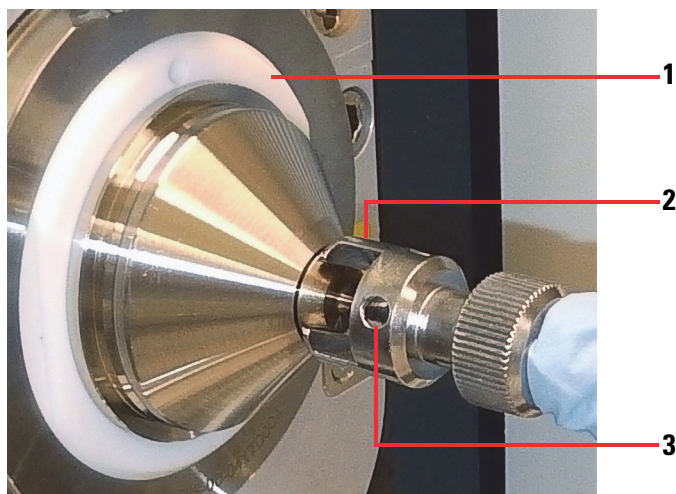
- TSQ Quantis Plus
- TSQ Quantis
- TSQ Fortis Plus
- TSQ Fortis
- TSQ Endura

❖ To remove the ion transfer tube

1. Align the hook end of the ion transfer tube removal tool with the flat edges of the ion transfer tube's nose cone.
2. 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 79. Ion transfer tube removal tool (for tube with a threaded nose cone)



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

3. 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 80 shows how to pull the ion transfer tube out of the API source interface.

Figure 80. Pulling the tube out of the spray cone

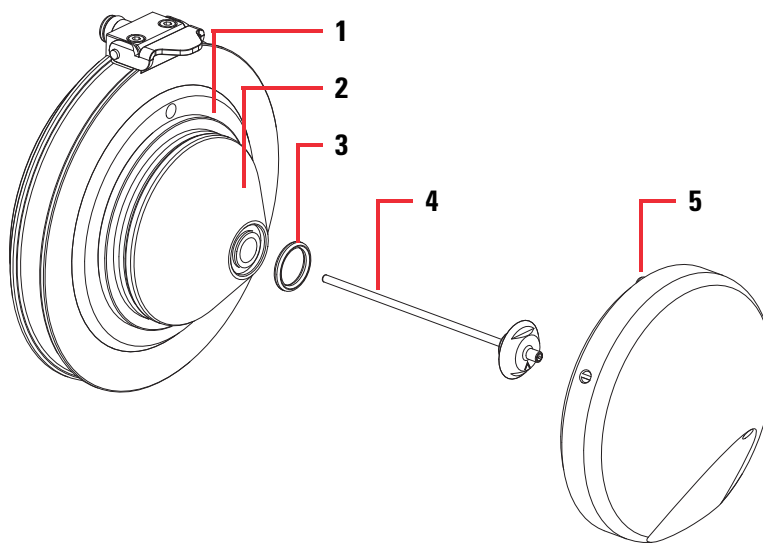


Clean the spray cone

❖ To clean the spray cone and its seal

1. Remove the sweep cone and the ion transfer tube. See “Remove the ion sweep cone” on page 145 and “Remove the ion transfer tube” on page 146.
2. Soak a lint-free tissue or a chamois-tipped swab in a 50:50 solution of methanol/water, and then clean the exterior surface of the spray cone.

Figure 81. Spray cone, seal, ion transfer tube, and ion sweep cone



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

3. If you see a leak at the seal, do the following:
 - a. Remove and inspect the seal located in the spray cone under the entrance end of the ion transfer tube (Figure 81).
 - b. Clean the seal with a wipe with methanol or replace the seal, if necessary.
 - c. 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.

- d. Reinstall the seal in the spray cone.

Clean the ion sweep cone and the ion transfer tube

Before you can clean the ion transfer tube and the ion sweep cone, you must first remove them from the API source interface. See “Remove the ion sweep cone” on page 145 and “Remove the ion transfer tube” on page 146.

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

❖ To clean the ion sweep cone and the transfer tube after you remove them from the API source interface

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-free 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. Rotating the ion transfer tube helps push the vent prevent ball out of the way.

Reinstall the ion transfer tube

After you remove the ion transfer tube to clean it or replace it or to access other components of the API source interface, follow these instructions to reinstall it.

❖ To reinstall the ion transfer tube

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

Note As you insert the tube, you feel a slight resistance from the vent prevent ball. After you push the vent prevent ball out of the way, the system vacuum draws the tube further into the API source housing.

3. Depending on the ion transfer tube type, do one of the following:
 - For an ion transfer tube that has a quarter-turn pin behind its cone face, align the tube's pin with the slot in the API source interface. Then, use the flat end of the 1/4 turn ion transfer tube removal tool to turn the tube clockwise by a quarter turn.
 - For an ion transfer tube that has a threaded fitting behind its cone face, 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.

Reinstall the ion sweep cone

❖ To reinstall the ion sweep cone

1. Align the pins on the back of the ion sweep cone with the receptacles on the API source interface.

Figure 82. Back and side views of the ion sweep cone

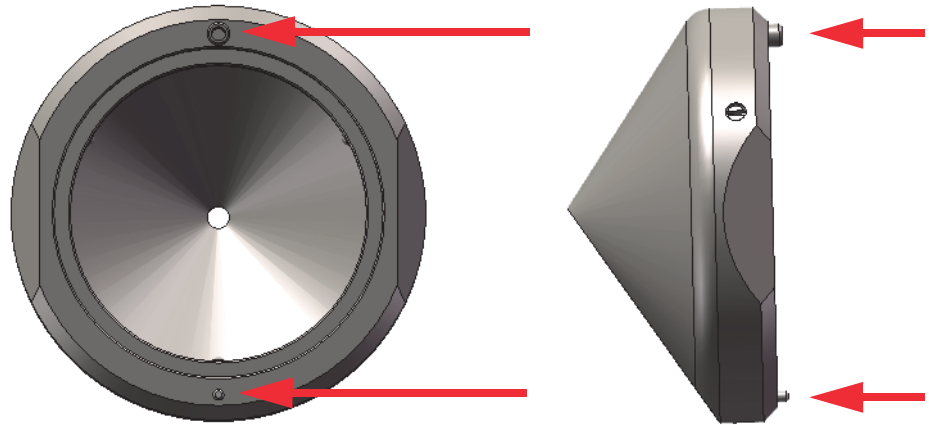
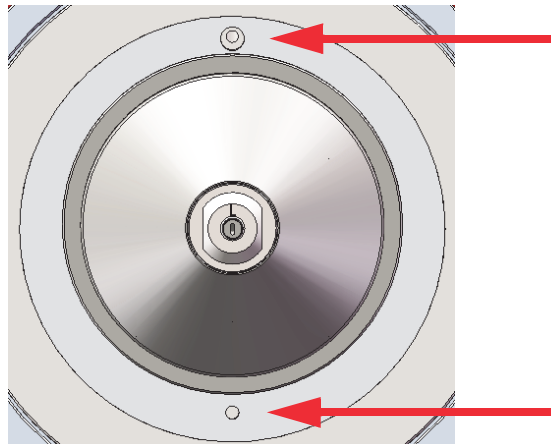


Figure 83. View of the white ceramic ring and the two receptacles for the ion sweep cone above and below the spray cone.



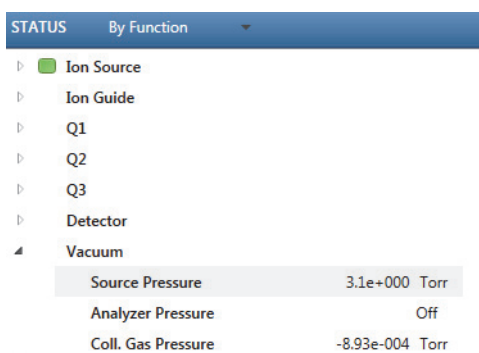
2. As you fit the ion sweep cone onto the spray cone, press the ion sweep cone firmly so that there are no gaps between the sweep cone and the white ceramic ring on the API source interface.

Verify the cleaning process for the external components of the API source

After you remove, clean, and reinstall the external components of the API source, follow this procedure to check for any blockage.

❖ To verify that the cleaning process unblocked the ion transfer tube

1. In the Tune window, open the Status pane, and then double-click **Vacuum**.



2. Verify that the Source Pressure and Analyzer Pressure readback values are below the operating threshold limits.

Normal readback measurements show a green square (■). If the ion transfer tube is blocked, the values are closer to 0 than those in [Table 28](#). Replace the tube if it is still blocked. A leak results in higher values than those in [Table 28](#).

Table 28. Vacuum specification with ion transfer tube installed and unblocked

MS model	Source pressure (Torr)
TSQ Altis Plus	< 3.8
TSQ Altis	< 3.8
TSQ Quantis Plus	< 2.0
TSQ Quantis	< 2.0
TSQ Fortis Plus	< 2.0
TSQ Fortis	< 2.0
TSQ Endura	< 2.5
TSQ Quantiva	< 4.5

Maintain the internal components of the API source interface

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 first vent the system, remove the components from the MS, and then remove the lenses from the source interface cage.

Table 29. Internal components of the API source interface by model

MS model	Internal API source components that require maintenance
All the TSQ models except for the TSQ Fortis and TSQ Fortis Plus	Exit lens, MP00 multipole, L0 lens, and the RF lens
TSQ Fortis Plus and TSQ Fortis	Skimmer and tube lens (MSIG), MP00 multipole, and L0 lens

IMPORTANT Thermo Fisher Scientific recommends wearing nitrile or powder-free gloves for cleaning the API source.

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

1. “Vent the mass spectrometer and remove the API source interface” on page 155
2. Remove the lenses from the source interface cage by following the applicable procedure:

MS model	Procedure
TSQ Fortis and TSQ Fortis Plus	“Remove the MP00 assembly, the skimmer, and the tube lens (TSQ Fortis and TSQ Fortis Plus only)” on page 159
All the other models	“Remove the MP00 assembly, the RF lens, and the exit lens from the source interface cage” on page 156

3. Clean the lenses and the MP00 multipole:
 - “Clean the lenses” on page 163
 - “Clean the MP00 multipole” on page 165
4. “Reinstall the components of the API source interface cage” on page 165
5. “Reinstall the API source interface cage” on page 169

Vent the mass spectrometer and remove 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 [Shut down the MS system completely for planned service or storage](#) before you start this procedure.

❖ To vent the MS and remove the API source interface

1. Shut down and vent the mass spectrometer as described in “[Shut down the MS system completely for planned service or storage](#)” on [page 88](#).
2. Let the API source housing cool to room temperature.

Venting the MS can take several minutes.



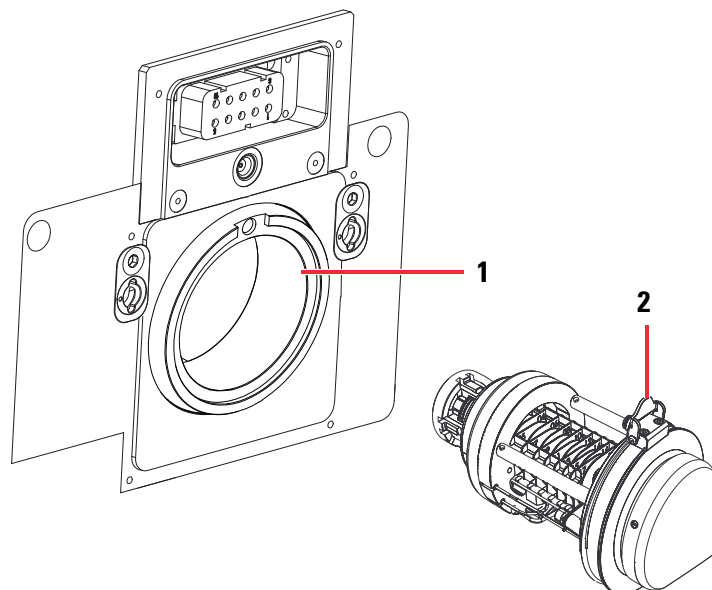
CAUTION Hot surface. The external surface of the spray insert, housing, and entry to the ion transfer tube can become hot enough to burn your skin. Before you touch or remove heated parts, allow the part to cool to room temperature (approximately 20 minutes) before you touch it.

