

# Exactive Series

Exactive Plus, Exactive Plus EMR, Q Exactive, Q Exactive Focus, Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X

## Operating Manual

BRE0012255 Revision A April 2017



# Exactive Series

**Exactive Plus, Exactive Plus EMR, Q Exactive,  
Q Exactive Focus, Q Exactive Plus,  
Q Exactive HF, and Q Exactive HF-X**

## **Operating Manual**

BRE0012255 Revision A April 2017

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## Original Operating Instructions

Published by:

Thermo Fisher Scientific (Bremen) GmbH, Hanna-Kunath-Str. 11, 28199 Bremen, Germany

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Release History: Revision A released in April 2017.

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# Contents

<b>Chapter 1</b>	<b>Using this Manual</b> .....	<b>1-1</b>
	About this Manual .....	1-1
	Exactive Series Mass Spectrometers .....	1-1
	Typographical Conventions .....	1-3
	Signal Word.....	1-3
	Viewpoint Orientation.....	1-3
	Data Input .....	1-3
	Topic Headings.....	1-4
	Reference Documentation.....	1-5
	Contacting Us.....	1-7
	Assistance .....	1-7
	Suggestions to the Manual .....	1-7
<b>Chapter 2</b>	<b>Scope of Delivery</b> .....	<b>2-1</b>
	Standard System Components .....	2-1
	Optional System Components .....	2-2
<b>Chapter 3</b>	<b>Functional Description</b> .....	<b>3-1</b>
	General Description .....	3-2
	Layout of the Exactive Plus and Exactive Plus EMR Mass Spectrometers.....	3-2
	Layout of the Q Exactive, Q Exactive Focus, Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X Mass Spectrometers.....	3-4
	Control Elements.....	3-10
	System Status LEDs .....	3-10
	Power Panel .....	3-11
	Power Column.....	3-14
	Vacuum System Controls.....	3-16
	API Source .....	3-17
	Ion Max API Source.....	3-17
	Ion Source Interface .....	3-20
	Ion Optics.....	3-24
	Ion Optics of Exactive Plus and Exactive Plus EMR Mass Spectrometers.....	3-24
	Ion Optics of Q Exactive, Q Exactive Focus, Q Exactive Plus, and Q Exactive HF Mass Spectrometers.....	3-26
	Curved Linear Trap .....	3-31
	Orbitrap Analyzer .....	3-32
	Extraction of Ion Packets .....	3-32

Measuring Principle .....	3-33
Ion Detection.....	3-34
HCD Cell.....	3-35
Additional Hardware.....	3-36
Syringe Pump .....	3-36
Switching Valves .....	3-37
Vacuum System .....	3-40
Source Vacuum Pumps .....	3-41
Auxiliary Forepump .....	3-42
Turbomolecular Pumps.....	3-43
System Bakeout.....	3-45
Cooling Fans.....	3-45
Gas Supply.....	3-46
Gas Distribution in the Instrument.....	3-46
Printed Circuit Boards .....	3-48
Preamplifier .....	3-48
Data Acquisition Board (DAQ Board).....	3-48
Internal Computer (Data Acquisition Unit).....	3-48
Source Board.....	3-49
8 kV Power Supply .....	3-49
Ion Optic Supply DC Board .....	3-49
Ion Optic Supply RF Board .....	3-50
Quadrupole Board .....	3-50
FT Adapter Board .....	3-50
Vacuum Control Board.....	3-51
C-Trap RF Board.....	3-51
CE HV Supply Board .....	3-52
CE Pulser Board.....	3-52
Power Supply DAQ Board.....	3-52
I/O Board .....	3-53
S-Lens RF Generator.....	3-53
Funnel RF Generator .....	3-53
Forepump On/Off Board.....	3-53

<b>Chapter 4</b>	<b>Safety.....</b>	<b>4-1</b>
	Safety Symbols and Signal Words in this Manual.....	4-2
	Observing this Manual.....	4-2
	Safety Symbols on the Instrument.....	4-3
	Rating Plate.....	4-5
	Intended Use.....	4-6
	Qualification of the Personnel.....	4-6
	Permitted Materials.....	4-7
	Electric Safety Precautions .....	4-8
	In Case of Emergency .....	4-9
	Residual Hazards.....	4-11
	Personal Protective Equipment .....	4-12

<b>Chapter 5</b>	<b>Installation .....</b>	<b>5-1</b>
------------------	---------------------------	------------

Safety Guidelines for Installation.....	5-2
Placing the Instrument.....	5-3
Instrument Dimensions .....	5-3
Workbench for Instrument .....	5-5
Moving the Instrument.....	5-5
Laboratory Conditions.....	5-9
Power Supply.....	5-9
Gas Supply.....	5-11
Laboratory Temperature .....	5-12
Humidity.....	5-12
Ventilation and Fume Exhaust.....	5-13
Vibration .....	5-13
Airborne Noise Emission .....	5-14
Setting Up Instrument Hardware and Adjusting System Parameters.....	5-15
Configuring the Ion Source.....	5-16
Changing the Ion Source Housing.....	5-16
Changing the API Probe .....	5-17
Connecting Frequently Used Devices.....	5-18
Connecting the API Probe to the Mass Spectrometer .....	5-18
Connecting the Inlet Plumbing.....	5-19
User I/O Connections.....	5-36
Obtaining Calibration Solutions .....	5-39
About Calibration Solutions.....	5-39
Obtaining Ready-to-Use Calibration Solutions .....	5-39
Preparing Calibration Solutions .....	5-40
<b>Chapter 6</b>	<b>Operation..... 6-1</b>
Safety Guidelines for Operation .....	6-2
Before Operating the System.....	6-4
Checking the Forepumps .....	6-4
Checking the Nitrogen Supply.....	6-4
Checking the System Vacuum Levels .....	6-5
Checking the Disk Space on the Data System .....	6-5
Checking the Mass Accuracy of the Instrument .....	6-6
Setting the System in Standby Condition.....	6-7
Shutting Down the System .....	6-8
Starting Up the System after a Shutdown.....	6-10
Starting Up the Instrument.....	6-10
Setting Up Conditions for Operation.....	6-12
Resetting the System .....	6-14
After Operating the System .....	6-15
Flushing Sample Transfer Line, Sample Tube, and API Probe .....	6-15
Flushing Ion Sweep Cone and Ion Transfer Capillary .....	6-16
Purging the Oil in the Source Vacuum Pump .....	6-19
Emptying the Solvent Waste Container .....	6-19

<b>Chapter 7</b>	<b>Troubleshooting</b> .....	<b>7-1</b>
	Safety Guidelines for Troubleshooting .....	7-2
	Fault Table.....	7-3
	Main Power Failure.....	7-4
	Vacuum Leak.....	7-5
	Failure of UHV Chamber Heating Control .....	7-7
	Turbomolecular Pump is not Running .....	7-8
	Failure of Source Heaters / Capillary Heaters .....	7-9
<b>Chapter 8</b>	<b>Maintenance</b> .....	<b>8-1</b>
	Safety Guidelines for Maintenance.....	8-2
	General Advice for Maintenance .....	8-4
	Inspection- and Servicing Plan .....	8-5
	Cleaning the Surface of the Instrument.....	8-6
	Checking Warning Labels .....	8-6
	Leak-Checking Gas Lines.....	8-7
	Checking Condition of Tubings and Hoses .....	8-7
	Maintaining the Vacuum System .....	8-8
	Pumps Maintenance.....	8-8
	Baking Out the System .....	8-12
	Maintenance of the Fan Filters.....	8-14
	API Source Maintenance.....	8-16
	Frequency of Cleaning .....	8-16
	Removing and Reinstalling the Ion Max API	
	Source Housing.....	8-16
	API Source Housing Maintenance .....	8-21
	Removing, Cleaning, and Reinstalling the Ion	
	Transfer Capillary .....	8-22
	API Probe Maintenance .....	8-29
	Ion Source Interface Maintenance.....	8-43
	Maintaining LCs or Autosamplers.....	8-51
	Consumables.....	8-51
	Thermo Fisher Scientific Service .....	8-52
	Returning Parts .....	8-52
	Services to be Performed by Thermo Fisher	
	Scientific Service Only .....	8-53
<b>Chapter 9</b>	<b>Replaceable Parts</b> .....	<b>9-1</b>
	Ion Source Probes and Parts.....	9-2
	Ion Source Interface Parts .....	9-2
	Parts for Ion Source with S-Lens .....	9-2
	Parts for Ion Source with Ion Funnel .....	9-2
	Source Accessory Parts .....	9-2
	Source Drain Parts .....	9-3
	Instrument Parts .....	9-4
<b>Appendix A</b>	<b>Legal Documents</b> .....	<b>A-1</b>



**Appendix B Component Suppliers' Documents ..... B-1**

**Glossary..... G-1**

**Index ..... I-1**



# Technical Data for Exactive Series Systems

The table summarizes the most important technical data of the Exactive Series systems. See the respective chapters of the manual for details and additional instrument properties.

**Table 1-1.** Technical Data for Exactive Series Systems (Sheet 1 of 2)

Parameter	Specification	Value	
<b>Instrument Properties</b>			
Mass spectrometer	Length × width × height	830 × 910 × 950 <sup>a</sup> (940 <sup>b</sup> ) mm	
	Weight	182 <sup>a</sup> (175 <sup>b</sup> ) kg	
Source Vacuum Pump SOGEVAC SV 65 BI	Length × width × height	530 × 330 × 360 mm	
	Weight	60 kg	
Source Vacuum Pump Agilent MS120 <sup>d</sup>	Length × width × height	750 × 516 × 538 mm	
	Weight	106 kg	
Auxiliary Forepump Pfeiffer DUO 11 <sup>d</sup>	Length × width × height	411 × 127 × 191 mm	
	Weight	17 kg	
Complete system (incl. data system)	Noise emission	Below 70 dB(A)	
	Heat generation	3000 W <sup>c</sup> (3300 W) <sup>d</sup>	
<b>Power Requirements</b>			
Mass spectrometer	Input	Nominal voltage	230 V AC, 50/60 Hz
		Power	apparent power: 800 VA (1150 VA) <sup>d</sup> ; effective power: 750 W (1100 W) <sup>d</sup>
		Fuse <sup>e</sup>	15/16 A
	Output 2×		230 V AC, 50/60 Hz, max. 10 A
	Protection type		IP 20
Source Vacuum Pump	Input	Nominal voltage	200–240 V AC, 50/60 Hz
		Power	SOGEVAC SV 65 BI: 1.5 kW (Agilent MS120: 1.8 kW) <sup>d</sup>
		Fuse <sup>e</sup>	15/16 A (tripping characteristic C)
Auxiliary Forepump	Input	Nominal voltage	200–240 V AC, 50/60 Hz
		Power	0.3 kW
		Fuse	10 A
Data system	Input	Nominal voltage	200–240 V AC, 50/60 Hz
		Fuse <sup>e</sup>	15/16 A
<b>Gas Requirements (Nitrogen)</b>			
Source gas (minimum requirement)	Purity		99% or better (high purity)
	Supply rate		max. 30 L/min (max. 50 L/min for high-flow applications)
	Pressure		0.8 ± 0.03 MPa (8 ± 0.3 bar)
HCD gas (recommended)	Purity		99.999% or better (ultra high purity)
	Supply rate		max. 2 mL/min
	Pressure		0.8 ± 0.03 MPa (8 ± 0.3 bar)

**Table 1-1.** Technical Data for Exactive Series Systems (Sheet 2 of 2)

Parameter	Specification	Value
<b>Operating Environment</b>	Laboratory temperature	15–26 °C
	Max. temperature fluctuation	1 °C/10 min
	Humidity	40–70%, non-condensing and non-corrosive atmosphere
	Max. altitude	2000 above sea level
<b>Exhaust Requirements</b>	Inrush flow rate	3 L/min
	Continuous flow rate	1 L/min

<sup>a</sup> Q Exactive, Q Exactive Focus, Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X mass spectrometers

<sup>b</sup> Exactive Plus and Exactive Plus EMR mass spectrometers

<sup>c</sup> Consider additional heat production of peripheral devices connected to MS power outlets.

<sup>d</sup> In case of a Q Exactive HF-X MS.

<sup>e</sup> dedicated wall outlet

## Chapter 1 Using this Manual

Welcome to the Thermo Scientific™ Exactive™ Series system! Exactive Series systems are members of the Thermo Scientific family of mass spectrometer (MS) detectors that are powered by Orbitrap™ technology.

### Contents

- [About this Manual on page 1-1](#)
- [Exactive Series Mass Spectrometers on page 1-1](#)
- [Typographical Conventions on page 1-3](#)
- [Reference Documentation on page 1-5](#)
- [Contacting Us on page 1-7](#)

## About this Manual

This *Exactive Series Operating Manual* contains precautionary statements that can prevent personal injury, instrument damage, and loss of data if properly followed. It also describes the modes of operation and principle hardware components of your Exactive Series instrument. In addition, this manual provides step-by-step instructions for cleaning and maintaining your instrument.

Designed, manufactured and tested in an ISO9001 registered facility, this instrument has been shipped to you from our manufacturing facility in a safe condition. This instrument must be used as described in this manual. Any use of this instrument in a manner other than described here may result in instrument damage and/or operator injury.

## Exactive Series Mass Spectrometers

Exactive Series instruments are designed to be placed on a bench in the laboratory and comprise the following mass spectrometers:

- The Exactive Plus, an instrument with an API source with S-lens ion optics technology for LC/MS high-throughput applications. It offers an inject flatpole and octapole for ion transfer and collision cell for all-ion-fragmentation. The Exactive Plus is equipped with Orbitrap mass analyzer.

- The Exactive Plus EMR, an instrument with an API source with S-Lens ion optics technology and a collision cell, for analysis of very large molecules, offering a mass range up to  $m/z$  20000. The Exactive Plus EMR is equipped with Orbitrap mass analyzer.
- The Q Exactive, an instrument with an API source with S-lens ion optics technology, a quadrupole mass filter for precursor ion selection, and a collision cell for performing MS/MS experiments. The Q Exactive is equipped with Orbitrap mass analyzer.
- The Q Exactive Focus, an instrument with an API source with S-lens ions optics technology, an inject flatapole, a hyperbolic quadrupole mass filter for precursor ion selection, and a collision cell for performing MS/MS experiments. The Q Exactive Focus offers a mass range up to  $m/z$  2000 and is equipped with Orbitrap mass analyzer.
- The Q Exactive Plus, an instrument with an API source with S-lens ion optics technology, an injection flatapole with mass resolving capabilities, a segmented quadrupole mass filter for optimal precursor ion selection, and a collision cell for performing MS/MS experiments. The Q Exactive Plus is equipped with Orbitrap mass analyzer.
- The Q Exactive HF, an instrument with an API source with S-lens ion optics technology, an injection flatapole with mass resolving capabilities, a segmented quadrupole mass filter for optimal precursor ion selection, and a collision cell for performing MS/MS experiments. The Q Exactive HF is equipped with an ultra-high-field Orbitrap mass analyzer resulting in an increased scan speed compared to the other Exactive Series instruments.
- The Q Exactive HF-X, an instrument with a brighter API source with a high-capacity transfer tube and mini ion funnel ion optics technology, an injection flatapole with mass resolving capabilities, a segmented quadrupole mass filter for optimal precursor ion selection, and a collision cell for performing MS/MS experiments. The Q Exactive HF-X is equipped with an ultra-high-field Orbitrap mass analyzer resulting in an increased scan speed. Compared to the Q Exactive HF, it provides faster scanning (with lower resolution setting).

## Typographical Conventions

This section describes typographical conventions that have been established for Thermo Fisher Scientific manuals.

### Signal Word

Make sure that you follow the precautionary statements presented in this manual. The special notices appear different from the main flow of text:

**NOTICE** Points out possible material damage and other important information in connection with the instrument. ▲

### Viewpoint Orientation

The expressions *left* and *right* used in this manual always refer to the viewpoint of a person that is facing the front side of the instrument.

### Data Input

Throughout this manual, the following conventions indicate data input and output with the computer:

- Messages displayed on the screen are represented by capitalizing the initial letter of each word and by italicizing each word.
- Input that you enter by keyboard is identified by quotation marks: single quotes for single characters, double quotes for strings.
- For brevity, expressions such as “choose **File > Directories**” are used rather than “pull down the File menu and choose Directories.”
- Any command enclosed in angle brackets < > represents a single keystroke. For example, “press <F1>” means press the key labeled *F1*.
- Any command that requires pressing two or more keys simultaneously is shown with a plus sign connecting the keys. For example, “press <Shift> + <F1>” means press and hold the <Shift> key and then press the <F1> key.
- Any button that you click on the screen is represented in bold face letters. For example, “click **Close**.”

## **Topic Headings**

The following headings are used to show the organization of topics in a chapter:

### **Chapter 1 Chapter Name**

#### **Second Level Topics**

#### **Third Level Topics**

#### **Fourth Level Topics**



## Reference Documentation

This *Exactive Series Operating Manual* represents the Original Operating Instructions. In addition to this manual, Thermo Fisher Scientific provides other documents for Exactive Series mass spectrometers that are not part of the Original Operating Instructions. Reference documentation for Exactive Series mass spectrometers includes the following:

- *Exactive Series Pre-Installation Requirements Guide*
- *Exactive Plus Software Manual* and *Exactive Plus QuickStart Guide* (with Exactive Plus system)
- *Exactive Plus EMR Software Manual* and *Exactive Plus EMR QuickStart Guide* (with Exactive Plus EMR system)
- *Q Exactive Software Manual* and *Q Exactive QuickStart Guide* (with Q Exactive system)
- *Q Exactive Focus Software Manual* and *Q Exactive Focus QuickStart Guide* (with Q Exactive Focus system)
- *Q Exactive Plus Software Manual* and *Q Exactive Plus QuickStart Guide* (with Q Exactive Plus system)
- *Q Exactive HF Software Manual* and *Q Exactive HF QuickStart Guide* (with Q Exactive HF system)
- *Q Exactive HF-X Software Manual* and *Q Exactive HF-X QuickStart Guide* (with Q Exactive HF-X system)
- *Ion Max and Ion Max-S API Source Hardware Manual*
- *HESI-II Probe User Guide*

You can access PDF files of the documents listed above and of this manual from the data system computer. The software also provides Help.

### ❖ To view product manuals

Go to **Start > All Programs > Thermo Exactive Series > Manuals**.

Printed versions of this *Exactive Series Operating Manual* and the *Ion Max and Ion Max-S API Source Hardware Manual* are shipped with the instrument. A printed version of the *Exactive Series Pre-Installation Requirements Guide* is part of the Preinstallation Kit. This kit is sent to your laboratory before the arrival of the Exactive Series mass spectrometer.

Refer also to the user documentation that is provided by the manufacturers of third-party components:

- Forepumps
- Turbomolecular pumps
- Syringe pump
- Switching valve
- Data system computer and monitor
- Safety data sheets

## Contacting Us

There are several ways to contact Thermo Fisher Scientific.

### Assistance

For brochures and ordering information, please visit:

[www.thermofisher.com/orbitrap](http://www.thermofisher.com/orbitrap)

Service contact details are available under:

[www.unitylabservices.com](http://www.unitylabservices.com)

Visit our customer SharePoint to download current revisions of user manuals and other customer-oriented documents for your product. Translations into other languages and software packages may be available there as well.

With the serial number (S/N) of your instrument, request access as a customer via [www.thermoscientific.com/Technicaldocumentation](http://www.thermoscientific.com/Technicaldocumentation). For the first login, you have to create an account. Follow the instructions given on screen. Please accept the invitation within six days and log in with your created Microsoft™ password.

### Suggestions to the Manual

#### ❖ To suggest changes to this manual

- Send your comments to:  
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Thermo Fisher Scientific (Bremen) GmbH  
Hanna-Kunath-Str. 11  
28199 Bremen  
Germany
- Send an e-mail message to the Technical Editor at  
[documentation.bremen@thermofisher.com](mailto:documentation.bremen@thermofisher.com)

You are encouraged to report errors or omissions in the text or index. Thank you.

## Using this Manual

Contacting Us

## Chapter 2 Scope of Delivery

This chapter lists the standard components of your Exactive Series LC/MS system and optional components.

### Contents

- [Standard System Components](#) on page 2-1
- [Optional System Components](#) on page 2-2

## Standard System Components

The Exactive Series standard system has the following components:

- Exactive Series mass spectrometer
- API Source with heated-electrospray ionization (HESI) probe
- Data system computer with monitor
- One or two forepumps
- Noise reduction cover and drip pan for one forepump
- Syringe pump
- Switching valve
- Holder for syringe pump and switching valves
- Installation Kit including
  - Equipment for connecting the above components (hoses, cables)
  - Computer equipment
  - Tools for installation and maintenance
  - Spare parts
- Pair of lifting devices
- Printed manuals
  - *Exactive Series Operating Manual*
  - *Ion Max and Ion Max-S API Source Hardware Manual*

In addition to these printed manuals, other documents for the Exactive Series mass spectrometer are available as PDF files on the data system computer. See [“Reference Documentation”](#) on page 1-5 for a list.

## Optional System Components

For reference, the following list contains components that are frequently shipped with the standard Exactive Series LC/MS system. They are not part of the standard system and may therefore not be present in your laboratory:

- High Speed LCs (Thermo Scientific UltiMate™ 3000 Series or Vanquish system)
- Probes for APCI, APPI, or ESI technique
- Nanospray Ion Source

## Chapter 3 Functional Description

This chapter provides an overview of the functional elements of the Exactive Series mass spectrometer.

### Contents

- [General Description](#) on page 3-2
- [Control Elements](#) on page 3-10
- [API Source](#) on page 3-17
- [Ion Optics](#) on page 3-24
- [Curved Linear Trap](#) on page 3-31
- [Orbitrap Analyzer](#) on page 3-32
- [HCD Cell](#) on page 3-35
- [Additional Hardware](#) on page 3-36
- [Vacuum System](#) on page 3-40
- [Cooling Fans](#) on page 3-45
- [Gas Supply](#) on page 3-46
- [Printed Circuit Boards](#) on page 3-48

## General Description

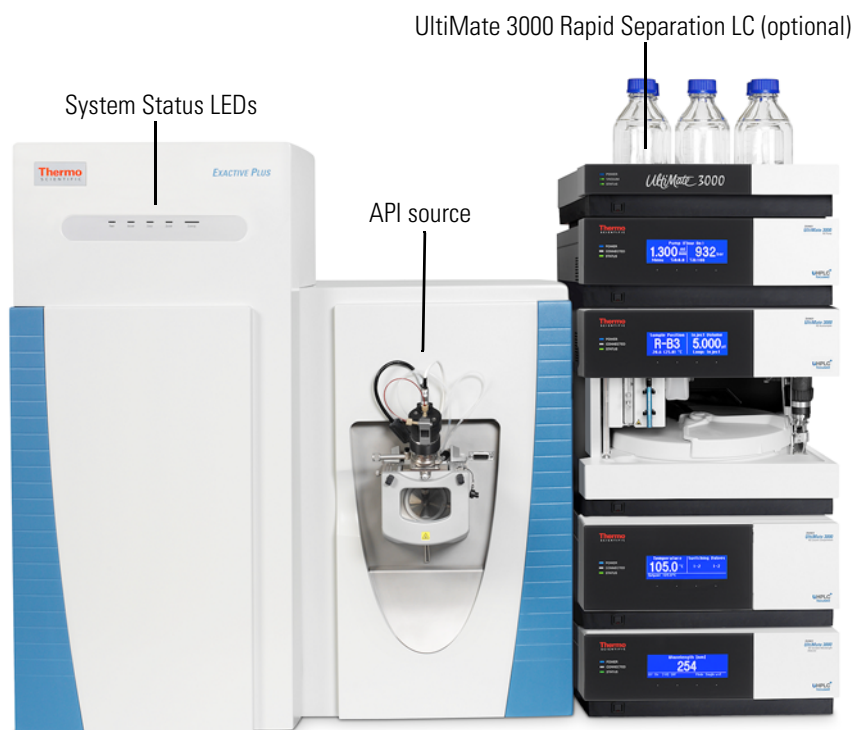
Exactive Series mass spectrometers are stand-alone Orbitrap™ instruments with an atmospheric pressure ionization (API) source for liquid chromatography (LC) mass spectrometry (MS) high-throughput applications. The instruments are designed to be placed on a bench in the laboratory. This chapter describes the principal components of Exactive Series systems and their respective functions.

### Layout of the Exactive Plus and Exactive Plus EMR Mass Spectrometers

Exactive Plus and Exactive Plus EMR mass spectrometers consist of four main components, which are described in the following topics:

- Ion source
- Intermediate storage device (C-Trap) for short pulse injection
- Optional<sup>1</sup> collision cell for performing HCD (Higher Energy Collisional Dissociation) experiments
- Orbitrap analyzer for Fourier transform mass analysis

Figure 3-1 shows a front view of an Exactive Plus MS. For a schematic view of the instrument layout, see Figure 3-14 on page 3-26.



**Figure 3-1.** Exactive Plus MS front view

<sup>1</sup> Exactive Plus EMR MS are always equipped with an HCD collision cell.



## Operating Modes of Exactive Plus and Exactive Plus EMR MS

Samples can be introduced into the API source at the front side by a variety of methods including direct infusion (with a syringe pump) or an U-HPLC system (for example, Thermo Scientific UltiMate™ 3000). The source is similar to the commercial source of the Thermo Scientific LTQ Velos™. See “API Source” on page 3-17 for details.

The ions are transferred into the C-Trap through four stages of differential pumping. See “Ion Optics” on page 3-24 for details. In the C-Trap, the ions are accumulated and their energy is dampened with a bath gas (nitrogen). The ions are then injected through three further stages of differential pumping by a lens system (Z-lens) into the Orbitrap analyzer where mass spectra are acquired by image current detection. The vacuum inside the Orbitrap analyzer is maintained below 1E-9 mbar. See “Orbitrap Analyzer” on page 3-32 for details.

Ions are passed through the C-Trap into the HCD cell, if the instrument is equipped with it. The HCD cell adds a Higher Energy Collision Induced Dissociation capability to the instrument. This allows performing all-ion fragmentation (AIF) experiments. After the ions have been fragmented in the HCD cell, the HCD cell voltages are ramped up and the ions are transferred back into the C-Trap from where they are injected into the Orbitrap analyzer for detection. See page 3-35 for a description of the HCD cell.

## Measurement Properties of Exactive Plus and Exactive Plus EMR MS

**Table 3-1.** Measuring properties of the Exactive Plus mass spectrometer

<b>Mass Range for Full Scans</b>	$m/z$ 50–6000 (Scan range: last mass $\leq 15 \times$ first mass)
<b>Mass Resolution</b>	17500 at $m/z$ 200 (12500 at $m/z$ 400) at a scan rate of 12 Hz 35000 at $m/z$ 200 (25000 at $m/z$ 400) at a scan rate of 7 Hz 70000 at $m/z$ 200 (50000 at $m/z$ 400) at a scan rate of 3 Hz 140000 at $m/z$ 200 (100000 at $m/z$ 400) at a scan rate of 1.5 Hz
<b>Mass Accuracy</b>	<3 ppm with external calibration (under defined conditions) <1 ppm using internal standard, lock masses (under defined conditions)
<b>Polarity Switching</b>	One full cycle in < 1 sec (one full scan positive mode and one full scan negative mode at resolution setting of 35000)
<b>Dynamic Range</b>	>5000 within a single scan
<b>Sensitivity</b>	S/N of a flow injection of Buspirone for the selected mass chromatogram of the $[M+H]^+$ ion ( $m/z = 386.2551$ ): Full Scan: 500 fg on column 100:1