3. Unplug the mass spectrometer’s power supply cord from the laboratory electrical outlet.



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

4. Remove the API source housing. Refer to the ion source guide.
5. Remove the API source interface as follows:
 - a. Lift up the release latch and firmly push it to unseal the API source interface from the vacuum manifold.
 - b. Grasp the API source interface with your fingers, and then carefully pull it out of the vacuum manifold ([Figure 84](#)).

Figure 84. API source interface removed from the vacuum manifold

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

Go to the appropriate procedure to remove the components from the API source interface:

- For all TSQ Series II mass spectrometers (except the TSQ Fortis and TSQ Fortis Plus), go to the next procedure, “[Remove the MP00 assembly, the RF lens, and the exit lens from the source interface cage](#)” on page 156.
- For the TSQ Fortis and TSQ Fortis Plus, go to “[Remove the MP00 assembly, the skimmer, and the tube lens \(TSQ Fortis and TSQ Fortis Plus only\)](#)” on page 159.

Remove the MP00 assembly, the RF lens, and the exit lens from the source interface cage

Follow this procedure for all the TSQ Series II mass spectrometers except for the TSQ Fortis and TSQ Fortis Plus models.

Preconditions

The MS is vented and cooled to room temperature.

Required tools

2 mm Allen wrench and L0 lens removal tool

❖ **To remove the MP00 assembly, the RF lens, and the exit lens from the source interface**

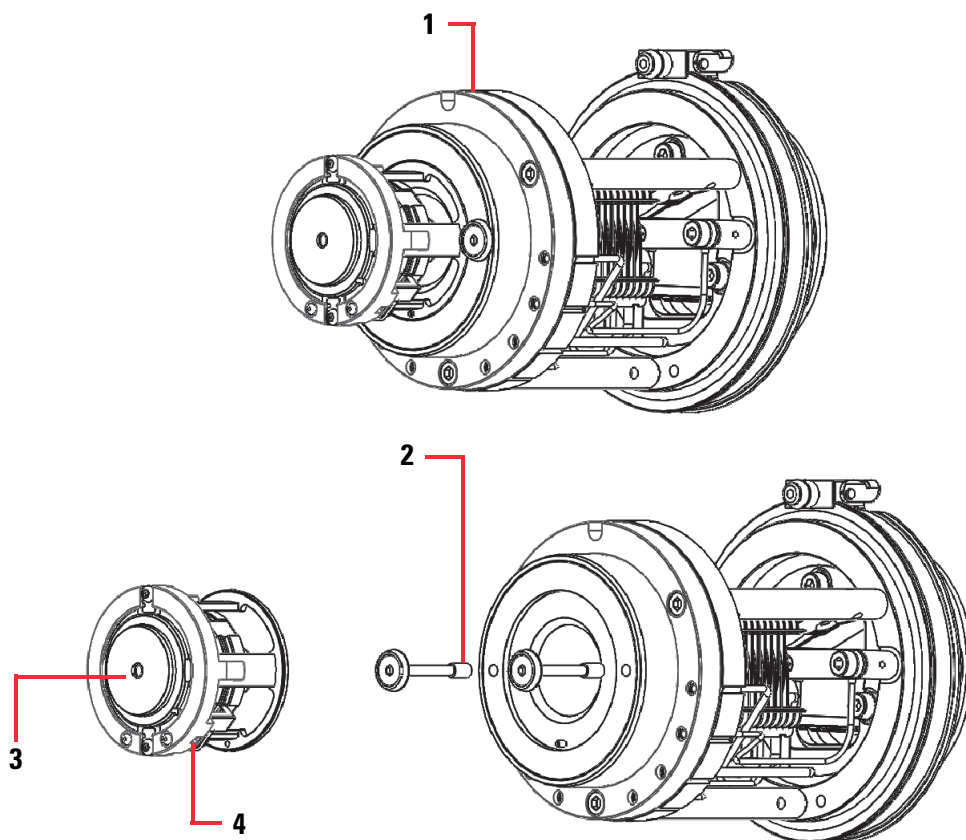
1. Wearing clean, lint-free and powder-free gloves, use a 2-mm Allen wrench to loosen and extend (if captive) or remove the two Allen screws that secure the exit lens, the MP00 multipole, and the L0 lens to the cage.

Note In the TSQ Endura and TSQ Quantiva mass spectrometers and older versions of the TSQ Altis and TSQ Quantis mass spectrometers, two captive screws secure the MP00 assembly to the cage. In newer versions of the TSQ Altis and TSQ Quantis and all versions of the TSQ Altis Plus and TSQ Quantis Plus mass spectrometers, you can remove the two Allen screws from the cage.

2. Pull the MP00 assembly off of the cage, and place the assembly on a clean, lint-free surface.

Figure 85 shows the location of the multipole and the two Allen screws that secure the exit lens, the MP00 multipole, and L0 lens to the cage.

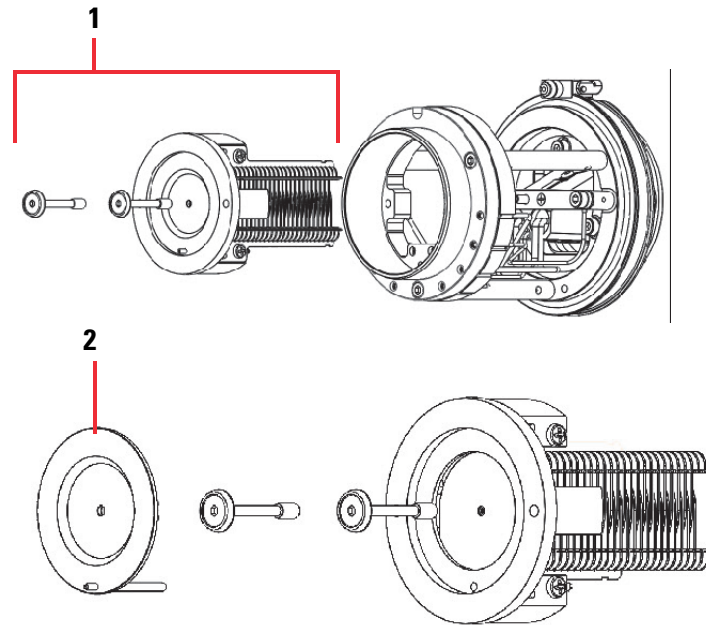
Figure 85. Removing the multipole MP00 and L0 lens assembly



No.	Description	No.	Description
1	API source interface cage	2	Allen screws removed from the cage
3	L0 lens	4	MP00 assembly (mount cage, multipole, and L0 lens)

Figure 86 shows the exit lens removed from the RF lens.

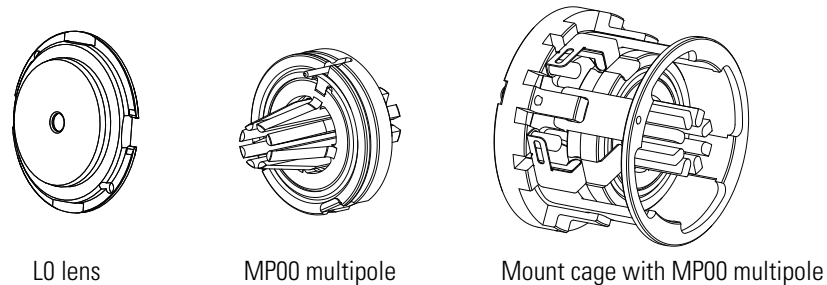
Figure 86. Removing the RF lens and the exit lens



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

3. If the Allen screws are captive, grasp them and carefully pull the RF lens with the exit lens straight out of the cage. Otherwise, push the RF lens out of the cage.
4. Separate the exit lens from the RF lens. Place both on a clean surface.
5. Using the L0 lens removal tool (or plastic tweezers), rotate the L0 lens to free it from the assembly, and then push the MP00 multipole out of the mount cage (Figure 87). Place the components on a clean surface.

Figure 87. L0 lens, MP00 multipole, and mount cage with multipole (from left-to-right)



Remove the MP00 assembly, the skimmer, and the tube lens (TSQ Fortis and TSQ Fortis Plus only)

Follow this procedure to remove the components of the source interface cage of a TSQ Fortis MS or a TSQ Fortis Plus MS.

Preconditions

The MS is vented and cooled to room temperature.

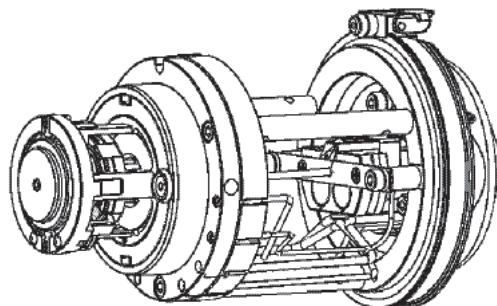
Required tools

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

❖ To remove the MP00 assembly, the skimmer, and the tube lens

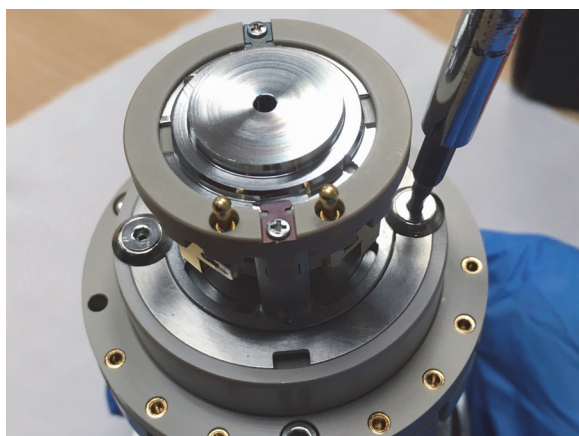
1. Wearing clean, lint-free and powder-free gloves, remove the source interface cage from the MS.

Figure 88. API source interface for the TSQ Fortis MS and TSQ Fortis Plus MS



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

Figure 89. Removing the Allen screws that secure the MP00 assembly to the cage



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

Figure 90. MP00 assembly removed from the cage (TSQ Fortis and TSQ Fortis Plus)



4. To remove the skimmer from the cage, use a small flat-head screwdriver (Figure 91) to free the skimmer from the cage. Then, lift the skimmer evenly from both sides to prevent bending the voltage contact pin.



CAUTION Because the voltage contact pin is easily bent, take care when removing the skimmer from the cage. Figure 92 shows the voltage contact pin.