**Table 3-2.** Measuring properties of the Exactive Plus EMR mass spectrometer

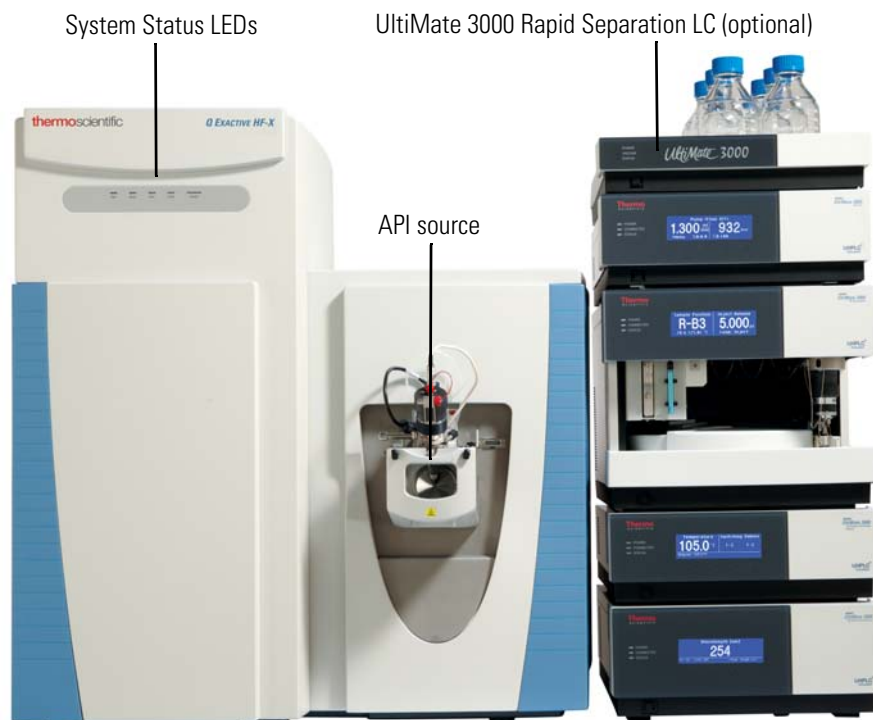
<b>Mass Range for Full Scans</b>	<i>m/z</i> 350–20 000
<b>Mass Resolution</b>	8750 at <i>m/z</i> 200 (6250 at <i>m/z</i> 400) at a scan rate of 12 Hz 17500 at <i>m/z</i> 200 (12500 at <i>m/z</i> 400) at a scan rate of 12 Hz 35000 at <i>m/z</i> 200 (25000 at <i>m/z</i> 400) at a scan rate of 7 Hz 70000 at <i>m/z</i> 200 (50000 at <i>m/z</i> 400) at a scan rate of 3 Hz 140000 at <i>m/z</i> 200 (100000 at <i>m/z</i> 400) at a scan rate of 1.5 Hz
<b>Mass Accuracy</b>	<3 ppm with external calibration (under defined conditions) <1 ppm using internal standard, lock masses (under defined conditions)
<b>Mass Accuracy in EMR Mode</b>	External: <5 ppm RMS for <i>m/z</i> 6001–10000 External: <10 ppm RMS for <i>m/z</i> 10001–15000 External: <25 ppm RMS for <i>m/z</i> 15001–20000, (all under defined conditions)
<b>Polarity Switching</b>	One full cycle in < 1 sec (one full scan positive mode and one full scan negative mode at resolution setting of 35000)
<b>Dynamic Range</b>	>5000 within a single scan
<b>Sensitivity</b>	S/N of a flow injection of Buspirone for the selected mass chromatogram of the [M+H] <sup>+</sup> ion ( <i>m/z</i> = 386.2551): Full Scan: 500 fg on column 100:1

## Layout of the Q Exactive, Q Exactive Focus, Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X Mass Spectrometers

The Q Exactive and Q Exactive Focus mass spectrometers consist of five main components; the Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X mass spectrometers consist of six main components. They are described in the following topics:

- Ion source
- In the Q Exactive Plus, Q Exactive HF and Q Exactive HF-X MS, an injection flatapole with mass resolving capabilities
- Quadrupole mass filter for precursor ion selection
- Intermediate storage device (C-Trap) for short pulse injection
- Collision cell for performing HCD (Higher Energy Collisional Dissociation) experiments
- Orbitrap analyzer for Fourier transform mass analysis

For a schematic view of the instrument layout, see [Figure 3-14](#) on [page 3-26](#). [Figure 3-2](#) shows a front view of the Q Exactive HF-X MS.



**Figure 3-2.** Q Exactive HF-X MS front view

## Operating Modes of the Q Exactive, Q Exactive Focus, Q Exactive Plus, Q Exactive HF , and Q Exactive HF-X MS

Samples can be introduced into the API source at the front side by a variety of methods including direct infusion (with a syringe pump) or an U-HPLC system (for example, Thermo Scientific UltiMate 3000). The sources of the Q Exactive, Q Exactive Focus, Q Exactive Plus, and Q Exactive HF MS MS are similar to the commercial source of the Thermo Scientific LTQ Velos™. The source of the Q Exactive HF-X mass spectrometer is derived from the commercial source of the Thermo Scientific Orbitrap Fusion Lumos™ MS. See “[API Source](#)” on [page 3-17](#) for details.

The injection flatpole transmits ions from the source to the quadrupole. Besides ion transmission, in the Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X MS, the injection flatpole also performs coarse pre-filtering of ions according to their mass-to-charge ratios. See “[Source Ion Optics of the Q Exactive, Q Exactive Focus, Q Exactive Plus, and Q Exactive HF MS](#)” on [page 3-26](#) for details.

The quadrupole rod assembly operates as ion transmission device with the possibility to filter the transmitted ion according to its mass-to-charge ratios. By applying RF and DC voltages to the rods, the filter characteristic is configured. See “[Quadrupole Mass Filter](#)” on [page 3-29](#) for details.

The ions are transferred into the C-Trap through four stages of differential pumping. See “[Ion Optics](#)” on [page 3-24](#) for details. In the C-Trap, the ions are accumulated and their energy is dampened with a bath gas (nitrogen). The ions are then injected through three further stages of differential pumping by a lens system (Z-lens) into the Orbitrap analyzer where mass spectra are acquired by image current detection. The Q Exactive, Q Exactive Focus, and Q Exactive Plus MS are equipped with a standard Orbitrap analyzer, whereas the Q Exactive HF and the Q Exactive HF-X MS are equipped with an ultra-high-field Orbitrap analyzer for increased scan speed. The vacuum inside the Orbitrap analyzer is maintained below 1E-9 mbar. See “[Orbitrap Analyzer](#)” on [page 3-32](#) for details.

Ions are passed through the C-Trap into the HCD cell. The HCD cell adds a Higher Energy Collision Induced Dissociation capability to the instrument. In combination with the quadrupole mass filter this allows MS/MS experiments or all-ion fragmentation (AIF) in case of a broad range of selected mass-to-charge ratios. After the ions have been fragmented in the HCD cell, the HCD cell voltages are ramped up and the ions are transferred back into the C-Trap from where they are injected into the Orbitrap analyzer for detection. See [page 3-35](#) for a description of the HCD cell.

**Table 3-3.** Measuring properties of the Q Exactive and Q Exactive Plus MS

<b>Mass Range for Full Scans</b>	$m/z$ 50–6000 (Scan range: last mass $\leq 15 \times$ first mass)
<b>Precursor Ion Selection</b>	
$50 < m/z \leq 400$	Any isolation widths between 0.4 amu and full scan
$400 < m/z \leq 700$	Any isolation widths between 0.7 amu and full scan
$700 < m/z \leq 1000$	Any isolation widths between 1.0 amu and full scan
$1000 < m/z \leq 2000$	Any isolation widths between 2.0 amu and full scan
$2000 < m/z \leq 2500$	Any isolation widths between 3.0 amu and full scan
$2500 < m/z$	No precursor ion isolation
<b>Mass Resolution</b>	17500 at $m/z$ 200 (12500 at $m/z$ 400) at a scan rate of 12 Hz 35000 at $m/z$ 200 (25000 at $m/z$ 400) at a scan rate of 7 Hz 70000 at $m/z$ 200 (50000 at $m/z$ 400) at a scan rate of 3 Hz 140000 at $m/z$ 200 (100000 at $m/z$ 400) at a scan rate of 1.5 Hz 280000 at $m/z$ 200 (200000 at $m/z$ 400) at a scan rate of 0.7 Hz
Q Exactive Plus MS with Enhanced Resolution Option	
<b>Mass Accuracy</b>	<3 ppm with external calibration (under defined conditions) <1 ppm using internal standard, lock masses (under defined conditions)
<b>Polarity Switching</b>	One full cycle in < 1 sec (one full scan positive mode and one full scan negative mode at resolution setting of 35000)
<b>Dynamic Range</b>	>5000 within a single scan
<b>Sensitivity</b>	S/N of a flow injection of Buspirone for the selected mass chromatogram of the $[M+H]^+$ ion ( $m/z = 386.2551$ ): Full Scan: 500 fg on column 100:1 SIM: 50 fg on column 100:1

**Table 3-4.** Measuring properties of the Q Exactive Focus MS

<b>Mass Range for Full Scans</b>	$m/z$ 50–2000 (Scan range: last mass $\leq 15 \times$ first mass)
<b>Precursor Ion Selection</b>	
$50 < m/z \leq 400$	Any isolation widths between 0.4 amu and full scan
$400 < m/z \leq 700$	Any isolation widths between 0.7 amu and full scan
$700 < m/z \leq 1000$	Any isolation widths between 1.0 amu and full scan
$1000 < m/z \leq 2000$	Any isolation widths between 2.0 amu and full scan
<b>Mass Resolution</b>	17500 at $m/z$ 200 (12500 at $m/z$ 400) at a scan rate of 12 Hz 35000 at $m/z$ 200 (25000 at $m/z$ 400) at a scan rate of 7 Hz 70000 at $m/z$ 200 (50000 at $m/z$ 400) at a scan rate of 3 Hz
<b>Mass Accuracy</b>	<3 ppm with external calibration (under defined conditions) <1 ppm using internal standard, lock masses (under defined conditions)
<b>Polarity Switching</b>	One full cycle in < 1 sec (one full scan positive mode and one full scan negative mode at resolution setting of 35000)
<b>Dynamic Range</b>	>5000 within a single scan
<b>Sensitivity</b>	S/N of a flow injection of Buspirone for the selected mass chromatogram of the $[M+H]^+$ ion ( $m/z = 386.2551$ ): Full Scan: 500 fg on column 100:1 SIM: 50 fg on column 100:1

**Table 3-5.** Measuring properties of the Q Exactive HF MS

<b>Mass Range for Full Scans</b>	$m/z$ 50–6000 (Scan range: last mass $\leq 15 \times$ first mass)
<b>Precursor Ion Selection</b>	
$50 < m/z \leq 400$	Any isolation widths between 0.4 amu and full scan
$400 < m/z \leq 700$	Any isolation widths between 0.7 amu and full scan
$700 < m/z \leq 1000$	Any isolation widths between 1.0 amu and full scan
$1000 < m/z \leq 2000$	Any isolation widths between 2.0 amu and full scan
$2000 < m/z \leq 2500$	Any isolation widths between 3.0 amu and full scan
$2500 < m/z$	No precursor ion isolation
<b>Mass Resolution</b>	15 000 at $m/z$ 200 at a scan rate of 18 Hz 30 000 at $m/z$ 200 at a scan rate of 12 Hz 45 000 at $m/z$ 200 at a scan rate of 10 Hz 60 000 at $m/z$ 200 at a scan rate of 7 Hz 120 000 at $m/z$ 200 at a scan rate of 3 Hz 240 000 at $m/z$ 200 at a scan rate of 1.5 Hz
<b>Mass Accuracy</b>	<3 ppm with external calibration (under defined conditions) <1 ppm using internal standard, lock masses (under defined conditions)
<b>Polarity Switching</b>	One full cycle in < 1 sec (one full scan positive mode and one full scan negative mode at resolution setting of 60 000)
<b>Dynamic Range</b>	>5 000 within a single scan
<b>Sensitivity</b>	S/N of a flow injection of Buspirone for the selected mass chromatogram of the $[M+H]^+$ ion ( $m/z = 386.2551$ ): Full Scan: 500 fg on column 100:1 SIM: 50 fg on column 100:1

**Table 3-6.** Measuring properties of the Q Exactive HF-X MS

<b>Mass Range for Full Scans</b>	$m/z$ 50–6000 (Scan range: last mass $\leq 15 \times$ first mass)
<b>Precursor Ion Selection</b>	
50 < $m/z$ $\leq$ 400	Any isolation widths between 0.4 amu and full scan
400 < $m/z$ $\leq$ 700	Any isolation widths between 0.7 amu and full scan
700 < $m/z$ $\leq$ 1000	Any isolation widths between 1.0 amu and full scan
1000 < $m/z$ $\leq$ 2000	Any isolation widths between 2.0 amu and full scan
2000 < $m/z$ $\leq$ 2500	Any isolation widths between 3.0 amu and full scan
2500 < $m/z$	No precursor ion isolation
<b>Mass Resolution</b>	7500 at $m/z$ 200 at a scan rate of 40 Hz 15 000 at $m/z$ 200 at a scan rate of 20 Hz 30 000 at $m/z$ 200 at a scan rate of 12 Hz 45 000 at $m/z$ 200 at a scan rate of 10 Hz 60 000 at $m/z$ 200 at a scan rate of 7 Hz 120 000 at $m/z$ 200 at a scan rate of 3 Hz 240 000 at $m/z$ 200 at a scan rate of 1.5 Hz
<b>Mass Accuracy</b>	<3 ppm with external calibration (under defined conditions) <1 ppm using internal standard, lock masses (under defined conditions)
<b>Polarity Switching</b>	One full cycle in < 1 sec (one full scan positive mode and one full scan negative mode at resolution setting of 60 000)
<b>Dynamic Range</b>	>5 000 within a single scan
<b>Sensitivity</b>	S/N of a flow injection of Buspirone for the selected mass chromatogram of the $[M+H]^+$ ion ( $m/z = 386.2551$ ): Full Scan: 200 fg on column 100:1 SIM: 20 fg on column 100:1

## Control Elements

Exactive Series mass spectrometers are mainly operated from the desktop computer (data system). LEDs at the front side of the MS give general information about the system status. Switches and ports for other devices of the LC/MS system (for example, a syringe pump or switching valves) are at the power panel on the left side of the MS. The mains inlet, power outlets for syringe pump and switching valves, the port for the relay control cable of the source vacuum pump, and the Ethernet port are at the rear side of the MS. This section describes the control elements for important system functions.

### System Status LEDs

Five system status LEDs at the front side (See [Figure 3-3.](#)) indicate main functions of the system. They are controlled by the source board (See [page 3-49.](#)). [Table 3-7](#) explains the function of the LEDs.



**Figure 3-3.** System status LEDs

**Table 3-7.** System status LEDs of the Exactive Series mass spectrometer

LED	Status	Information
Power	Green	Electronics service switch on (Operating mode)
	Off	Electronics service switch off (Service mode)
Vacuum	Green	Operating vacuum reached
	Yellow	Vacuum insufficient for measurements, RF can be switched on <sup>a</sup>
	Green/Yellow flashing	System bakeout in progress
	Off	Vacuum insufficient for measurements, RF cannot be switched on <sup>a</sup>
Status	Green	Instrument in operating mode
	Yellow	Warn status, does not prevent measurement, however proper operation could be affected <sup>a</sup>
	Off	Grave failure detected that does prevent measurement <sup>a</sup>
System	Green	System on
	Yellow	System in Standby mode
	Off	System off
Scanning	Blue flashing	Instrument scanning
	Off	Instrument not scanning

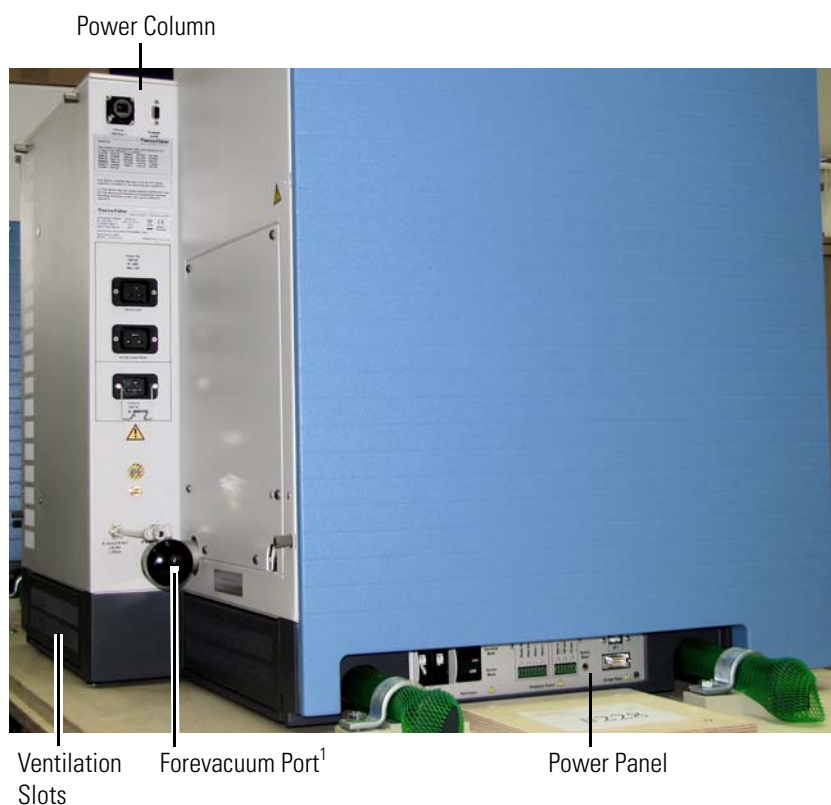
<sup>a</sup> Refer to the Tune software for detailed information about malfunctions of system components.



**NOTICE** The system status LEDs give a quick overview of the general system status; they do not have any function for the safety status of the instrument. Before you perform any maintenance on the instrument, make sure that the main power circuit breaker switch (labeled Main Power) is in the Off (O) position and that the power cords of *mass spectrometer and source vacuum pump* are disconnected. It is not sufficient that the Power LED is off because it might be defective. All system status LEDs are off, when the electronics service switch is in the Service Mode position. ▲

## Power Panel

Figure 3-4 shows the rear side of the instrument. Visible are the power panel, power column, forevacuum port<sup>1</sup>, and ventilation slots.



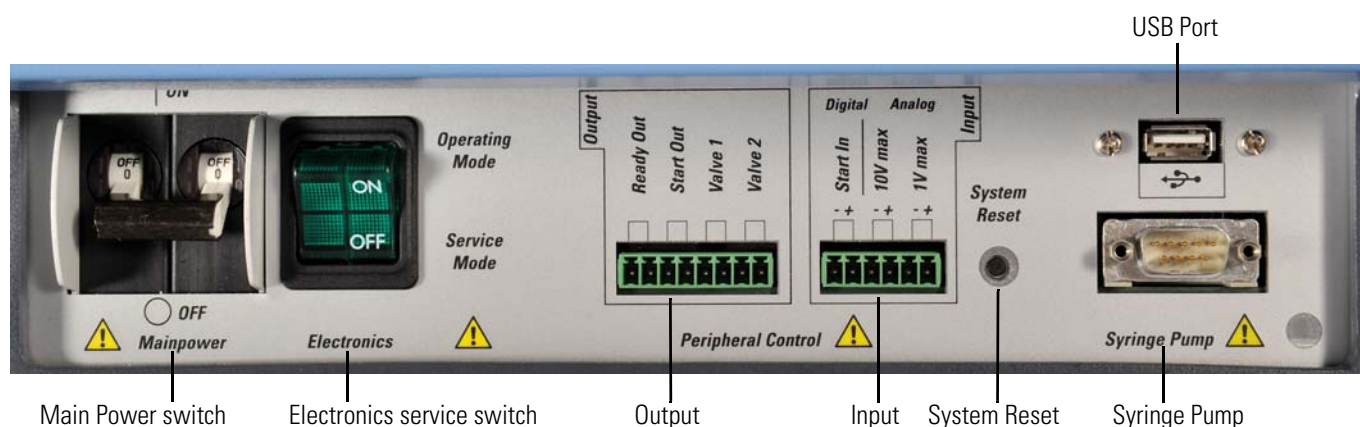
**Figure 3-4.** Rear side of instrument (partial view)

The *main power circuit breaker switch* (labeled Main Power) is located on the power panel at the left side of the mass spectrometer. See Figure 3-5. In the Off (O) position, the circuit breaker removes all power to the mass spectrometer, including the vacuum pumps. In the On (I) position, power is supplied to the mass spectrometer. In the standard operational mode, the circuit breaker is kept in the On (I) position.

<sup>1</sup> The Q Exactive HF-X MS has an additional smaller vacuum port for the auxiliary forepump. See Figure 3-28 on page 3-42.

**NOTICE** Power is to remain on. The mass spectrometer should remain on and pumping continuously for optimum performance. ▲

The *electronics service switch* is located on the power panel. See [Figure 3-5](#). In the Service Mode position, the switch removes power to all components of the mass spectrometer except the vacuum system. In the Operating Mode position, power is supplied to all components of the mass spectrometer.



**Figure 3-5.** Power panel

Both switches contain circuit breakers that protect the electrical wiring of the instrument from an overloaded (overcurrent) condition when it is exposed to more electrical current than it is designed to handle. In case of a thermal overload they interrupt the power supply to the instrument. After cooling down (and removal of the overload), the circuit breakers close and both switches can be used again. If you cannot reset the instrument to the operating mode despite repeated tries, the circuit breaker inside the switch is blown. In this case, call a Thermo Fisher Scientific field service engineer to replace it.

## Peripheral Control

The *peripheral control output* connection allows transmitting *digital* contact closure signals from the Exactive Series mass spectrometer to other devices of the LC/MS system:

- The *Ready Out* port allows the mass spectrometer to provide ready status through contact closure for an external receiving device.
- The *Start Out* port allows the mass spectrometer to provide a programmable contact closure output signal to the inputs of an external receiving device (a fraction collector, for example).

Refer to the Software Manual or the Tune Help of your instrument for information about setting up contact closure signals.

- The *Valve 1* port and the *Valve 2* port allow the mass spectrometer to provide contact closure signals for two switching valves. A suitable two-position switching valve is available from Thermo Fisher Scientific (Rheodyne MXT 715-000, see [Chapter 9, “Replaceable Parts”](#)). See [“Establishing Power Supply and Communication for the Switching Valve\(s\)”](#) on [page 5-34](#) for instructions about connecting switching valves to the mass spectrometer.

Any connected switching valve is controlled with the Tune software or the Xcalibur software. Refer to the Help for details.

The contact closure signals are transmitted through a trigger cable that connects the respective port to the external device. A suitable plug connector for the peripheral control output connection is provided with the Installation Kit. See [“User I/O Connections”](#) on [page 5-36](#) for specifications of the peripheral control output connection ports.

The *peripheral control input* connection allows transmitting signals from other devices of the LC/MS system to the mass spectrometer:

- The *Start In* port allows the mass spectrometer to start data acquisition upon receiving a *digital* contact closure signal from an external device.
- The *10 V max* port and the *1 V max* port allow the mass spectrometer to record an *analog* signal from an external device with the mass spectrometer data. Use the *10 V max* port if the output signal from the analog device is between 0 and +10 V; use the *1 V max* port if the output signal from the analog device is between 0 and +1 V. Both ports may be used simultaneously, allowing to record two data channels.

The contact closure signals are transmitted through a trigger cable that connects the respective port to the external device. A suitable plug connector for the *peripheral control input* connection is provided with the Installation Kit. See [“User I/O Connections”](#) on [page 5-36](#) for specifications of the peripheral control input connection ports.

The *reset button* is also located on the power panel. When you press the reset button, the instrument software is reloaded from the data system. See [“Resetting the System”](#) on [page 6-14](#) for information on resetting the mass spectrometer.

The *USB port* allows the internal computer to communicate with other devices of the LC/MS system. Do not connect any device to this port other than dedicated Thermo Fisher Scientific devices.

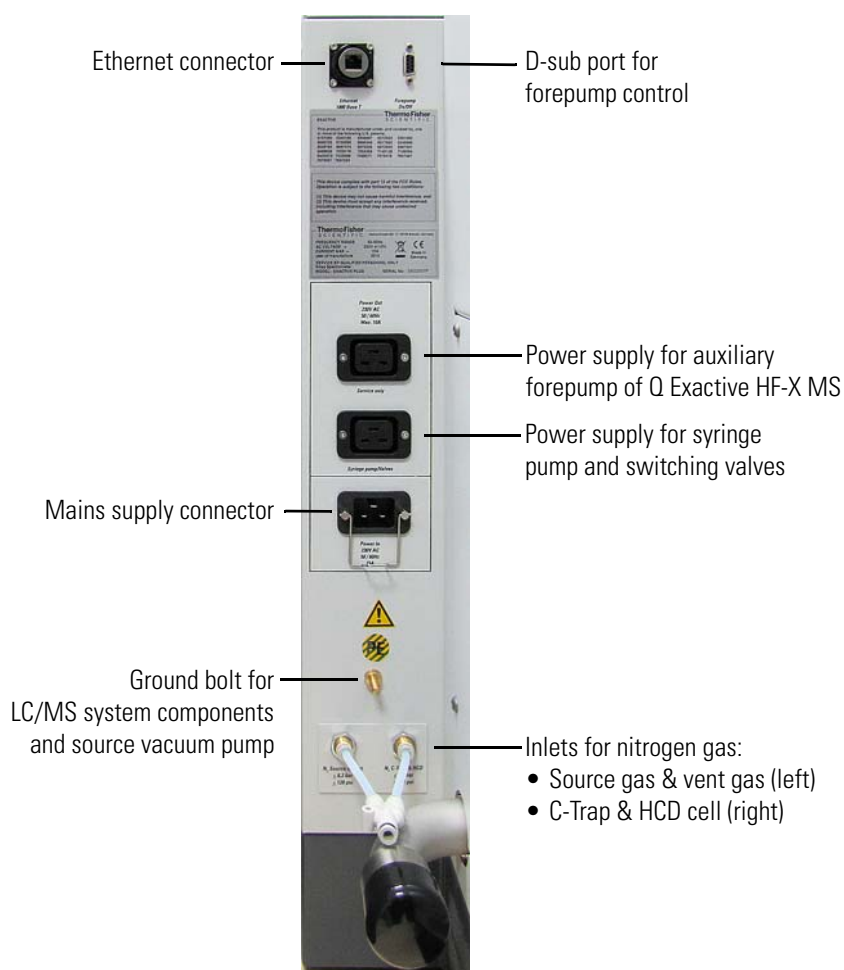
The *syringe contact* allows controlling established syringe pumps by the instrument software by means of the RS-232 serial interface. A suitable syringe pump is available from Thermo Fisher Scientific (Chemyx Fusion 100, see [Chapter 9, “Replaceable Parts”](#)). See also [“Syringe](#)

Pump” on page 3-36. See “Establishing Power Supply and Communication for the Syringe Pump” on page 5-33 for instructions about connecting a syringe pump to the mass spectrometer.

**NOTICE** Any connected syringe pump is controlled with the Tune software or the Xcalibur software. Refer to the Help for details. ▲

## Power Column

The power column at the rear side of the instrument provides external connections for mains supply, gas, and Ethernet communication. See Figure 3-6.



**Figure 3-6.** Power column

Use the Ethernet port at the top left side to connect the mass spectrometer to the data system computer.

Use the D-sub port at the top right side to connect the relay control cable that is used for switching the source vacuum pump with a contact closure (relay output) signal. See also “Forepump On/Off Board” on page 3-53 and “Source Vacuum Pumps” on page 3-41.

Use the outlet labeled *Syringe pump/Valves* on the power column to supply electric power for other devices of the LC/MS system (for example, a syringe pump or switching valves).

Use the outlet labeled *Auxiliary Forepump* to supply electric power for the auxiliary forepump of the Q Exactive HF-X MS. On all other Exactive Series instruments, the second outlet is labeled *Service only* and can be used for service purposes.

These outlets (230 V AC, 50/60 Hz, 10 A maximum) are controlled by the main power circuit breaker switch and not by the electronics service switch.

The power connector for the mains supply is located below the two power outlets. The Exactive Series instrument is designed to operate at a nominal voltage of 230 V AC, 50/60 Hz. See “[Power Supply](#)” on [page 5-9](#) for details.

**NOTICE** Use wall outlets to supply electrical power for the source vacuum pump, the data system, or devices of the LC/MS systems. ▲

Above the gas ports, a ground bolt provides a grounding connection for the ground wires of the source vacuum pump and devices of the LC/MS system. Use the ports for nitrogen gas to connect Teflon™ hoses from the gas supply of the laboratory to the instrument. (See “[Gas Supply](#)” on [page 3-46](#).) The required gas pressure is  $800 \pm 30$  kPa ( $8 \pm 0.3$  bar,  $116 \pm 4$  psi).

## Vacuum System Controls

An interface for RS-485 data connects the TMPs to the vacuum control board. The vacuum gauges of the mass spectrometer are controlled by the same board. (See “[Vacuum Control Board](#)” on [page 3-51](#).)

### Vacuum Gauges

As shown in [Table 3-8](#), vacuum in the mass spectrometer is measured in three regions.