Figure 91. Removing the skimmer from the cage (TSQ Fortis and TSQ Fortis Plus)

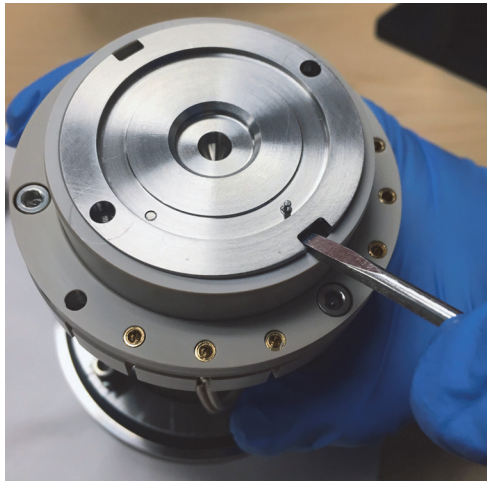
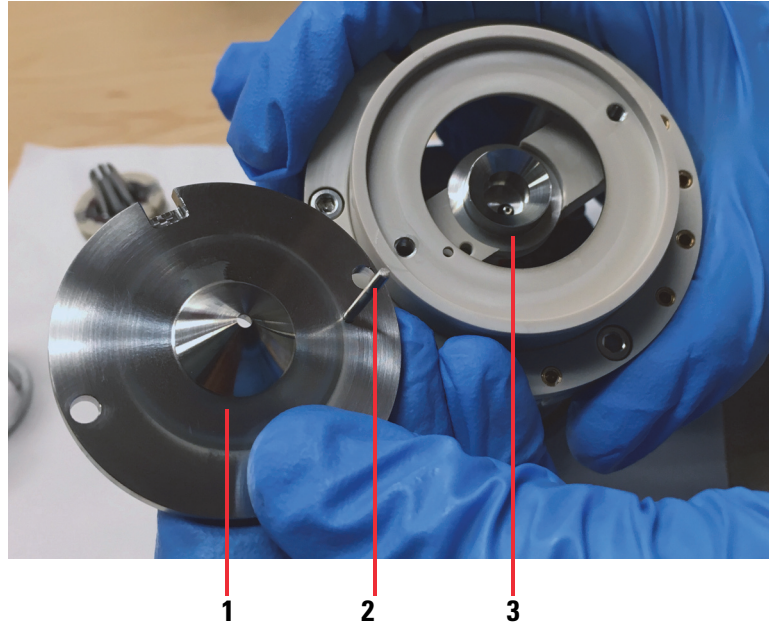


Figure 92. Skimmer removed from the cage (TSQ Fortis and TSQ Fortis Plus)

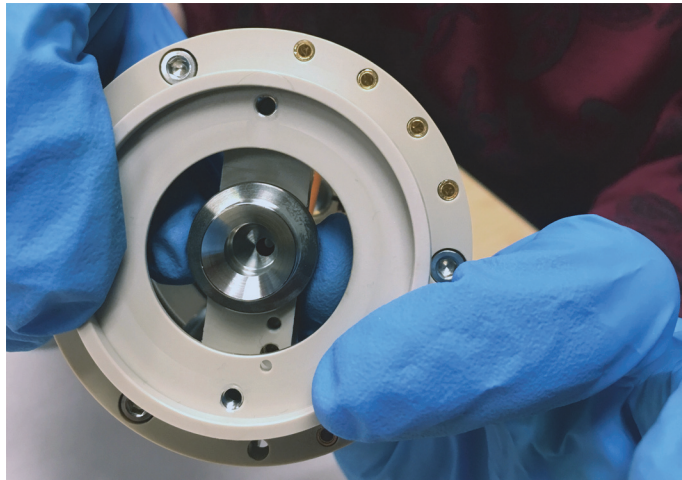


No.	Description	No.	Description	No.	Description
1	Skimmer	2	Voltage contact pin	3	Tube lens

- To remove the tube lens, push it out of the cage (Figure 93).

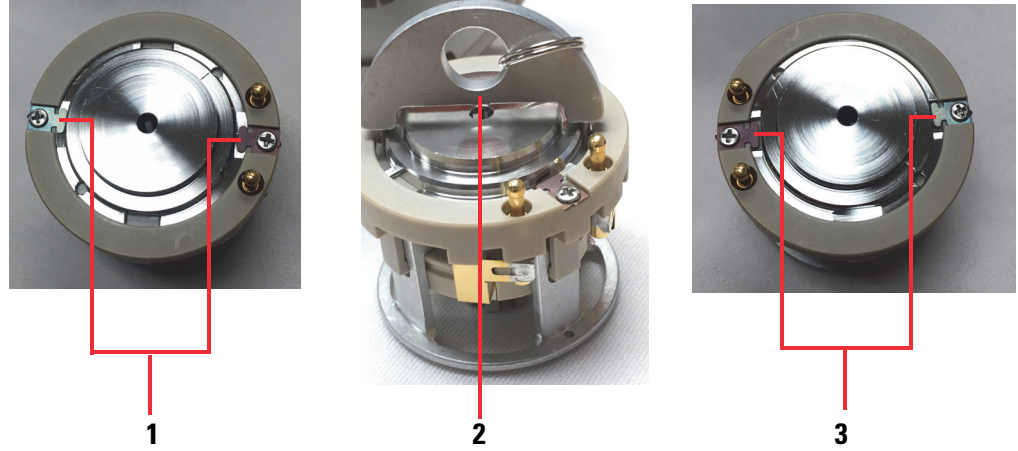
Note It can take quite a bit of force to push out the tube lens the first few times you remove it.

Figure 93. Pushing the tube lens out of the cage (TSQ Fortis and TSQ Fortis Plus)



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

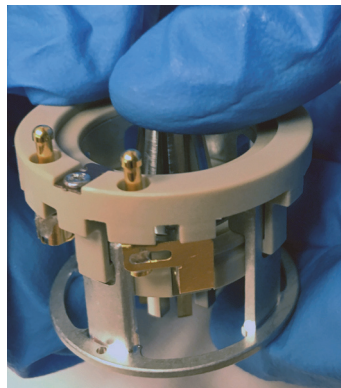
Figure 94. Using the L0 lens removal tool to rotate L0 lens



No.	Description
1	L0 lens secured to the MP00 assembly by two tabs
2	Rotating the L0 lens by a quarter turn
3	L0 lens released (but not removed) from the MP00 assembly

- Push the MP00 multipole out of the mounting cage.

Figure 95. Pushing the MP00 multipole out of the mounting cage



- Place the components on a clean surface.

Figure 96. Tube lens, skimmer, L0 lens, and MP00 multipole (from left-to-right)



Clean the lenses

Preconditions

The MS is vented and cooled to room temperature. The API source interface is removed from the MS, and the lenses are removed from the source interface cage.

Chemicals

Liquinox, UHPLC grade water, UHPLC grade methanol

Materials and equipment

- Magnification device
- Sonication bath
- Chamois-tipped swabs and 6000 grit MICRO-MESH polishing swabs

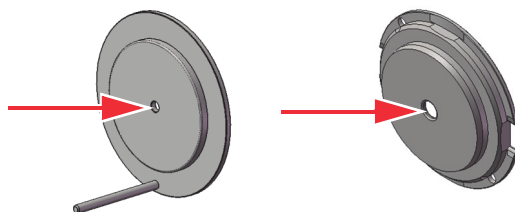


CAUTION Do not clean the lenses with abrasives, acidic or caustic substances, or detergents not specified in this chapter.

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

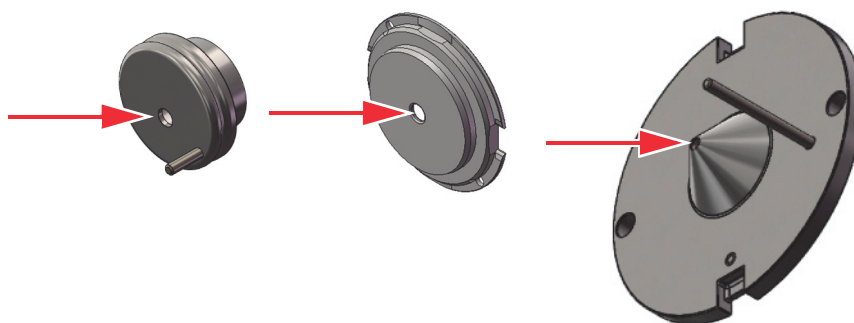
❖ To clean the lenses

- Using a magnification device, inspect the components for any lint, particulates, and sample buildup or coatings.
- Clean the bores of the lenses as follows:
 - All TSQ Series II mass spectrometers except the TSQ Fortis and TSQ Fortis Plus
For the exit lens and L0 lens, use the 6000 grit MICRO-MESH polishing swabs to clean the bore.

Figure 97. Exit lens on the left and L0 lens on the right

- TSQ Fortis and TSQ Fortis Plus

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

Figure 98. Tube lens, L0 lens, and skimmer (from left-to-right)

3. For 10 minutes, sonicate the components in a 1% solution of Liquinox in water.
4. 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.

Note Thermo Fisher Scientific recommends the use of a sonication bath to clean the lenses. If you do not have a sonication bath, consider purchasing one.

5. Thoroughly rinse the components 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. Thoroughly dry the components 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 the lint and particulates.

Clean the MP00 multipole

Preconditions

The MS is vented and cooled to room temperature. The API source interface is removed from the MS, and the lenses are removed from the source interface cage.

Chemicals

- Liquinox
- UHPLC-grade water
- UHPLC-grade methanol

Materials and equipment

- Soft toothbrush
- Chamois-tipped swabs
- Magnification device or loupe

❖ To clean 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. Thoroughly rinse the multipole 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.

Reinstall the components of the API source interface cage

After you remove the components of the API source interface cage and clean them, follow these topics as applicable to reinstall the components:

- [Reassemble the MP00 Assembly](#)
- [Reinstall the lenses and the MP00 assembly in any TSQ Series II MS except for a TSQ Fortis MS or a TSQ Fortis Plus MS](#)
- [Reinstall the lenses and the MP00 assembly \(TSQ Fortis MS or TSQ Fortis Plus MS\)](#)

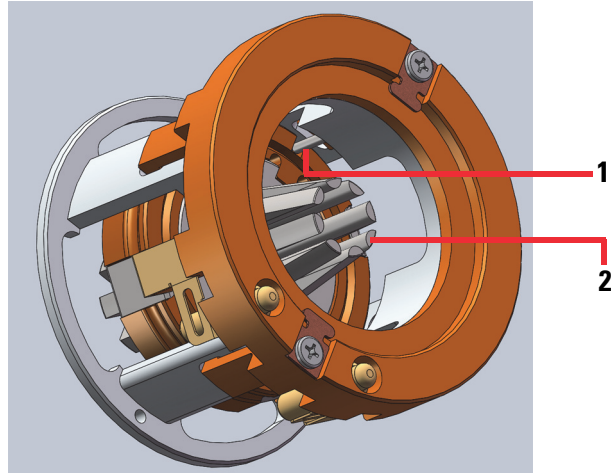
Reassemble the MP00 Assembly

Follow this procedure after you remove the MP00 assembly for cleaning.

❖ To reassemble the MP00 assembly

Align the MP00 multipole with the alignment pin in the mounting cage, and then insert the multipole into the cage.

Figure 99. Inserting the MP00 multipole into the mounting cage



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

Reinstall the lenses and the MP00 assembly in any TSQ Series II MS except for a TSQ Fortis MS or a TSQ Fortis Plus MS

After you clean the lenses, follow this procedure to reinstall the RF lens, the exit lens, the MP00 assembly, and L0 lens in the source interface cage of any TSQ Series II MS, except for the TSQ Fortis MS and the TSQ Fortis Plus MS.

❖ To reinstall the components of the source interface cage

1. Reassemble the MP00 assembly.
2. Attach the exit lens to the RF lens, and then reinsert the RF lens into the cage ([Figure 86](#) on [page 158](#)).
3. Attach the MP00 assembly to the cage, and then attach the L0 lens.

Reinstall the lenses and the MP00 assembly (TSQ Fortis MS or TSQ Fortis Plus MS)

After you remove and clean the lenses and MP00 assembly, follow this procedure to reinstall the lenses and MP00 multipole in a TSQ Fortis MS or a TSQ Fortis Plus MS.

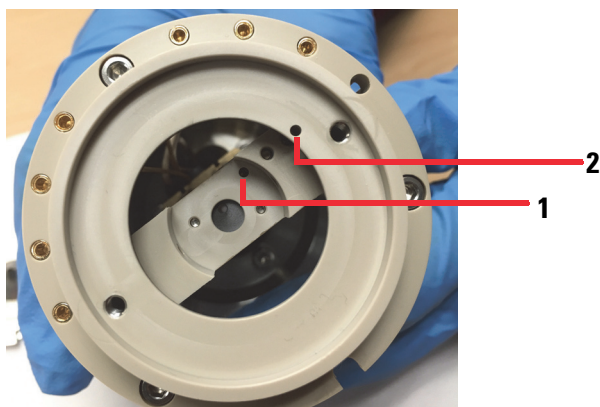
Required tools

L0 lens removal tool

❖ To reinstall the lenses and the MP00 assembly

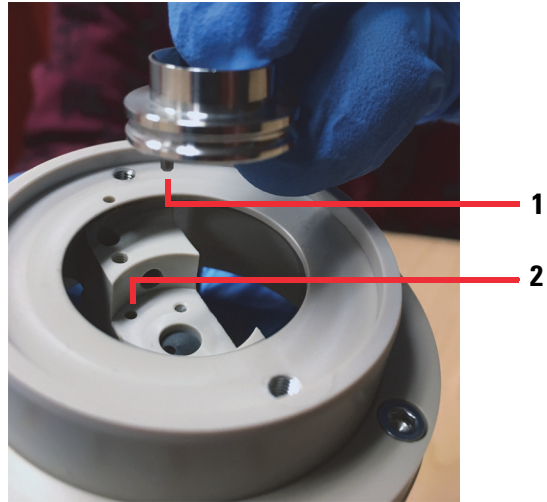
1. Reassemble the MP00 assembly. See “Reassemble the MP00 Assembly” on page 166.
2. Align the two slots in the outer ring of the L0 lens with the tabs on the mounting cage. Then, use the L0 lens removal tool to turn the L0 lens by a quarter turn.
3. Align the tube lens pin to the port in the inner circle of the API source interface cage, and then insert the lens into the cage and snap it into place.