**Table 3-8.** Vacuum measurement regions in Exactive Series mass spectrometers

Region	Typical values	Gauge type	Name in Tune software
S-lens region (Exactive Plus, Exactive Plus EMR, Q Exactive, Q Exactive Focus, Q Exactive Plus, and Q Exactive HF MS)	about 2 mbar (depends on temperature of heated capillary)	Pirani	Forevacuum
Funnel region (Q Exactive HF-X MS)	about 3.5 mbar (depends on temperature of heated capillary)		
Transfer multipole region (Exactive Plus MS)	3E-05 mbar		
Transfer multipole region (Exactive Plus EMR MS)	from 1E-05 mbar to 1E-04 mbar	Cold cathode	High Vacuum
Quadrupole region (Q Exactive, Q Exactive Focus, Q Exactive Plus, and Q Exactive HF MS)	3E-05 mbar		
Orbitrap analyzer (Exactive Plus, Q Exactive, Q Exactive Focus, Q Exactive Plus, and Q Exactive HF MS)	< 8E-10 mbar	Cold cathode	Ultra High Vacuum
Orbitrap analyzer (Exactive Plus EMR MS)	from 1E-10 mbar to 1E-09 mbar		

The vacuum is monitored by three vacuum gauges:

- The vacuum in the S-lens region/funnel region is monitored by an Active Pirani gauge (TPR 280, manufacturer: Pfeiffer Vacuum) connected to the forevacuum line.
- The vacuum in the transfer multipole/quadrupole region is monitored by a Compact Cold Cathode Gauge (IKR 251, manufacturer: Pfeiffer Vacuum).
- The vacuum in the Orbitrap analyzer chamber is monitored by a Compact Cold Gauge (IKR 270, manufacturer: Pfeiffer Vacuum).

## API Source

The atmospheric pressure ionization (API) source forms gas-phase sample ions from sample molecules that are contained in solution. The API source also serves as the interface between LC and mass spectrometer. See [Figure 3-7](#).



**Figure 3-7.** Ion Max API source with HESI probe attached

Additionally, you can operate the API source with atmospheric pressure chemical ionization (APCI), atmospheric pressure photoionization (APPI), or nanospray ionization (NSI) techniques.

The API source consists of the Ion Max™ API source and the ion source interface, which are described in the following topics.

### Ion Max API Source

The Ion Max API source is the part of the ion source that is at atmospheric pressure. The Ion Max API source can be configured to operate in any of several API modes, including electrospray ionization (ESI), atmospheric pressure chemical ionization (APCI), and atmospheric pressure photoionization (APPI). See [Figure 3-7](#). A separate nanospray ionization (NSI) probe is necessary to operate in NSI mode. The ions produced in the API source are transmitted by the ion optics into the Orbitrap mass analyzer, where they are separated according to their mass-to-charge ratio.



## Ion Source Housing

The Ion Max API source housing enables you to quickly switch between ionization modes without the need for specialized tools. A safety relay switches off the high voltage supply (8 kV) when the source is removed from the mass spectrometer.

Ventilating the ion source housing keeps the housing cool and easy to handle. Pressure in the ion source housing is kept at atmospheric levels. This reduces the chemical noise that can be caused by nebulized gases when they are not properly evacuated from the ion source. The probe mounting angle is fixed at the optimum angle for signal intensity and ion source robustness. Minor adjustment of the probe position in the X, Y, and Z dimensions is allowed, with marked adjustments to allow for freedom in probe position during ionization optimization. View ports are placed at the front and at the side of the ion source housing to permit viewing the probe position during ESI operation and the easy addition of accessories.

The Ion Max API source is equipped with special features to ensure maximum lifetime. The drain size and angle prevent ion source corrosion by allowing eluants to flow directly from the probe into the drain when auxiliary gases are off. For liquids that do not enter the drain directly, the floor of the ion source interior is sloped to enable maximum drainage of collected eluants. Additionally, the zero dead volume LC grounding union that connects the LC flow to the ESI sample inlet is offset from the ion source. This is to prevent LC leaks from dripping directly on the ion source housing.

The Ion Max API source has a universal mounting platform and interface for use with ESI, APCI, NSI, and APPI probes. See below. For more information on the analysis of ions produced by the ion source, refer to the *Ion Max and Ion Max-S API Source Hardware Manual*.

## Solvent Drainage

Because the Ion Max API source can accommodate high flow rates, you must collect the waste solvent in a manner that does not build up pressure in the source. The Ion Max API source is fitted with a 25.4-mm (1.0-in.) OD outlet for solvent drainage. A 25.4-mm to 12.7-mm (1-in. to 0.5-in.) reducing fitting connects to a waste container, both of which come with the system. To prevent pressure buildup in the source, make sure that the 1-inch diameter hose from the API source drain to the reducing fitting is as long as possible. The 25.4-mm (1-in.) diameter Tygon™ tubing that comes with the system is 1.52 m (5 ft) long. See [“Connecting the Source Housing Drain to the Waste Container”](#) on [page 8-20](#) for additional information.

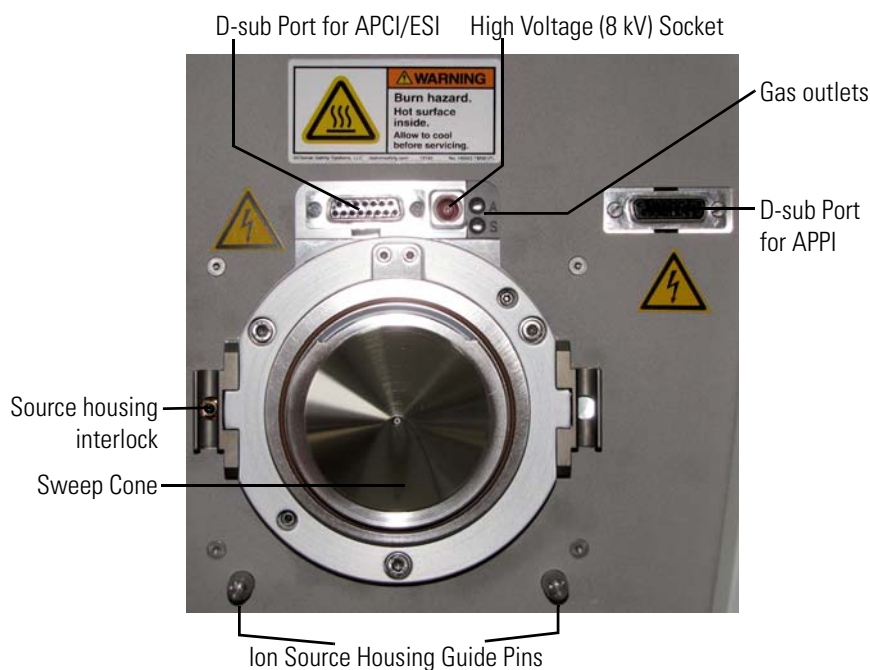


## Ion Source Mount

The ion source mount on the front side of the mass spectrometer allows interchanging ESI, APCI, and APPI probes without using tools. The mount has high-voltage electrical connections for the electrospray needle (ESI and H-ESI) and for the vaporizer and corona discharge needle (APCI). See [Figure 3-8](#). A high-voltage safety interlock switch turns off the following voltages when the ion source is removed:

- ESI and H-ESI spray voltage (or APCI corona discharge voltage)
- All API source and lens voltages, including the ion transfer capillary offset voltage
- The voltages on the ion guides

The above voltages are also turned off if the APCI vaporizer cable (APCI mode) is not plugged into the APCI vaporizer cable interlock connector on the source housing.



**Figure 3-8.** Ion source mount

**NOTICE** When the source housing is removed, the Tune software displays a message box to indicate that the ion source is open. After the source is open for 60 minutes, the system automatically switches into Off mode. ▲

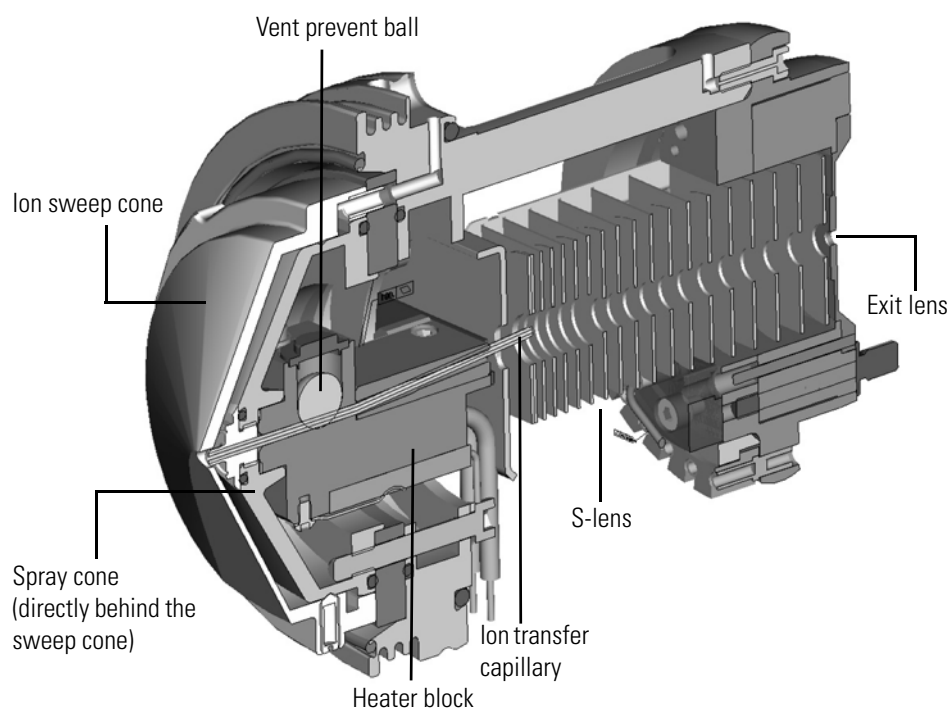
## Ion Source Interface

The ion source interface consists of the components of the API source that are held under vacuum (except for the atmospheric pressure side of the ion sweep cone). Exactive Series instruments have two types of ion source interfaces:

- The ion source interface with an S-Lens is used with the Exactive Plus, Exactive Plus EMR, Q Exactive, Q Exactive Plus, Q Exactive Focus, and Q Exactive HF MS.
- The ion source interface with an ion funnel is used with the Q Exactive HF-X MS.

### Ion Source Interface with S-Lens

The ion source interface in the mass spectrometer (Figure 3-9) includes an ion transfer capillary, two cartridge heaters, a heater block, a sensor, a vent prevent ball, an ion sweep cone, an S-lens, and an exit lens.



**Figure 3-9.** Ion source interface (cross section)

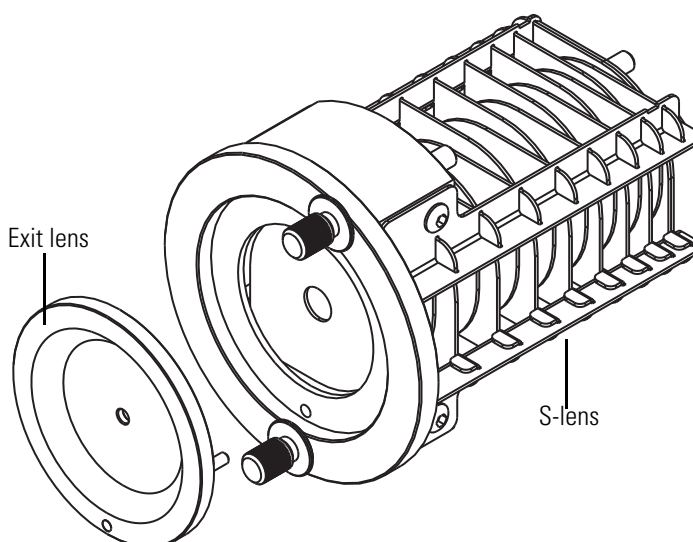
The *ion transfer capillary* assists in desolvating ions that are produced by the API probe. The capillary is an elongated cylindrical tube made of metal. Two heater cartridges are embedded in the heater block. The heater block surrounds the ion transfer capillary and heats it to temperatures up to 400 °C. A probe sensor measures the temperature of the heater block. A decreasing pressure gradient draws ions into the ion transfer capillary in the atmospheric pressure region and transports them to the ion transfer S-lens region of the vacuum manifold. The *vent*

*prevent ball* prevents air from entering the vacuum manifold when the capillary is removed so that you can remove the ion transfer capillary for cleaning without venting the system.

The *ion sweep cone*, also made of metal, fits over the capillary. The ion sweep cone acts as a physical barrier that protects the entrance of the capillary and increases source robustness.

Ions from the ion transfer capillary enter the S-lens. The *S-lens* is an ion transmission device consisting of progressively-spaced, stainless-steel electrodes (Figure 3-10).

An RF is applied to the electrodes of the S-lens to focus the ions toward the opening of the exit lens. Adjacent electrodes have voltages of opposite phase. As the RF amplitude increases, ions of progressively higher mass-to-charge ratios pass through to the exit lens. When you tune the mass spectrometer, adjust the S-lens RF to maximize sensitivity. During the tune procedure, the mass spectrometer determines the mass-dependent RF amplitudes for optimum transmission of ions through the lens.

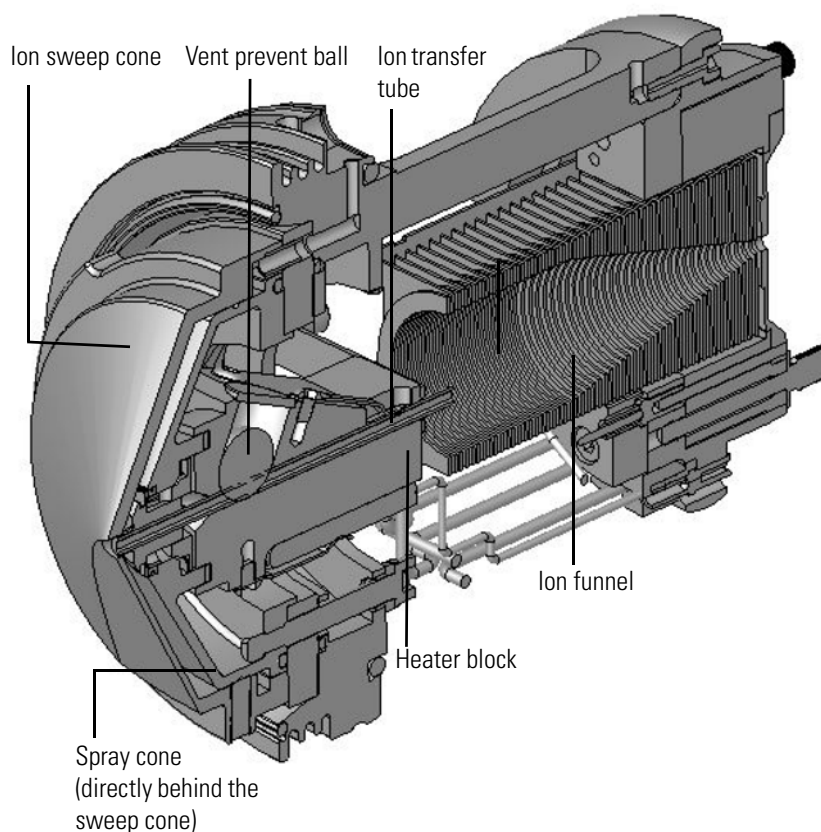


**Figure 3-10.** Exit lens and S-lens (rear view)

Ions from the S-lens pass through the exit lens and move toward the injection flatpole. The S-lens and the exit lens act as a vacuum baffle between the higher-pressure ion source interface region and the lower-pressure ion optics region of the vacuum manifold. The S-lens and exit lens mount to the ion source interface cage. The ion source interface is enclosed in a vacuum chamber that is evacuated by the source vacuum pump.