Figure 100. 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

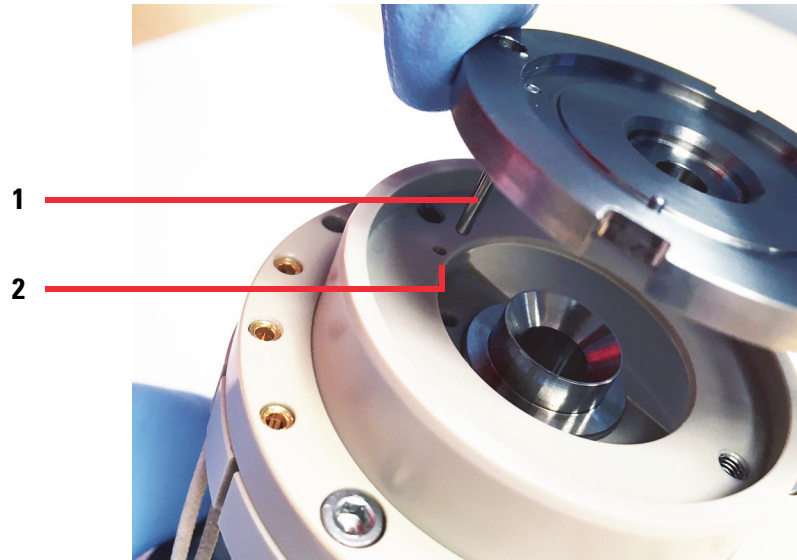
Figure 101. Installing the tube lens



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

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

Figure 102. Inserting the skimmer into the cage



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

- 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.

Reinstall the API source interface cage

After you reinstall the API source interface components in the cage, reinstall the API source interface cage in the MS, reinstall the external components of the API source interface, and reinstall the API source housing.

❖ To reinstall the API source interface cage

1. Orient the cage with the release latch at the top ([Figure 84 on page 156](#)).
2. Carefully insert the cage into the vacuum manifold.
3. Reinstall the ion transfer tube. See [“Reinstall the ion transfer tube” on page 151](#).
4. (Optional) Reinstall the ion sweep cone.
5. Reinstall the API source housing. Refer to the ion source user guide.
6. Start up the system as described in [“Restart the MS system after a complete shutdown” on page 89](#).

Maintain the forepumps

There are two forepump options for the TSQ Series II mass spectrometers:

- Roots vacuum pumps: Leybold EcoDry pump or Edwards nXL110i pump
- Oil-sealed rotary vane vacuum pumps: Oerlikon Leybold Vacuum™, SOGEVAC™ SV 65 BI

Roots vacuum pumps cannot be serviced in the field. For service or to extend the life of the forepump to prevent downtime, Thermo Fisher Scientific recommends purchasing a factory reconditioning service using the following time frame:

- Leybold EcoDry pump—Every 4 years
- Edwards nXL110i pump—Every 5 years

Maintaining the oil-sealed forepumps requires inspecting, adding, purging (ballasting), and changing the pump oil. Refer to the manufacturer’s manual for instructions.

See these topics:

- [Check the level of the forepump oil before daily use](#)
- [Purge or change the oil](#)

Check the level of the forepump oil before daily use

❖ To check the oil level

1. Make sure that the oil level is visible in the oil-level sight glass between the MIN and MAX marks.
2. If the oil level is below the MIN mark, add oil.

Purge or change the oil

New oil has a translucent, light amber color. If the oil is cloudy or discolored, purge (ballast) 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.

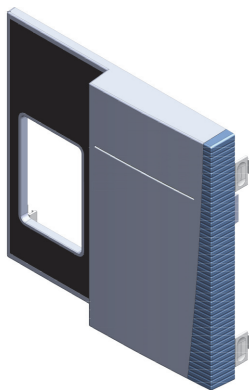
Maintain the air filter

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

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

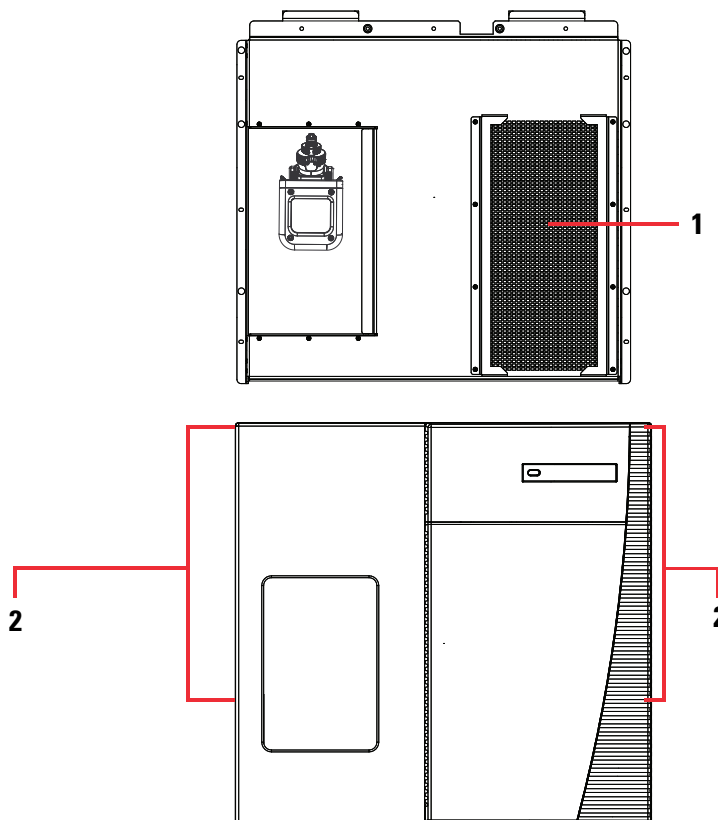
❖ To clean the air filter

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



- c. Remove the filter from the filter bracket (Figure 103).
3. Wash the air filter in a solution of soap and water.
4. Rinse the filter with tap water, and then allow it to air dry.
5. Reinstall the air filter and front cover.
6. Reconnect the plumbing tubing.

Figure 103. Air filter location in the MS with the front cover removed



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


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.

- Open the Tune window
- Set the instrument system controls
- Set the instrument power mode
- Check the instrument readback status
- Set the Tune preferences
- Use the mass list table in the Define Scan pane
- Use the History pane
- Use the Favorites pane to save the system settings

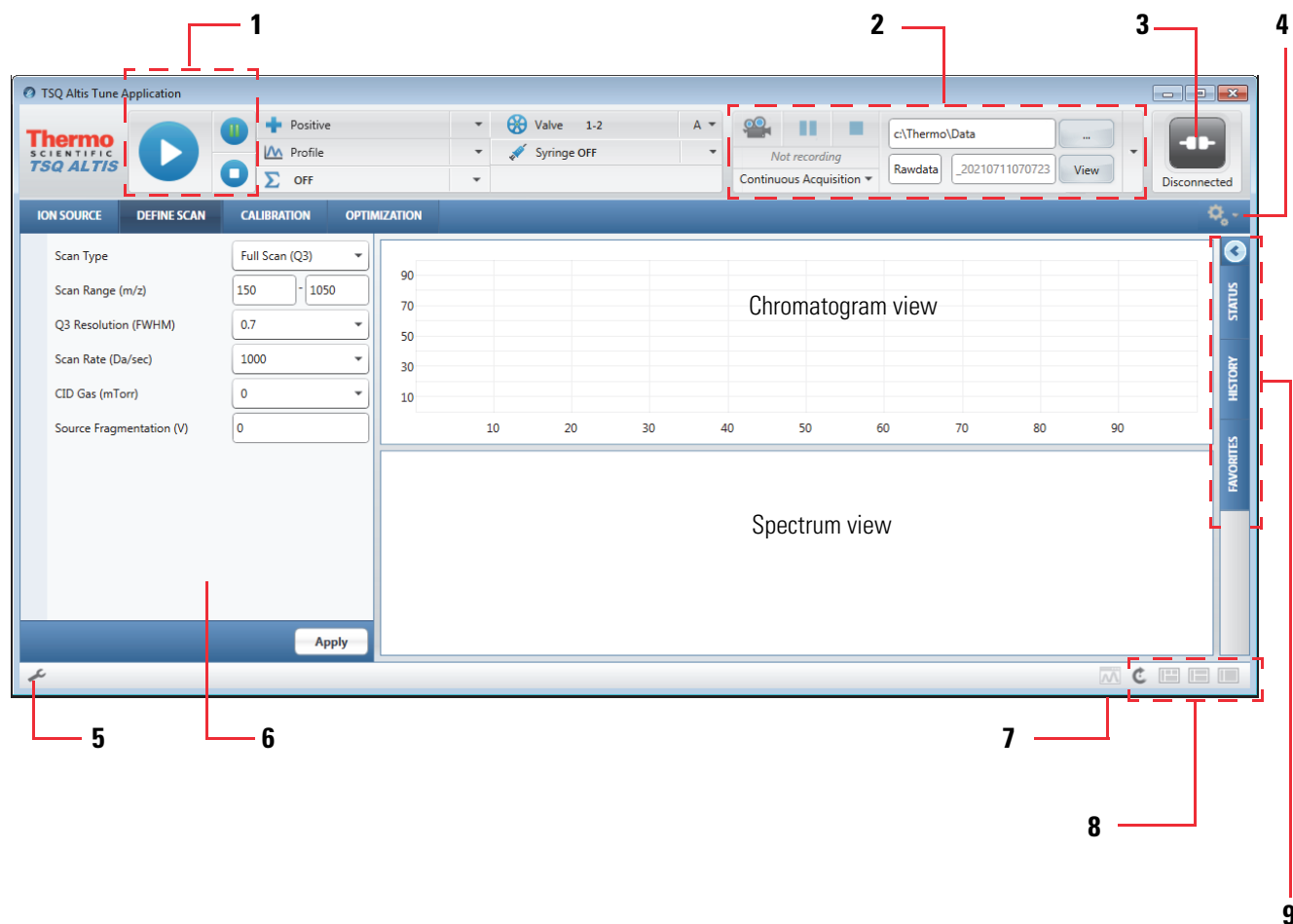
Open the Tune window

❖ To open the Tune window

From the Windows10 taskbar, click the **Start** icon, . Then, choose **Thermo Instruments > Model x.x Tune**.

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

Figure 104. Tune window showing the Define Scan pane



No.	Description	No.	Description
1	Three power mode icons (on/standby/off)	2	Manual data acquisition pane
3	Instrument readback status	4	Set Options or View Help icon
5	Diagnostics icon	6	Define Scan pane
7	Plot Chromatogram tool	8	Controls for the graphs
9	Panels: Status, History, and Favorites		

Set the instrument system controls

Table 30 shows the options for each of the system control buttons at the top of the Tune window.