## API Source Interface with Ion Funnel

The API source interface for the Q Exactive HF-X MS consists of the components of the API source that are held under vacuum (except for the atmospheric pressure side of the ion sweep cone) in a vacuum chamber that the source vacuum pump evacuates to a pressure of approximately 3.5 mbar. The API source interface includes an ion sweep cone, an ion transfer tube, two cartridge heaters, a heater block, a sensor, a vent prevent ball, and the ion funnel (Figure 3-11).



**Figure 3-11.** API source interface (Q Exactive HF-X MS)

The ion sweep cone is a metal cone over the ion transfer tube. The ion sweep cone channels the sweep gas toward the entrance of the ion transfer tube, acts as a physical barrier that protects the entrance of the ion transfer tube, and increases source robustness. The net result is a significant increase in the number of samples to analyze without a loss of signal intensity.

In addition, keeping the ion transfer tube entrance as clean as possible reduces the need for frequent maintenance. Install the ion sweep cone to improve ruggedness when analyzing complex matrices such as plasma or nonvolatile salt buffers. Remove the ion sweep cone before you perform NSI experiments.

The ion transfer tube is a metal tube of a rectangular cross section. It assists in desolvating ions that are produced by the API spray insert while transferring them into the vacuum system.

The heater block contains two heater cartridges, surrounds the ion transfer tube, and heats the tube to temperatures up to 400 °C (752 °F). A thermocouple measures the temperature of the heater block. Typical temperatures of the ion transfer tube are 270 °C (518 °F) for H-ESI and 250 °C (482 °F) for APCI, but these temperatures vary with the flow rate and the mobile phase composition. A decreasing pressure gradient draws ions into the ion transfer tube in the vacuum manifold. The mass spectrometer applies the same electrical potential (positive for positive ions and negative for negative ions) to the ion transfer tube and the ion funnel, which assists in transporting the ions from the tube to the ion funnel. When you remove the ion transfer tube (after it has cooled to room temperature), the vent prevent ball drops into place to stop air from entering the vacuum manifold. Therefore, you can remove the ion transfer tube for cleaning or replacement without venting the system.

Ions from the ion transfer tube pass through the ion funnel and then the ion funnel lens ([Figure 3-16 on page 3-28](#)). The ion funnel is an ion transmission device that consists of equally spaced, stainless-steel electrodes. The mass spectrometer applies an RF voltage to the electrodes, and adjacent electrodes have voltages of opposite phase. As the RF amplitude increases, ions of progressively higher mass-to-charge ratios pass through to the ion funnel lens and move toward the injection flatapole. The ion funnel lens acts as a vacuum baffle between the higher-pressure API source interface region and the lower-pressure ion optics region of the vacuum manifold. The ion funnel and ion funnel lens mount to the API source interface cage.

## Ion Optics

The ion optics focus the ions produced in the API source and transmit them to the C-Trap.

**NOTICE** In-source CID offset voltage and S-Lens Level or Funnel RF level are the only ion optics parameter that you can set in the Tune software. All other ion optics parameters are set automatically. Refer to the Software Manual or the Tune Help for details. ▲

### Ion Optics of Exactive Plus and Exactive Plus EMR Mass Spectrometers

Figure 3-12 shows the schematic view of the Exactive Plus mass spectrometers. Voltages for the elements of the ion optics are supplied by the ion optic supply DC board (See page 3-49.) and the ion optics supply RF board. (See page 3-50.)

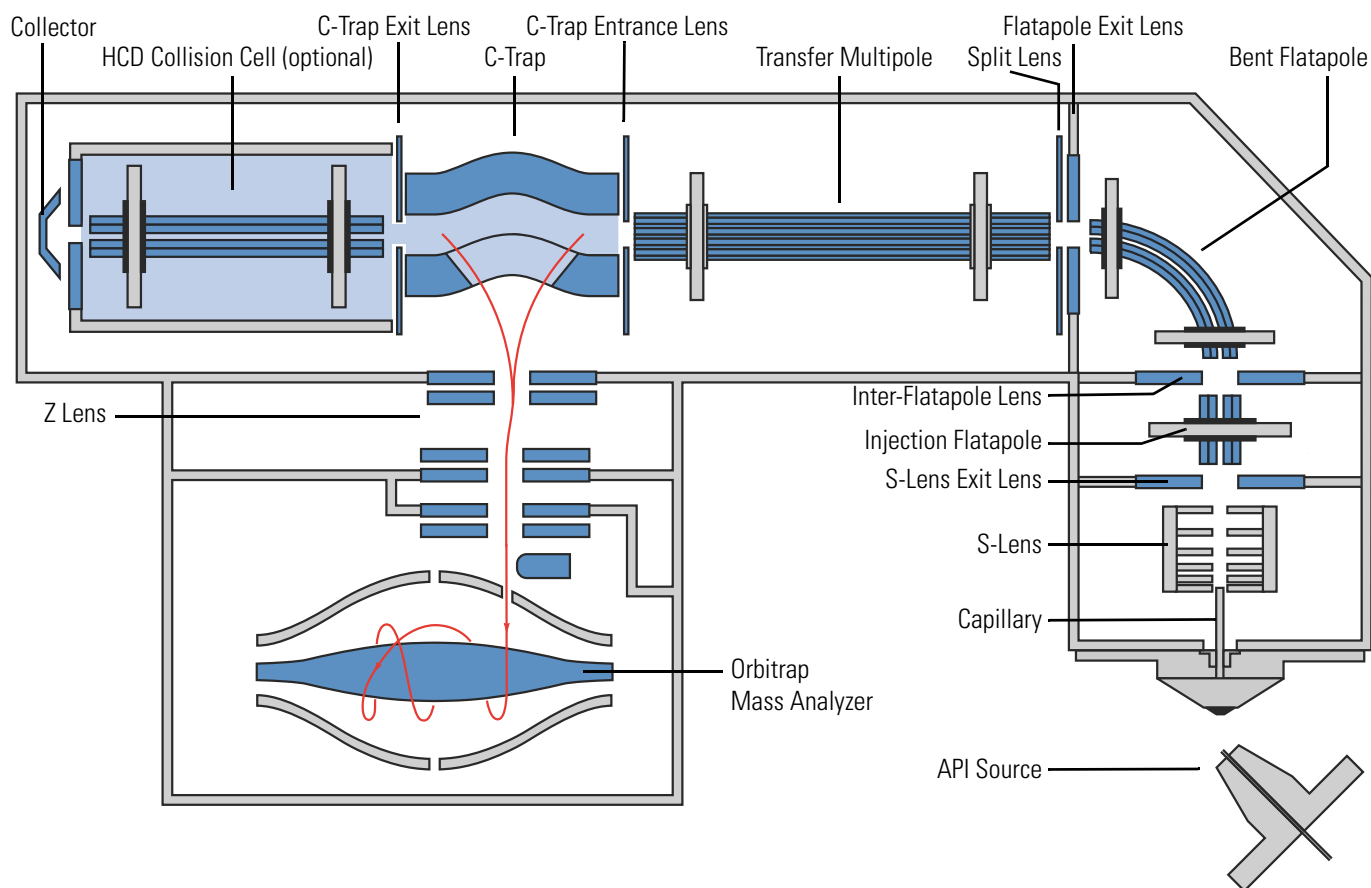
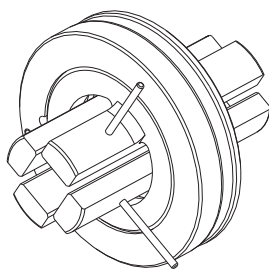


Figure 3-12. Schematic of the Exactive Plus and Exactive Plus EMR MS

## Source Ion Optics of the Exactive Plus and Exactive Plus EMR MS

The *injection flatapole* is a square array of flat metal electrodes that acts as an ion focusing device (Figure 3-13). An RF voltage that is applied to the electrodes (injection flatapole RF) gives rise to an electric field that focuses the ions along the axis of the lens. A DC offset voltage is applied to the injection flatapole (injection flatapole DC). During ion focusing, this voltage creates a negative potential difference with respect to the S-lens exit lens in positive ion mode. In negative ion mode this voltage difference is inverted. Increasing the voltage difference increases the translational kinetic energy of the ions emerging from the S-Lens exit lens.



**Figure 3-13.** Injection flatapole

The *inter-flatapole lens* is a metal plate with a small hole through which the ion beam can pass. A DC potential is applied to the lens to aid in ion transmission. The lens also acts as a vacuum baffle between the source and analyzer ion optics chambers.

## Analyzer Ion Optics of the Exactive Plus and Exactive Plus EMR MS

The *bent flatapole* always acts as an ion transmission device. It guides the ions through a 90° arc from the injection flatapole to the transfer multipole and removes the neutral gas jet and solvent droplets passing through S-lens and injection flatapole. Because of the bent shape of the flatapole, the neutral particles cannot follow the bent path of the flatapole. The region around the bent flatapole is pumped by the interstage inlet IS1 of the source TMP.

An RF voltage is supplied through a separate RF vacuum feedthrough to the bent flatapole electrodes. A common mode DC offset voltage (bent flatapole DC) can be set.

The *flatapole exit lens* focuses the ion beam into the transfer multipole. It also shields the bent flatapole from the RF voltage applied to the transfer multipole and vice versa. Additionally, the lens acts as vacuum baffle between bent flatapole and transfer multipole. Furthermore, the lens assembly ensures the accurate and automatic alignment of bent flatapole and transfer multipole. A potential in the range of  $\pm 25$  V is applied to the flatapole exit lens by the ion optic supply DC board.



The *split lens* is used to start and stop the injection of ions into the mass analyzer. It provides a high deflection voltage most of the time so that ions are deflected into a baffle except when they are to be allowed into the C-Trap. The fast switching of the ion beam ensures the precise determination of the ion injection time that is required for Automatic Gain Control (AGC).

After passing the RF-only *transfer multipole*, which acts as another transmission device, the ions enter the C-Trap through its entrance lens.

## Ion Optics of Q Exactive, Q Exactive Focus, Q Exactive Plus, and Q Exactive HF Mass Spectrometers

Figure 3-14 shows the schematic view of the Q Exactive, Q Exactive Focus, Q Exactive Plus, and Q Exactive HF mass spectrometers. With the exception of the quadrupole, voltages for the elements of the ion optics are supplied by the ion optic supply DC board and the ion optics supply RF board. The quadrupole voltages are supplied by a dedicated PCB. See page 3-49 for details.

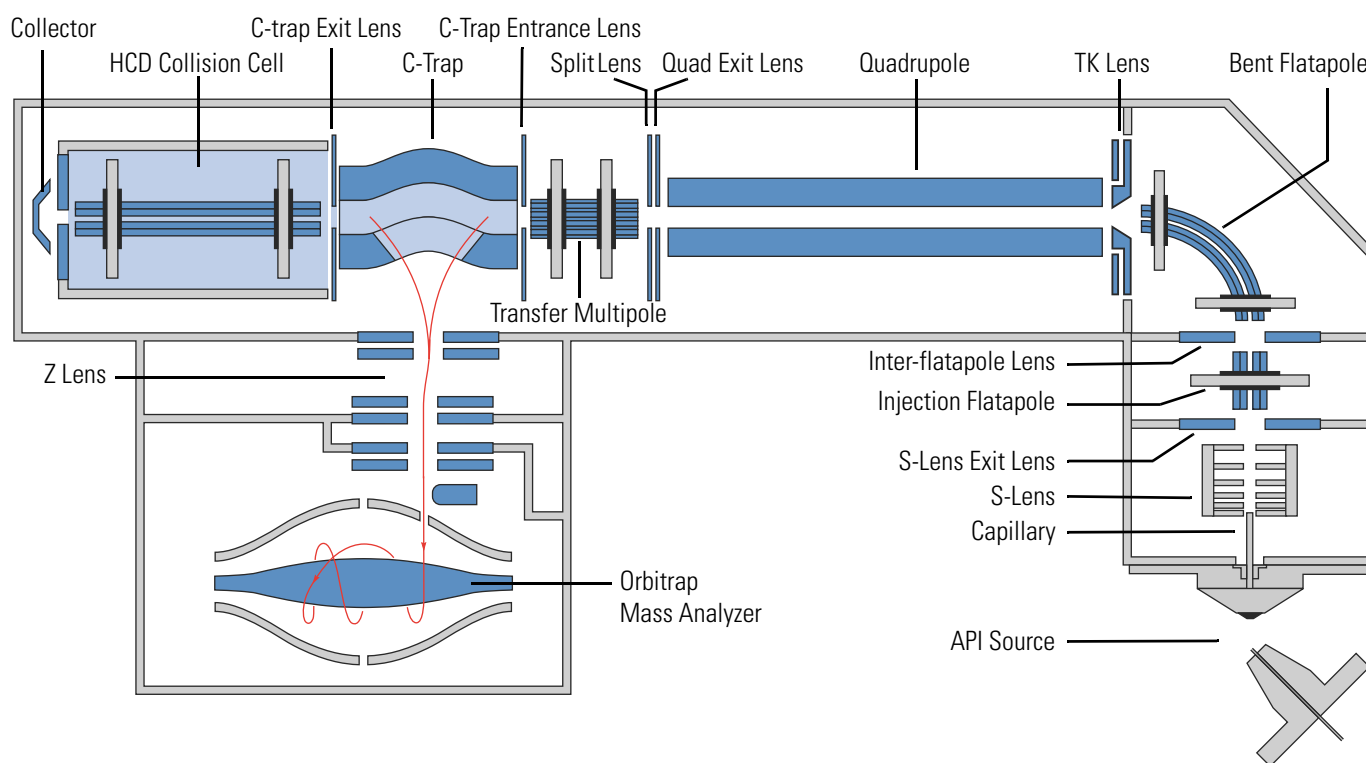


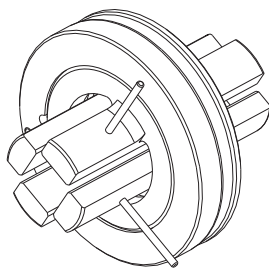
Figure 3-14. Schematic of the Q Exactive, Q Exactive Focus, Q Exactive Plus, and Q Exactive HF MS

### Source Ion Optics of the Q Exactive, Q Exactive Focus, Q Exactive Plus, and Q Exactive HF MS

The *injection flatapole* is a square array of flat metal electrodes that acts as an ion focusing device and, in the Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X MS, as an ion pre-filtering device (Figure 3-13).