Table 30. Procedures for using the instrument control buttons (Sheet 1 of 2)


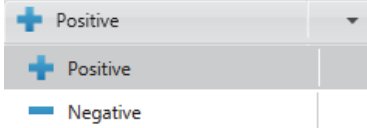
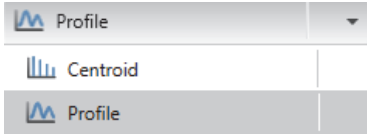
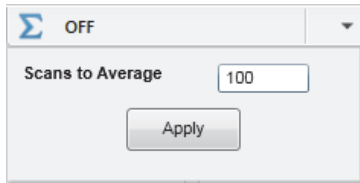
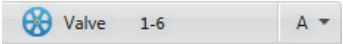
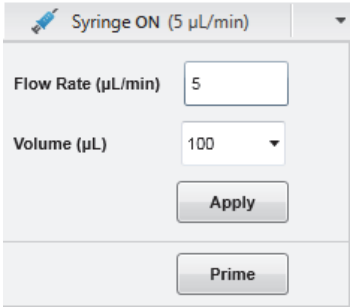
Button	Function	Procedure
	Power mode	<ul style="list-style-type: none"> ❖ To set the instrument power mode <p>Click the icon for the applicable power mode.</p> <p>The center of the selected icon changes from white to green. See Set the instrument power mode.</p>
	Ion polarity mode	<ul style="list-style-type: none"> ❖ To set the ion polarity mode <p>Click Positive (Negative) and select the ion polarity mode.</p>
	Data type	<ul style="list-style-type: none"> ❖ To set the data type <p>Click Centroid (Profile) and select the data type.</p>
	Spectrum scan averaging	<ul style="list-style-type: none"> ❖ To turn the scan averaging on or off <p>Click the button to switch between on and off.</p> <ul style="list-style-type: none"> ❖ To set the scan averaging value <p>Click the down arrow to enter the value, and then click Apply.</p>
	Divert/inject valve	<ul style="list-style-type: none"> ❖ To set the divert/inject valve module and position <p>Click the down arrow to select the valve, and then click Valve to set the position.</p>

Table 30. Procedures for using the instrument control buttons (Sheet 2 of 2)

Button	Function	Procedure
	Syringe pump	<ul style="list-style-type: none"> ❖ To turn the syringe pump on or off Click Syringe On (Off) to switch between on and off. ❖ To set the syringe pump parameters <ol style="list-style-type: none"> 1. Click the down arrow. Then, type or select 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.

Set the instrument power mode

Use the three power mode icons in the Tune window (Figure 104) to set the power mode for the MS (On, Standby, or Off).

When you remove the 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 source housing, 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 5, “System startup, shutdown, and reset.”

Check the instrument readback status

The system readback icon is located in the top right of the Tune window. Table 31 lists the various readback states.

Table 31. Instrument readback icons and their meanings (Sheet 1 of 2)







Icon	Background color	Meaning
	Green	The system parameters are within tolerance.
	Green	The system is initializing.

Table 31. Instrument readback icons and their meanings (Sheet 2 of 2)

Icon	Background color	Meaning
	Amber	One or more settings are changing.
	Red	An error has occurred or the mass calibration has expired.
	Gray	The MS is off.
	Gray	There is no communication between the MS and the data system.

Set the Tune preferences

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

❖ To set your preferences for the Tune application


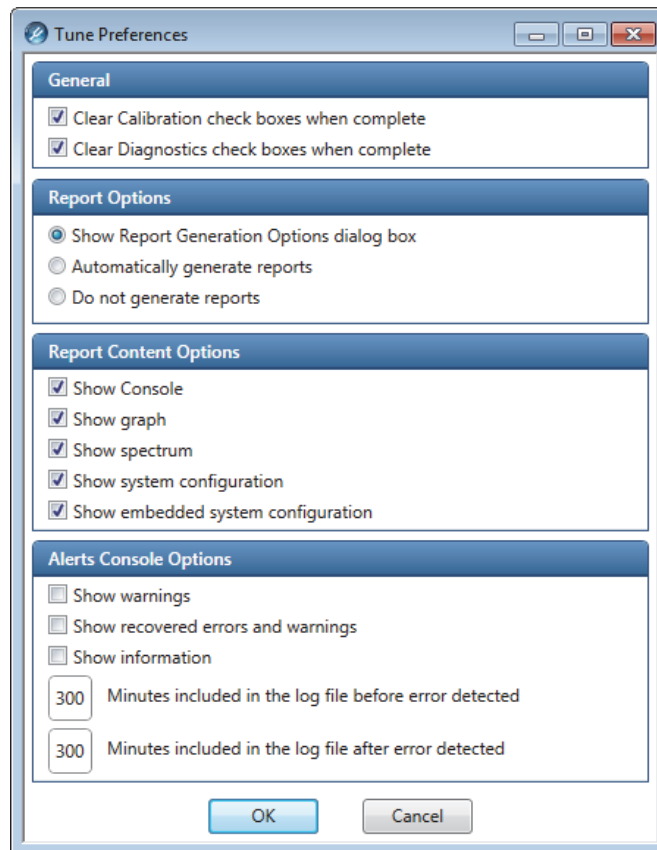
1. Click the **Set Options or View Help** icon, , and then choose **Preferences** from the dropdown menu to open the Tune Preferences dialog box (Figure 105).

Figure 105. Tune Preferences dialog box



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


Use 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.

Add a row to the table


❖ To add a row to the mass list table

Do one of the following:

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


Delete a row from the table

❖ To delete a row from the mass list 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.

Delete multiple rows from the table

❖ To delete multiple rows from the mass list 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.

Add or remove scan parameters from the scan type table

❖ To add or remove scan parameters from the scan type table


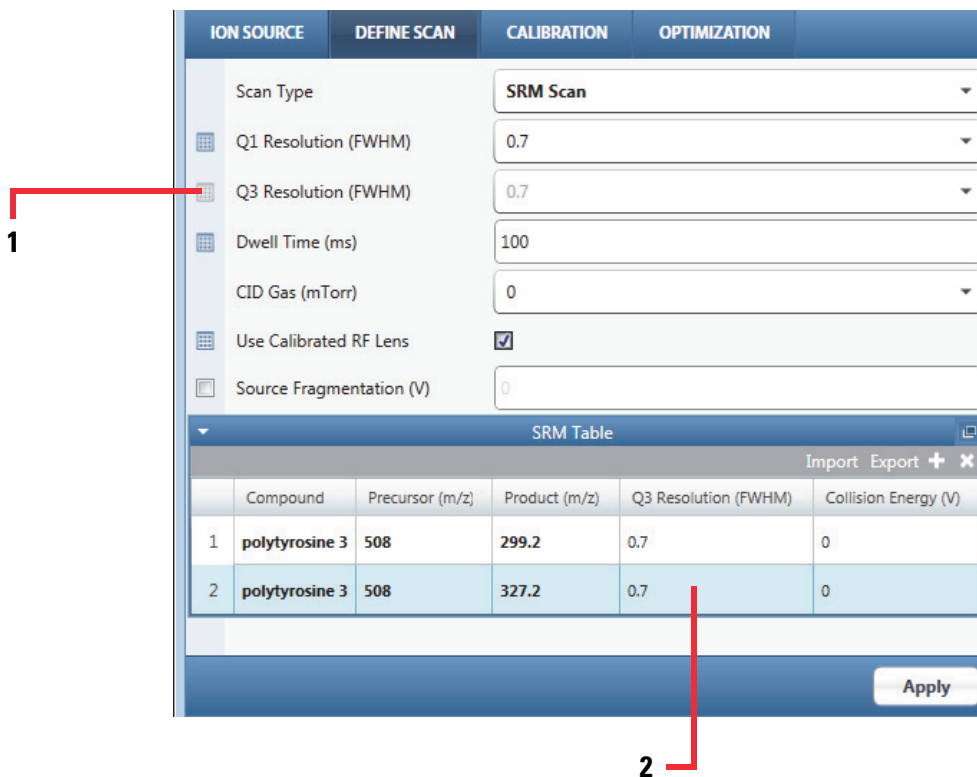
Click the **Table** icon, , once to add the adjacent scan parameter to the table. Click it again to remove the parameter from the table.

Figure 106 shows an example with Q3 Resolution added to the SRM Table.

Figure 106. Q3 Resolution selected and added to the SRM Table



The screenshot shows the 'DEFINE SCAN' pane with the following parameters:

- Scan Type: SRM Scan
- Q1 Resolution (FWHM): 0.7
- Q3 Resolution (FWHM): 0.7
- Dwell Time (ms): 100
- CID Gas (mTorr): 0
- Use Calibrated RF Lens:
- Source Fragmentation (V): 0

The SRM Table below contains the following data:

SRM Table					
Import Export + X					
	Compound	Precursor (m/z)	Product (m/z)	Q3 Resolution (FWHM)	Collision Energy (V)
1	polytyrosine 3	508	299.2	0.7	0
2	polytyrosine 3	508	327.2	0.7	0

An 'Apply' button is located at the bottom right of the pane.

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

Import a mass list from a file

You can use the contents of a mass list file to populate the columns in a scan type table in the Define Scan pane.

❖ **To import 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.

Export a mass list to a file

❖ **To export 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**.

Use 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 when they were created. The maximum number of change records is 100.
- You can display a change record's parameters by either double-clicking the record or right-clicking it and choosing **Load**. Parameters that are in bold differ from their currently set values.
- You can submit a change record's parameters to the MS by either double-clicking the record or by right-clicking it and choosing **Apply**.
- A change record is inactive if the source type of the change record differs from the current source type.

Use the Favorites pane to save the system settings

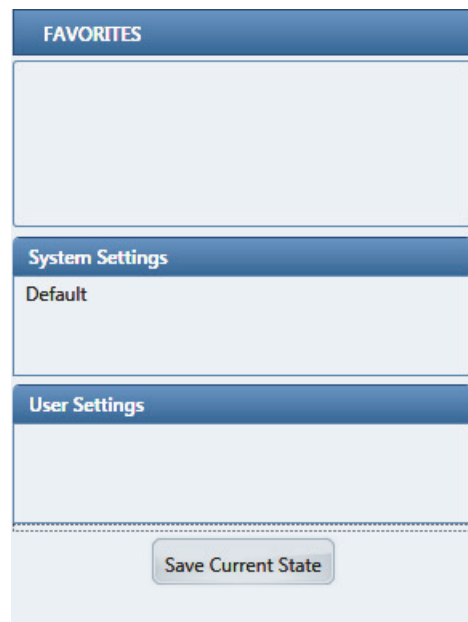
You can manually save the current settings for the source settings and scan parameters in the Favorites pane.

- 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

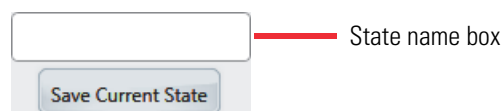
1. In the Tune window, modify the parameters in the Ion Source or Define Scan pane.
2. Click **Apply** or **Export**.
3. Click the **Favorites** tab to display the Favorites pane ([Figure 107](#)).

Figure 107. Favorites pane



4. Click **Save Current State**, and then type a unique name in the box ([Figure 108](#)).

Figure 108. 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**.

Set up the syringe and the syringe pump

To set up the syringe pump, see these topics:

- [Set up the syringe pump to infuse a sample from the syringe](#)
- [Connect the syringe union to the sample transfer line](#)

Set up the syringe pump to infuse a sample from the syringe

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

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.

❖ To set up the syringe pump

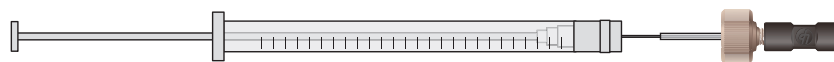
1. Load a clean, 500 μ L syringe with the sample solution.
2. Use a fingertight fitting to connect a 4 cm (1.5 in.) length of Teflon tubing to the (black) syringe union adapter.



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

3. Hold the plunger of the syringe in place and carefully insert the tip of the syringe needle into the free end of the Teflon tubing. Then, place the syringe on the syringe pump.

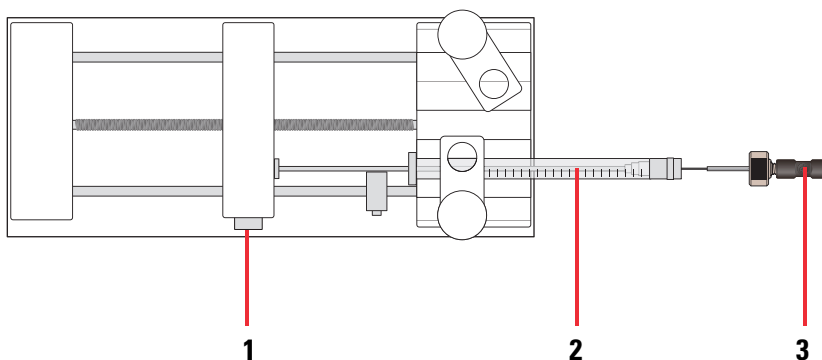
Figure 109. Syringe needle inserted into the Teflon tubing



Tip 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.

Figure 110. Syringe pump with syringe



No.	Description
1	Syringe pump release button on the pusher bar
2	Syringe with sample solution
3	Syringe needle and Teflon tubing connection to the union

Connect the syringe union to the sample transfer line

❖ To connect the syringe union to the sample transfer line

1. Using a polymeric tubing cutter, cut the ends of a 0.6 m (2 ft) length of red PEEK tubing so that they are square.

IMPORTANT Poorly cut tubing can cause flow restrictions.

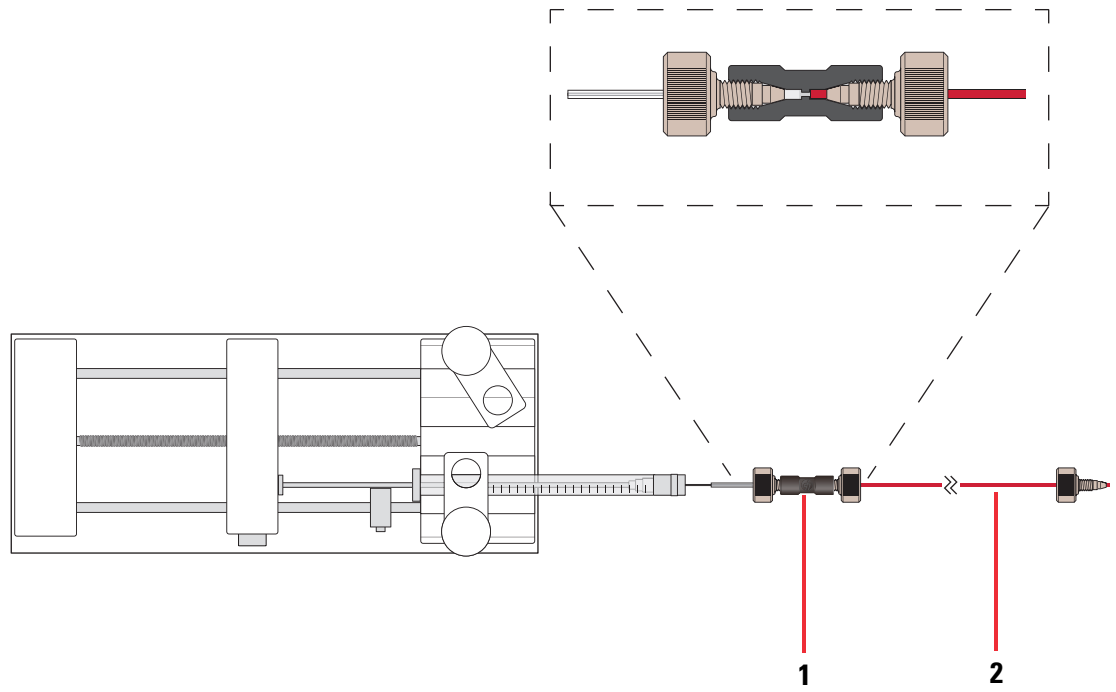
2. Make sure that the PEEK tubing is not crimped, kinked, or otherwise damaged.
3. Connect the PEEK tubing so that it contacts the bottom of the LC union's 10-32, coned-bottom receiving port.

IMPORTANT Tubing that is not properly seated can add dead volume to a chromatographic system.

4. Tighten the PEEK fittings by using only your fingers. Overtightening the PEEK fittings can cause leaks.

B Set up the syringe and the syringe pump
Connect the syringe union to the sample transfer line

Figure 111. Syringe connection to the sample transfer line



No.	Description
1	Syringe union
2	Sample transfer line

Divert/Inject valve

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

- [Divert/Inject valve positions](#)
- [Divert/Inject valve configurations](#)
- [Divert/Inject valve controls](#)

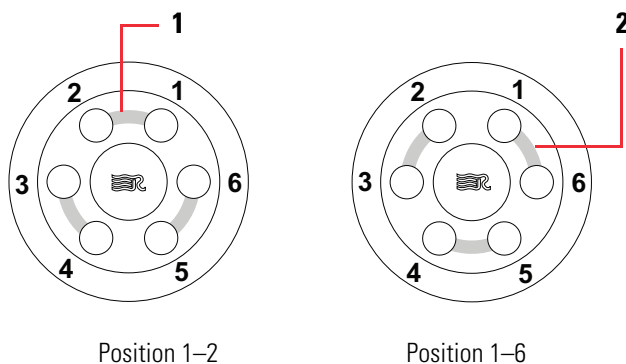
Divert/Inject valve positions

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 112](#) 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 112. Divert/inject valve positions



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

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 114](#) shows the divert valve configuration.

For details, see these topics:

- [Loop injection](#)
- [Divert valve](#)

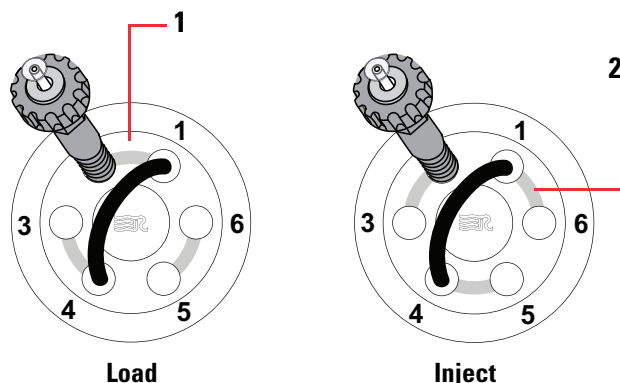
Loop injection

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 to the sample transfer line.

Figure 113. Loop injection positions



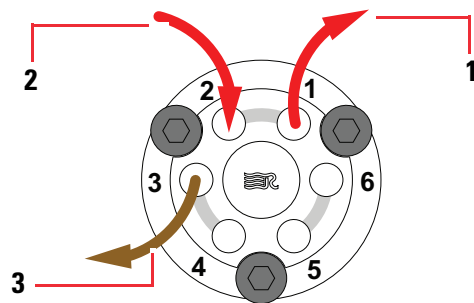
Divert valve

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 to the sample transfer line.

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

Figure 114. 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

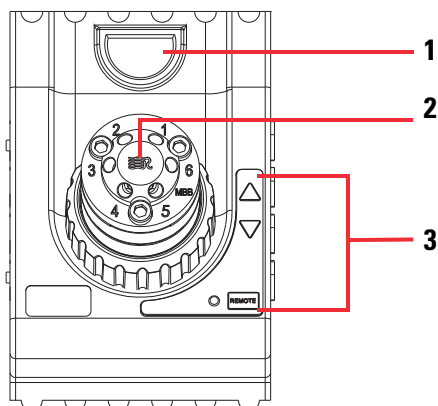
When the solvent flow is connected to a UV detector, use the setup shown in [Figure 121](#) on [page 197](#).

Divert/Inject valve controls

You can control the divert/inject valve by using the mass spectrometry data system or the control buttons on the valve:

- Use the data system to specify the parameters in the Divert Valve Properties pane of the Method Editor for the MS. For instructions, refer to the Method Editor Help for the MS.
- Use the valve's control buttons (Figure 115) 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 115. Divert/Inject valve (front view)



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

Sample introduction techniques

You can introduce samples into the MS by using the external syringe pump and the inject/divert valve or by using an LC system with an autosampler.

To connect the sample introduction plumbing, see these topics:

- [H-ESI or low-flow H-ESI direct infusion](#)
- [High-flow infusion without an autosampler](#)
- [Set up loop injections for a flow-injection analysis](#)
- [Set up injections using the autosampler](#)

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 perform this procedure, set up the syringe in the syringe pump as described in [Appendix B, “Set up the syringe and the syringe pump.”](#)

See the following topics:

- [Set up H-ESI direct infusion](#)
- [Set up low-flow H-ESI direct infusion](#)

Set up H-ESI direct infusion

If you are going to calibrate the MS, take care to avoid contaminating the calibration solution.

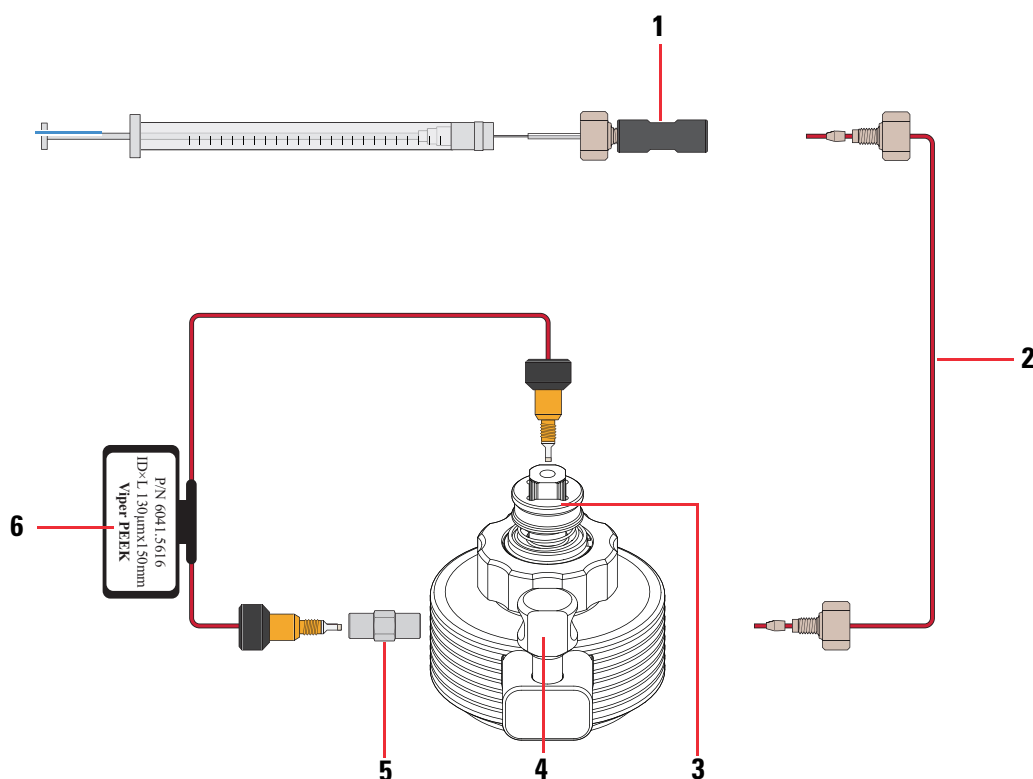
IMPORTANT Nitrile gloves are made with diphenylguanidine, which is soluble in EMRS. If diphenylguanidine contaminates the calibration solution, the solution's spectrum will include a peak at m/z 212.

Do not touch the tip of the needle or the ends of the transfer line tubing while you are filling the syringe, setting up the syringe pump, connecting the syringe to the transfer line, or connecting the transfer line to the grounding union.

❖ **To set up the system for direct infusion with the H-ESI ion source**

1. Fill the syringe with sample and connect it to the syringe union as described in “Set up the syringe pump to infuse a sample from the syringe” on page 183.
2. Insert the grounding union (4 in Figure 116) into the grounding union holder (3 in Figure 116).
3. Use two natural PEEK fingertight fittings and a length of red PEEK tubing (2 in Figure 116) to connect the syringe union to the grounding union.
4. Use a Viper PEEK capillary (6 in Figure 116) to connect the grounding union (5 in Figure 116) to the H-ESI spray insert (3 in Figure 116).