An RF voltage that is applied to the electrodes (injection flatapole RF) gives rise to an electric field that focuses the ions along the axis of the lens. A DC offset voltage is applied to the injection flatapole (injection flatapole DC). During ion focusing, this voltage creates a negative potential difference with respect to the S-lens exit lens in positive ion mode. In negative ion mode this voltage difference is inverted. Increasing the voltage difference increases the translational kinetic energy of the ions emerging from the S-Lens exit lens. In ion pre-filtering mode, additional DC voltages (of opposite sign but equal magnitude) are applied to opposite sets of electrodes to coarsely filter ions falling outside of a wide window around the much narrower window of ions passed by the quadrupole. This mode is available only on the Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X MS and is active when the mass resolving quadrupole (see [page 3-29](#)) is in isolation mode.



**Figure 3-15.** Injection flatapole

The *inter-flatapole lens* is a metal plate with a small hole through which the ion beam can pass. A DC potential is applied to the lens to aid in ion transmission. The lens also acts as a vacuum baffle between the source and analyzer ion optics chambers.

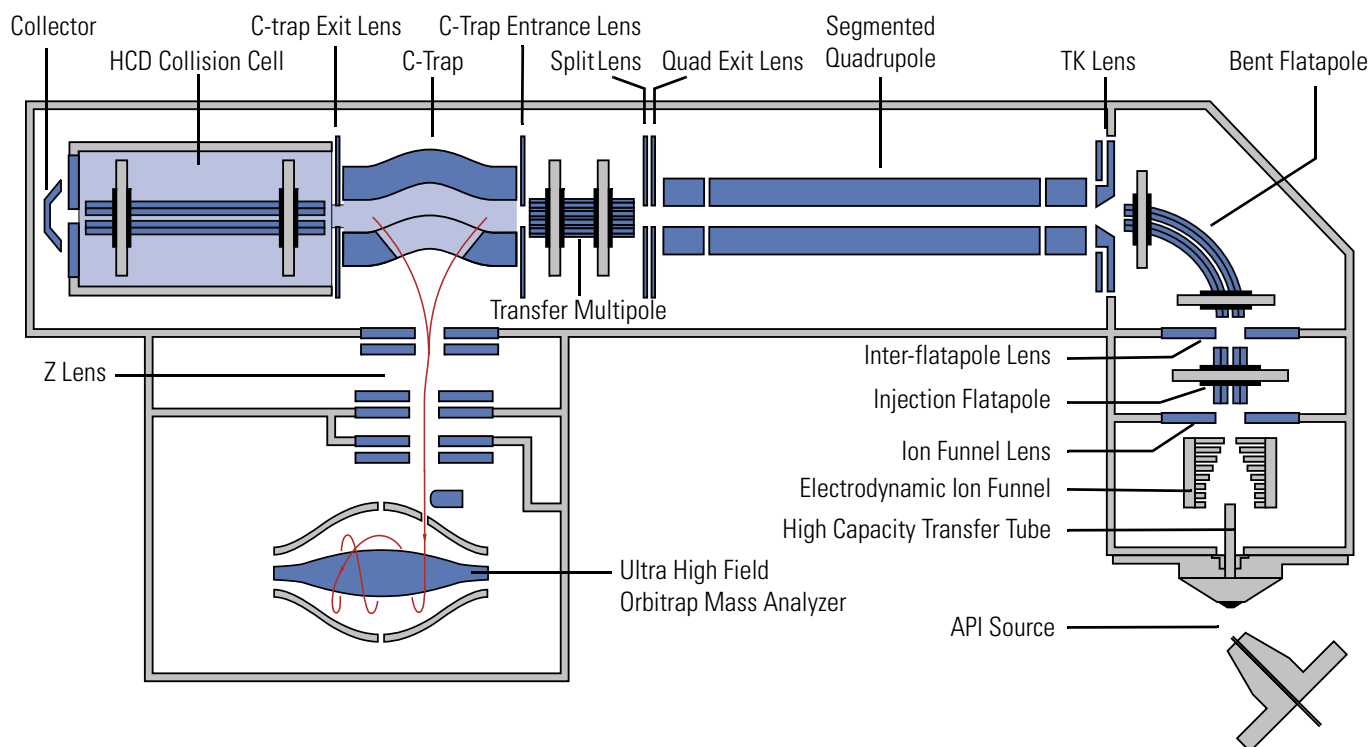
### Source Ion Optics of the Q Exactive HF-X MS

In the Q Exactive HF-X MS, the inlet stack includes a heated high-capacity ion transfer tube—with a rectangular cross section—that assists in desolvating ions. The ion transfer tube guides the ions to an ion transmission device, the ion funnel. This device consists of a stack of electrodes to which RF is applied to transport and focus the ions to the exit lens. From there, the ions move towards the injection flatapole and the bent flatapole. Both the ion optics and the operating pressure range differ from those on the Q Exactive HF MS.

## Functional Description

### Ion Optics

The ion funnel is controlled by the Funnel RF Driver, and its vacuum chamber is evacuated by the source vacuum pump.



**Figure 3-16.** Schematic of the Q Exactive HF-X MS

## Analyzer Ion Optics of the Q Exactive, Q Exactive Focus, Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X MS

The *bent flatapole* always acts as an ion transmission device. It guides the ions through a 90° arc from the injection flatapole to the quadrupole and removes the neutral gas jet and solvent droplets that pass through the S-lens or ion funnel and the injection flatapole. Because of the bent shape of the flatapole, the neutral particles cannot follow the bent path of the flatapole. The region around the bent flatapole is pumped by the interstage inlet IS1 of the source TMP.

An RF voltage is supplied through a separate RF vacuum feedthrough to the bent flatapole electrodes. A common mode DC offset voltage (bent flatapole DC) can be set. In the Q Exactive Plus, Q Exactive HF MS and Q Exactive HF-X, an additional axial DC gradient is applied to the bent flatapole to support the ion pre-filtering mode.

The combination of inner and outer *TK lens* (Turner-Kruger lens) focuses the ion beam into the quadrupole. It also shields the bent flatapole from the RF voltage applied to the quadrupole and vice versa. Additionally, the TK lens acts as vacuum baffle between bent flatapole and quadrupole. Furthermore, the lens assembly ensures the accurate and automatic alignment of bent flatapole and quadrupole.

The quadrupole is described in the next topic.

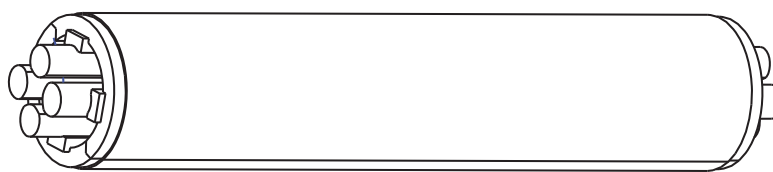
The *quad exit lens* focuses the ions coming from the quadrupole into the transfer multipole.

The *split lens* is used to start and stop the injection of ions into the mass analyzer. It provides a high deflection voltage most of the time so that ions are deflected into a baffle except when they are to be allowed into the C-Trap. The fast switching of the ion beam ensures the precise determination of the ion injection time that is required for Automatic Gain Control (AGC).

After passing the RF-only *transfer multipole*, which acts as another transmission device, the ions enter the C-Trap through its entrance lens.

## Quadrupole Mass Filter

The *quadrupole* is a square array of precision-machined and precision-aligned hyperbolic-profile round rods. See [Figure 3-17](#). Quartz spacers act as electrical insulators between adjacent rods.

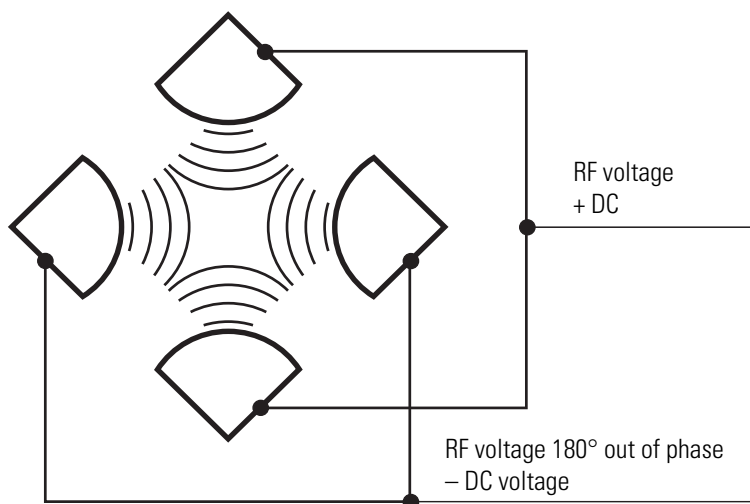


**Figure 3-17.** Quadrupole

The quadrupole assembly is located in the source chamber between the TK lens and the transfer multipole. See [Figure 3-14](#) on [page 3-26](#). In addition to the quadrupole, the assembly includes the exit lens and the split lens.

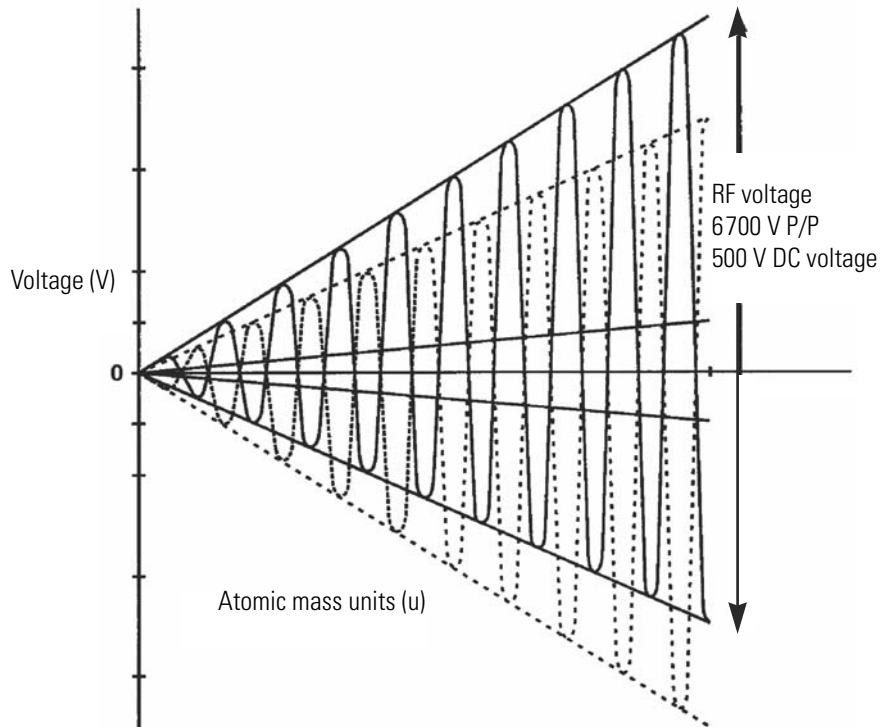
In a quadrupole rod assembly, rods opposite each other in the array are connected electrically. Thus, the four rods can be considered as two pairs of two rods each. RF and DC voltages are applied to the rods and these voltages are ramped during the scan. Voltages of the same amplitude and sign are applied to the rods of each pair. However, the voltages applied to the different rod pairs are equal in amplitude but opposite in sign. See [Figure 3-18](#).

The quadrupole board supplies the voltages for operating the quadrupole. See [page 3-50](#). The RF voltage applied to the quadrupole rods is of constant frequency (between 825–845 kHz) and varies from 0 to 6700 V peak-to-peak amplitude. The DC voltage varies from 0 to  $\pm 500$  V.



**Figure 3-18.** Polarity of the RF and DC voltages applied to the rods of the quadrupole mass filter

In [Figure 3-19](#), the solid line represents the combined RF and DC voltage applied to one rod pair, and the dashed line represents the combined RF and DC voltage applied to the other rod pair. The RF-to-DC-voltage ratios and their values determine the range of mass-to-charge ratios to be transmitted through the quadrupole mass filter.



**Figure 3-19.** Magnitude of the RF and DC voltages applied between the rods of the quadrupole mass filter

In the mass spectrometer, the rods of the quadrupole are supplied with a variable ratio of RF voltage and DC voltage (Figure 3-19). For each injection, controlled by the split lens, the quad RF amplitude and DC voltage are set to fixed values. Under these conditions, only ions of a certain range of  $m/z$  ratios are maintained within bounded oscillations as their velocity carries them through the mass filter. 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.

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

The Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X MS use advanced quadrupole technology (AQT). It comprises a hyperbolic segmented quadrupole, for higher transmission efficiency and optimized transmission window shape.

## Curved Linear Trap

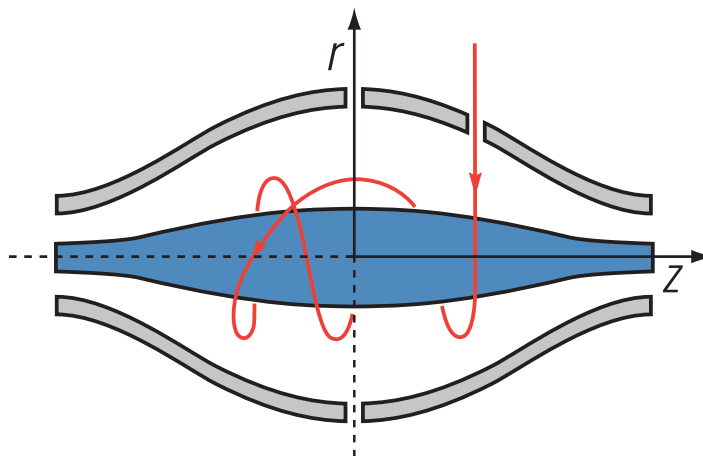
On their way from the ion source to the Orbitrap analyzer, ions move through the gas-free RF transfer multipole into the gas-filled curved linear trap (C-Trap). See Figure 3-14 on page 3-26. Ions entering the C-Trap lose their kinetic energy in collisions with nitrogen bath gas and get collected near the middle part of the C-Trap. The nitrogen collision gas (bath gas) is used for dissipating the kinetic energy of injected ions and for cooling them down to the axis of the C-Trap.