Figure 116. H-ESI direct infusion (numbered in clockwise order, starting with 1 at the top)



No.	Description
1	Syringe union
2	Fingertight PEEK fittings and red PEEK tubing (sample transfer line connection between the syringe union and the grounding union)
3	H-ESI spray insert
4	Grounding union holder
5	Grounding union
6	Viper PEEK capillary (recommended to prevent solvent leaks and dead volume)

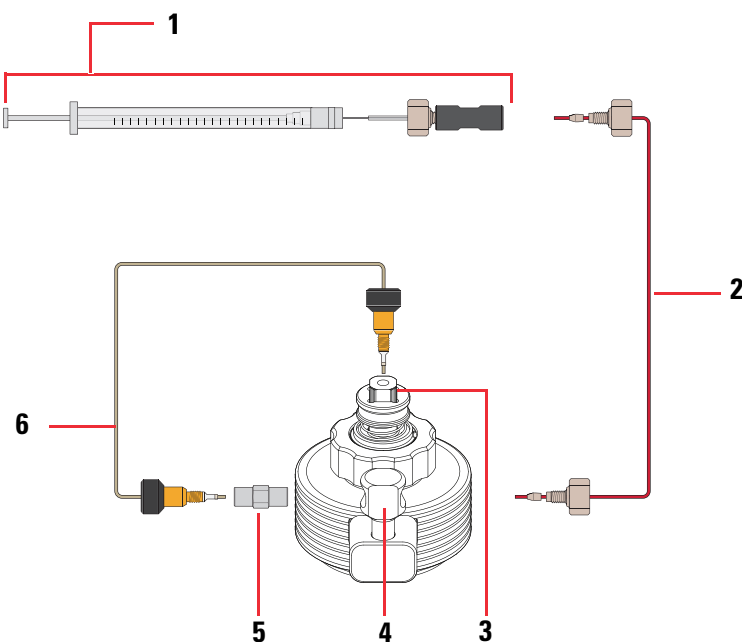
Set up low-flow H-ESI direct infusion

Note Use Viper fittings on the natural-colored PEEK tubing. Use a PEEK fitting to connect one end of the red PEEK tubing to the syringe union and a PEEK fitting to connect the other end of the tubing to the right side of the grounding union.

❖ To set up the H-ESI source for low-flow direct infusion

1. Place sample in the syringe (1 in Figure 117). The syringe pump is not shown.
2. Insert the grounding union (4 in Figure 117) into the grounding union holder (3 in Figure 117).
3. Use natural PEEK tubing and Viper fittings (5 in Figure 117) to connect the grounding union to the H-ESI spray insert (6 in Figure 117).
4. Use PEEK fingertight fittings to connect a length of red PEEK tubing between the syringe union and the grounding union (2 in Figure 117). This is the infusion line.

Figure 117. Low-flow H-ESI direct infusion (numbered in clockwise order, starting with 1 at the top)



No.	Description
1	Syringe and syringe adapter
2	Sample transfer line consisting of red PEEK tubing and PEEK fingertight fittings
3	Low-flow H-ESI needle in the H-ESI spray insert
4	Grounding union holder
5	Grounding union
6	Natural PEEK tubing and Viper fittings

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. Use this infusion method to perform experiments at a higher flow rate with an LC system. The high-flow infusion method lets you optimize the source parameters (such as sheath gas and vaporizer temperature) at the flow rate and mobile phase composition of the instrument method.

Before you begin, complete the procedures in [Appendix B, “Set up the syringe and the syringe pump.”](#)

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

- For H-ESI or low-flow H-ESI, see [“H-ESI or low-flow H-ESI direct infusion”](#) on [page 190](#)
- For APCI, see [“Connect the sample flow to the APCI source”](#) on [page 97](#)

Note The inject/divert valve in [Figure 119](#) is an example. The valve in your system might be different.

❖ To set up the system for high-flow infusion without an autosampler

1. Fill the syringe (1 in [Figure 118](#)) with your sample and connect it to the syringe pump (not shown).
2. Using red PEEK tubing and natural PEEK fittings (2 in [Figure 118](#)), connect the syringe union to the base of the Tee union (4 in [Figure 118](#)).

This is the infusion line.

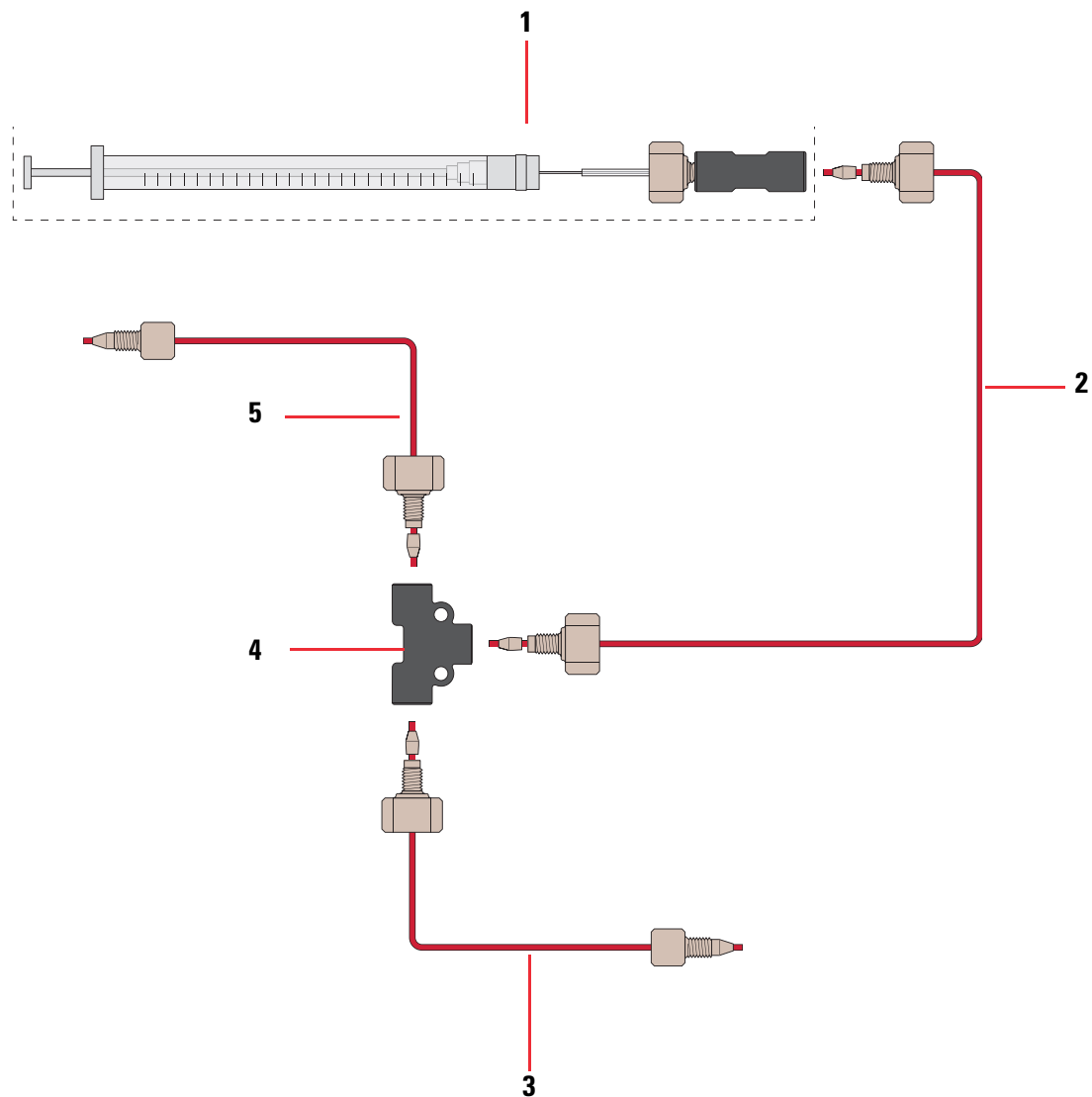
3. Use a fingertight fitting to connect a piece of red PEEK tubing (5 in [Figure 118](#)) to one side of the Tee union.

This connection adds the flow from the LC pump to the flow from the syringe pump.

4. Using red PEEK tubing and fittings (5 in [Figure 118](#)), connect the open end of the Tee union to the grounding of the union source.

This brings the flow to the MS.

Figure 118. High-flow infusion without an autosampler (numbered in clockwise order, starting with 1 at the top)



No.	Description
1	Syringe and union
2	Red PEEK tubing infusion line
3	Red PEEK tubing connecting the Tee valve to the MS
4	Tee union
5	PEEK tubing from the LC system

Set up loop injections for a flow-injection analysis

Use manual loop injections with or without an LC column. You can use this technique in H-ESI or APCI mode.

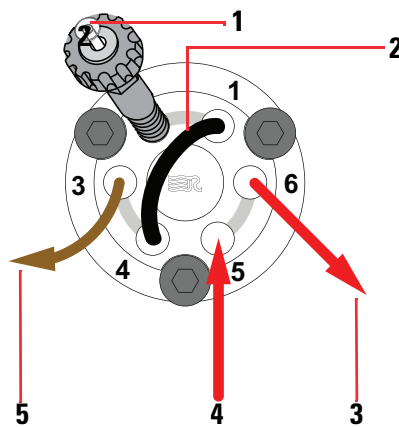
This technique requires attaching a sample loop, an injection port fitting (also known as a needle port or loop filler), and an LC pump to the divert/inject valve, and then connecting the valve to the API source (or to the API source after passing through an LC column). With the valve in the Load position, 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 119 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.

❖ To set up the system for manual loop injections

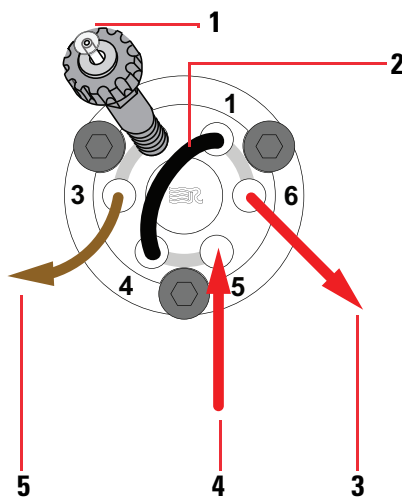
1. Connect a sample loop to Ports 1 and 4 of the valve.
2. Connect a needle port to Port 2.
3. Use a Rheodyne fitting to connect one end of Teflon or PEEK tubing (3 in Figure 119) to Port 3. Place the other end in a waste container, not shown.
4. Use red PEEK tubing and a fingertight fitting or an appropriately sized Viper line to connect Port 5 to the outlet of the LC system.
5. Connect the red PEEK tubing or an appropriately sized Viper line from Port 6 to the API source.
 - To connect to the H-ESI source, see “Connect the sample flow to the H-ESI source.”
 - To connect to the APCI source, see “Connect the sample flow to the APCI source.”

Figure 119. Injector valve in the Load position for loop injection (numbered in clockwise order, starting with 1 at the top)



No.	Description
1	The needle port (also known as a loop filler or an injection port) connects to port 2
2	The sample loop connects ports 1 and 4
3	Mobile phase from the LC pump exits from port 6 and flows to the API source
4	Mobile phase from the LC pump flows into port 5
5	Excess sample exits to waste through the Teflon or PEEK tubing connected to port 3

Figure 120. Injector valve in the Inject position for loop injection (numbered in clockwise order, starting with 1 at the top)



No.	Description
1	The needle port (also known as a loop filler or an injection port) connects to port 2.
2	The sample loop connects ports 1 and 4.
3	The mobile phase and sample mixture exits the injection valve through port 6 and flows to the API source.
4	Mobile phase from the LC pump flows into port 5 and enters the sample loop from the back through the connection between ports 5 and 4.
5	Teflon or PEEK tubing connects port 3 to waste.

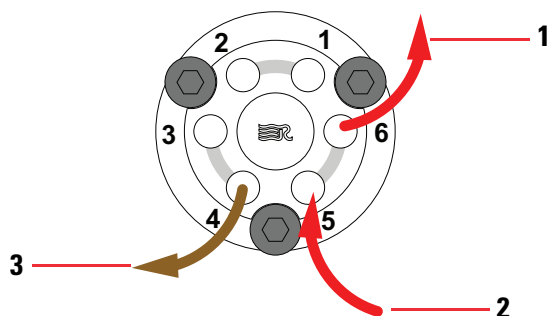
Set up injections using the autosampler

You can use the data acquisition software to 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 directing them into the API source, either H-ESI or APCI.

❖ To set up injections from an LC system with an autosampler

1. Use red PEEK tubing and a Rheodyne fitting to connect port 5 of the divert/inject valve to one of the following:
 - The outlet of the autosampler (not shown)
 - The outlet of a liquid chromatography 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 of the tubing in a waste container (not shown).
3. Connect red PEEK tubing to port 6 and the other end to the API source.

Figure 121. 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 column or autosampler.
3	Port 4 Teflon tubing is connected to waste.

Replaceable parts

The TSQ Series II mass spectrometers and older models 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 Solution Kits
- Calibration Kit
- Low Flow Needle and ESI Probe Calibration Kit
- Performance Specification Kit
- TSQ Source Installation Kit
- API source interface replaceable parts
- Miscellaneous replaceable parts

Test Solution Kits

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

Calibration Kit

Calibration Kit (Rev D)	80000-62013
Source LC Connection Kit (see Table 32)	80000-62057
Syringe, gas tight, 500 µL	00301-19016
Syringe Adapter Kit (see Table 33)	70005-62011

Table 32. 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 33. 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

Low Flow Needle and ESI Probe Calibration Kit

This kit contains the low-flow probe assembly with holder and the low-flow needle insert. See [Figure 122](#).

Low Flow Needle and ESI Probe Calibration Kit	Opton-20065
Assembly, low flow probe with holder	80111-60410
Needle insert, low flow	80000-60398

Figure 122. Low-flow needle insert with holder



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

TSQ Source Installation Kit

TSQ Source Installation Kit (Rev A)	
Ion transfer tube removal tool for ion transfer tubes with a 1/4 turn nose cone	70005-20972
Ion transfer tube removal tool for ion transfer tubes with a threaded nose cone	70111-20258
Lens L0 removal tool	70005-20900
Viper Capillary Kit (5 provided)	00109-99-00068
Capillary length tool	80000-20957

API source interface replaceable parts

TSQ Altis MS and TSQ Altis Plus MS

MP00 multipole	80100-20070
Ion sweep cone	80100-20646
Ion transfer tube, high-capacity transfer tube (HTTC) (58 mm L, 0.6×1.6 mm ID tube with an L-etched 1/4 turn nose cone) . .	80500-20045
O-ring, Vespel, graphite, 0.325 in. ID, 0.046 in. thick (behind the ion transfer tube)	70005-20922
Lens L0	80100-20548
SRIG lens stack (ion funnel)	80100-60036

TSQ Quantis MS and TSQ Quantis Plus MS

MP00 multipole	80100-20070
Ion sweep cone	80111-20646
Ion transfer tube (58 mm L, 0.58 mm ID tube with a threaded nose cone)	70005-20606
O-ring, Vespel, graphite (behind the ion transfer tube)	97055-20442
Lens L0	80100-20548
SRIG lens stack (S-lens)	80000-60136

TSQ Fortis MS and TSQ Fortis Plus MS

Ion transfer tube (101.6 mm L, 0.58 mm ID tube with a threaded nose cone)	80100-20062
O-ring, Vespel, graphite (behind the ion transfer tube)	97055-20442
Skimmer	80111-20064
Tube lens	80111-20162
Ion sweep cone	80111-20646
Lens L0	80100-20548

TSQ Quantiva MS

Exit lens	80000-20218
Ion sweep cone	80100-20646
Ion transfer tube (vertical orifice)	80100-20641
O-ring, Vespel, graphite (behind the ion transfer tube)	70005-20922
Lens L0	80100-20548
SRIG lens stack (ion funnel)	80100-60036

TSQ Endura MS

Exit lens	80000-20218
Ion sweep cone	80000-20895
Ion transfer tube (58.42 mm length, 0.58 mm ID tube with a threaded nose cone)	70005-20606
O-ring, Vespel, graphite, 0.325 in. ID, 0.046 in. thick (behind the ion transfer tube)	97055-20442

Lens L0	80100-20548
SRIG lens stack (S-lens)	80000-60136

Miscellaneous replaceable 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
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Air Filter

Air filter, metal mesh.	80000-10355
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Forepump Accessories

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

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 electrons, which enter the electron multiplier.

D

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

E

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

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

F

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

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

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

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

H

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

I

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 one ± 12 kVdc conversion dynode 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 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. The automated calibration process tunes these values for positive and negative ions.

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

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

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

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

multipole A symmetrical, parallel array of (usually) four, six, or eight 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 Q1 and Q3 scans 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 Q3 scan is a selected number of mass units lower than the Q1 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:

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

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 from a chromatographic column. 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.

S

scan 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 list of singular 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.



Index

A

- API gas valves, description 53
- API gases
 - See gases
- API modes 55
- API source
 - description 55
- API source interface
 - ion transfer tube 65
 - replaceable parts 201
- API spray inserts
 - gas plumbing, H-ESI 54
- auxiliary gas flow (figure) 54
- auxiliary gas, description 54

B

- buttons, on/standby/off 173

C

- calibration solution
 - See extended mass range reference solution (EMRS) 117
- cleaning procedures
 - exit lens 163
 - ion transfer tube 150
 - L0 lens 163
 - MP00 multipole 163
 - RF lens 163
 - skimmer 164
 - spray cone and seal 150
 - syringe 84
 - tube lens 164
- collision cell efficiency 76
- collision energy (Q2 offset voltage) 76
- collision gas 76
- collision pressure vacuum gauge 52
- communication connectors 34

- communication LED, description 31
- compliance
 - FCC 4
 - regulatory 3
- contact closure cable control, connecting with MS application 36
- contact closure interface 33
- contacting us 18
- contamination, preventing 139, 145, 183
- convection gauge, description 52
 - See also vacuum system, gauges
- cooling fans, description 38

D

- data acquisition
 - Record icon 132
- data type, setting 174
- data types 47
- direct infusion, description 190
- directives
 - regulatory 3
 - WEEE 5
- divert/inject valve, setting 174
- documentation, accessing 13
- dual-mode discrete dynode, description 77

E

- Electro Dynamic Ion Funnel (EDIF) 69
- electromagnetic compatibility 3
- electron multiplier gain 77
- Electronics service switch
 - description 33
- electronics service switch
 - location 32
- EMRS calibrant, ordering 198
- exit lens
 - cleaning 163

- description 68
- reinstalling 166

extended mass range reference solution (EMRS)
positive and negative ion peak lists 117

F

- fans, description 38
- favorite parameter states 181
- FCC compliance 4
- forepump, control connector, MS 33

G

- gas plumbing, H-ESI spray insert 54
- gases
 - nitrogen, description 53
 - supply levels, checking 82
- gloves, part numbers 142

H

- H-ESI mode
 - LC/MS operational guidelines 121
 - plumbing connection, direct infusion 190
- hyperquads Q1 and Q3, description 72

I

- ion detection system 77
- ion optics, cleaning 163
- ion polarity mode, setting 174
- ion polarity modes 48
- ion sweep cone
 - description 63
 - figure of 145
 - removing 145
- ion transfer tube 146
 - cleaning 150
 - description 65
 - drawing of 65, 149
 - installing 150
 - removal tools 146
- ion transmission device, rod assembly 40
- ionization gauge, description 52
- ionization technique, description 29

K

- kits
 - Calibration 198
 - Performance Specification 200
 - TSQ Source Installation 200

L

- L0 lens removal tool 162
- LC/MS analysis, description 28
- LC/MS operational guidelines
 - APCI mode 121
 - H-ESI mode 121
 - NSI mode 122
- LEDs 31
- lenses
 - L4 77
- lenses, cleaning 163
- line power, specification 32
- liquid chromatograph
 - solvent flow, turning off 86, 143

M

- main power switch, description 33
- maintenance
 - ion transfer tube 146
 - schedule 138
- mass analysis, discussion 75
- mass analyzer
 - RF and DC voltages 75
- mass analyzer description 40
- mass list
 - exporting from Tune 180
 - importing into Tune 179
- mass spectrometer
 - functional description 49
 - ion polarity modes 48
 - on/off status for components, voltages, and gas flows 94
 - power modes, setting 175
 - power panel 32
 - resetting 92
 - Standby mode 86
 - vacuum manifold 51
 - vacuum system 49
- Matrix Separator Ion Guide (MSIG) 69
- metal needle insert for H-ESI spray insert 138
- MP00 multipole
 - cleaning 163
 - description 70
- MS scan types 41–42
- MS/MS scan types
 - neutral loss scan type 44
 - product ion scan type 42
 - See scan types

N

- neutrals blocker 71
- nitrogen gas
 - inlets assembly, description 53
 - pressure 53

O

- offset voltage, quadrupole 76
- on/off status for MS components 94

P

- panes
 - Favorites 181
 - History 180
 - Optimization 126
- parts
 - See* replaceable parts
- polarity mode
 - See* ion polarity mode, setting
- power
 - entry module 32
 - LED description 31
 - specifications 32
- power switch, location 32
- pressure gauges, note about 91
- procedures
 - cleaning
 - ion transfer tube 150
 - lenses and MP00 multipole 154
 - spray cone and seal 149
 - favorite states, using 181
 - inlet, setting up for sample introduction 190
 - sample introduction techniques
 - autosampler 197
 - direct infusion, connecting the plumbing 190
 - high-flow infusion 193
 - loop injections 195
 - start instrument, selecting in Xcalibur 133
 - syringe pump, controlling 175
 - Tune preferences, setting 177

Q

- quadrupole mass analyzers
 - functional description 75
 - quadrupole offset voltage 76

R

- readback status, description 175
- readback values, vacuum gauges 52

- Record icon 132
- regulatory compliance 3
- relay switch circuit 36
- removal tool, L0 lens 162
- replaceable parts, part numbers 198
- reset button 33
- RF lens
 - cleaning 163
 - description 68
 - reinstalling 166
- Run Sequence dialog box (acquisition options) 134

S

- safety standards 3
- sample data, acquire by using Tune 130
- sample transfer line, flushing 83
- sample tube, flushing 83
- scan LED, description 31
- scan types
 - MS scans
 - full scan Q1 and Q3 41
 - selected ion monitoring (SIM) 42
 - MS/MS scans
 - neutral loss 44
 - precursor 43
 - product 42
 - selected reaction monitoring (SRM) 46
 - summary of 40
- seal, cleaning 150
- sequence run, start instrument in Xcalibur 133
- sheath gas flow (figure) 54
- sheath gas, description 53
- skimmer (TSQ Fortis)
 - description 70
 - removing 160
- solvent waste container, emptying 84
- source pressure vacuum gauge 52
- spray cone, cleaning 149
- spray insert, cleaning 83
- Stacked Ring Ion Guide (SRIG) 69
- Standby mode 86
- start instrument, configuring with Xcalibur 133
- sweep cone
 - See* ion sweep cone
- sweep gas, description 54
- switches, MS 32
- symbols, meaning 16
- syringe
 - cleaning 84
 - priming 175

system checks for argon and nitrogen supplies 82
system LED, description 31

T

time stamp, raw data file 131
tools, ion transfer tube removal 146
tube lens 69, 161
Tune application
 basic functions 172
 opening 172
 Preferences dialog box 177

V

vacuum LED
 description 31
 note about pressure 91
vacuum manifold
 description 51
vacuum pressure levels, checking 78
vacuum pumps
 See turbomolecular pumps
vacuum system
 description 49
 gauges
 collision pressure 52
 convection 52
 ion pressure 52
 source pressure 52
vent valve, description 53
voltages
 quadrupole offset 76
voltages, line power specifications 32

W

WEEE directive 5

X

Xcalibur file type, raw data (.raw) 131
Xcalibur file type, sequence (.sld) 133