Voltages on the end apertures of the C-Trap (entrance and exit apertures) are elevated to provide a potential well along its axis. These voltages may be later ramped up to squeeze ions into a shorter thread along this axis. The RF to the C-Trap (Main RF) as well as the entrance and exit DC voltages are supplied by the C-Trap RF main board. (See page 3-51.) High voltages to the lens system are supplied by the central electrode high-voltage power supply board. (See page 3-52.)

A *collector* is mounted behind the HCD collision cell. (On Exactive Plus instruments without HCD collision cell, the collector is mounted behind the C-Trap.) This collector is used for an independent C-Trap charge detection, which periodically (every 5–10 seconds) checks and adjusts the accuracy of the Automatic Gain Control. The collector is also used in some of the diagnostic procedures of the instrument.

## Orbitrap Analyzer

The heart of the Orbitrap™ analyzer is an axially-symmetrical mass analyzer. It consists of a spindle-shaped central electrode surrounded by a pair of bell-shaped outer electrodes. See [Figure 3-20](#). The Orbitrap analyzer employs electric fields to capture and confine ions. In the Q Exactive HF and Q Exactive HF-X MS, the Orbitrap analyzer is more compact than the Orbitrap analyzers in the other Exactive Series instruments and thus employs a higher electric field.



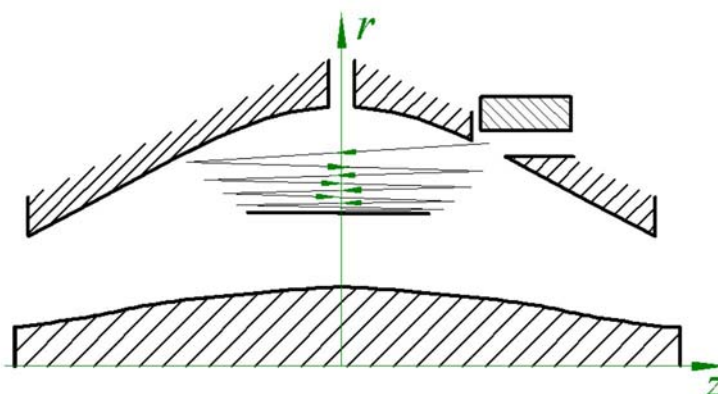
**Figure 3-20.** Schematic of Orbitrap cell and example of stable ion trajectory

## Extraction of Ion Packets

For ion extraction, the RF on the rods of the C-Trap is ramped off and extracting voltage pulses are applied to the electrodes, pushing ions orthogonally to the curved axis through a slot in the inner electrode. Because of the initial curvature of the C-Trap and the subsequent lenses, the ion beam converges on the entrance into the Orbitrap analyzer. The lenses that follow the C-Trap (Z-lens) also act as differential pumping slots and cause spatial focusing of the ion beam into the entrance of the Orbitrap analyzer. Ions are electrostatically deflected away from the gas jet, thereby eliminating gas carryover into the Orbitrap analyzer.

Owing to the fast pulsing of ions from the C-Trap, ions of each mass-to-charge ratio arrive at the entrance of the Orbitrap analyzer as short packets that are only a few millimeters long. For each mass-to-charge population, this corresponds to a spread of flight times of only a few hundred nanoseconds for mass-to-charge ratios of a few hundred Daltons per charge. Such durations are considerably shorter than a half-period of axial ion oscillation in the C-Trap. When ions are injected into the Orbitrap analyzer at a position offset from its equator (See [Figure 3-21](#).), these packets start coherent axial oscillations without the need for any additional excitation cycle.

The evolution of an ion packet during the increase of the electric field is shown schematically in Figure 3-21. When the injected ions approach the opposite electrode for the first time, the increased electric field (owing to the change of the voltage on the central electrode) contracts the radius of the ion cloud by a few percent. The applied voltages are adjusted to prevent collision of the ions with the electrode. A further increase of the field continues to squeeze the trajectory closer to the axis, meanwhile allowing for newly arriving ions (normally, with higher  $m/z$ ) to enter the C-Trap as well. After ions of all  $m/z$  have entered the Orbitrap analyzer and moved far enough from the outer electrodes, the voltage on the central electrode is kept constant and image current detection takes place.



**Figure 3-21.** Principle of electrodynamic squeezing of ions in the Orbitrap analyzer as the field strength is increased

**NOTICE** In contrast to Thermo Scientific LTQ Orbitrap Series instruments, Exactive Series instruments can fill the C-Trap in parallel to acquisition of the transient in the Orbitrap analyzer. ▲

## Measuring Principle

In the mass analyzer shown in Figure 3-20 on page 3-32, stable ion trajectories combine rotation around an axial central electrode with harmonic oscillations along it. The frequency  $\omega$  of these harmonic oscillations along the  $z$ -axis depends only on the ion's mass-to-charge ratio  $m/z$  and the instrumental constant  $k$ :

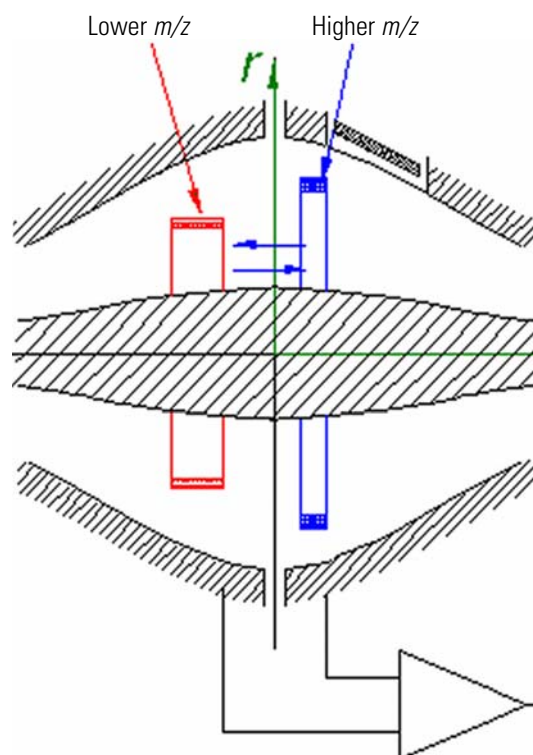
$$\omega = \sqrt{\frac{z}{m}} \times k$$

Owing to the ultra-high-field Orbitrap analyzer of the Q Exactive HF and the Q Exactive HF-X MS, the instrumental constant  $k$  of these instruments is higher compared to the other Exactive Series instruments.

Two split halves of the outer electrode of the Orbitrap analyzer detect the image current produced by the oscillating ions. By Fast Fourier Transformation (FFT) of the amplified image current, the instrument obtains the frequencies of these axial oscillations and therefore the mass-to-charge ratios of the ions.

## Ion Detection

During ion detection, the central electrode and the additional electrode, which deflects ions during injection and compensates electric field imperfections during the measurement (See [Figure 3-21](#) on [page 3-33](#).), are maintained at very stable voltages so that no mass drift can take place. The outer electrode is split in half at  $z=0$ , allowing the ion image current in the axial direction to be collected. The image current on each half of the outer electrode is differentially amplified and then undergoes analog-to-digital conversion before processing by the fast Fourier transform algorithm.



**Figure 3-22.** Approximate shape of ion packets of different  $m/z$  after stabilization of voltages

As mentioned above, stable ion trajectories in the Orbitrap analyzer combine axial oscillations along the  $z$ -axis with rotation around the central electrode and vibrations in the radial direction. (See [Figure 3-20](#) on [page 3-32](#).) For any given  $m/z$ , only the frequency of axial oscillations is completely independent of initial ion parameters, whereas rotational and radial frequencies exhibit strong dependence on initial radius and



energy. Therefore, ions of the same mass-to-charge ratio continue to oscillate along  $z$  together, remaining in-phase for many thousands of oscillations.

In contrast to the axial oscillations, the frequencies of radial and rotational motion will vary for ions with slightly different initial parameters. This means that in the radial direction, ions dephase orders of magnitude faster than in the axial direction, and the process occurs in a period of only 50–100 oscillations. After this, the ion packet of a given  $m/z$  assumes the shape of a thin ring, with ions uniformly distributed along its circumference. See [Figure 3-22](#). Because of this angular and radial smearing, radial and rotational frequencies cannot appear in the measured spectrum. Meanwhile, axial oscillations will persist, with axial thickness of the ion ring remaining small compared with the axial amplitude. Moving from one half outer electrode to the other, this ring will induce opposite currents on these halves, thus creating a signal to be detected by differential amplification.

## HCD Cell

The HCD cell<sup>1</sup> consists of a straight multipole mounted inside a metal tube, which is connected in direct line-of-sight to the C-Trap. It is supplied with a collision gas to supply increased gas pressure inside the multipole. The C-Trap is directly attached to the HCD cell, so part of the collision gas flows into the C-Trap to serve as bath gas. See “[Gas Supply](#)” on [page 3-46](#) for details. The ion optic supply DC board supplies all RF and DC voltages that are necessary to operate the HCD cell. (See [page 3-49](#).)

For HCD (Higher Energy Collisional Dissociation), ions are passed through the C-Trap into the HCD cell. The offset between the C-Trap and HCD is used to accelerate the precursor ions into the gas-filled cell. A potential gradient is applied to the HCD cell to provide fast extraction of ions, such that it returns ions at a reliable rate.

The spectra of fragments generated in the HCD cell and detected in the Orbitrap analyzer are comparable to the typical fragmentations patterns obtained on triple-quadrupole instruments. Refer to the QuickStart Guide for your instrument for more information.

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<sup>1</sup> This feature may not be present in your Exactive Plus mass spectrometer.

## Additional Hardware

In addition to connecting the Exactive Series mass spectrometer to an LC system, you can use the instrument with a syringe pump or switching valves. See [Figure 3-23](#).



**Figure 3-23.** Exactive Series MS with syringe pump and switching valve

A holder for syringe pump and switching valves is shipped with the instrument. Place the holder on the right side of the mass spectrometer, next to the API source. Place the syringe pump on the inclined plate on top of the holder and mount the switching valves to the right part of the holder.

**NOTICE** To prevent the holder from getting out of place, make sure that the top of the instrument housing is dry and free of dust before you put the holder in its position. ▲

## Syringe Pump

Exactive Series mass spectrometers can be connected to a syringe pump. The syringe pump delivers sample solution from the syringe into the API source. When the syringe pump is operating, a motor drives a pusher block that depresses the plunger of the syringe at a user selectable rate. Liquid flows out of the syringe needle and into the sample transfer line as the plunger is depressed. The syringe is held in place by a syringe holder. For instructions on setting up the syringe pump, see [“Setting Up the Syringe”](#) on [page 5-23](#).

A suitable syringe pump (Chemyx Fusion 100) is available from Thermo Fisher Scientific and shipped with the instrument.

An RS-232 serial interface allows controlling established syringe pumps by the instrument software. The external connection for the communication between mass spectrometer and syringe pump is located on the power panel. See [Figure 3-5](#) on [page 3-12](#). The mass spectrometer can supply electric power to the syringe pump with an outlet on the power column. See [Figure 3-6](#) on [page 3-14](#). Alternatively, use a properly grounded wall outlet. “[Connecting the Inlet Plumbing](#)” on [page 5-19](#) gives instructions on connecting the syringe pump to the mass spectrometer.

Syringe pump parameters can be set with the Tune software. The Tune software allows switching on/off the syringe pump by an instrument method or manually. Refer to the Software Manual or the Tune Help for details.

## Switching Valves

Exactive Series mass spectrometers allow connecting up to two external switching valves. Suitable switching valves (Rheodyne™ MX Series II™) are available from Thermo Fisher Scientific). One switching valve is shipped with the instrument. The valves are controlled by the instrument software by means of contact closures. The external connection for the valves is located on the power panel. See [Figure 3-5](#) on [page 3-12](#). The Universal Power Supply of the valve can be operated from inputs of 100–240 V AC, 50–60 Hz. The mass spectrometer can provide electric power to the valves with an outlet on the power column. See [Figure 3-6](#) on [page 3-14](#). Alternatively, use a properly grounded wall outlet.

You can configure (plumb) a switching valve as a loop injector for flow injection analysis or as a divert valve for direct infusion, high-flow infusion, or LC/MS experiments. Procedures for plumbing the valve in the loop injector or divert valve configuration are given in “[Connecting the Inlet Plumbing](#)” on [page 5-19](#).

You can control the switching valves with the Tune software. Refer to the Help for instructions on operating the switching valves.

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

## Divert Valve Positions

Use the switching valve to divert the solvent flow between the mass spectrometer and waste (Figure 3-24). The valve has two positions:

- Detector position—Solvent flow from the LC pump enters the valve through port 2 and exits the valve through port 3.
- Waste position—Solvent flow from the LC pump enters the valve through port 2 and exits the valve through port 1 to waste.

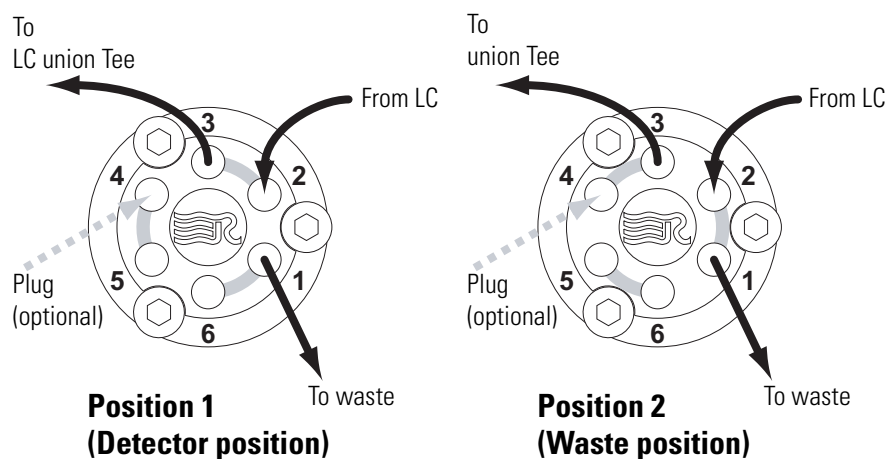
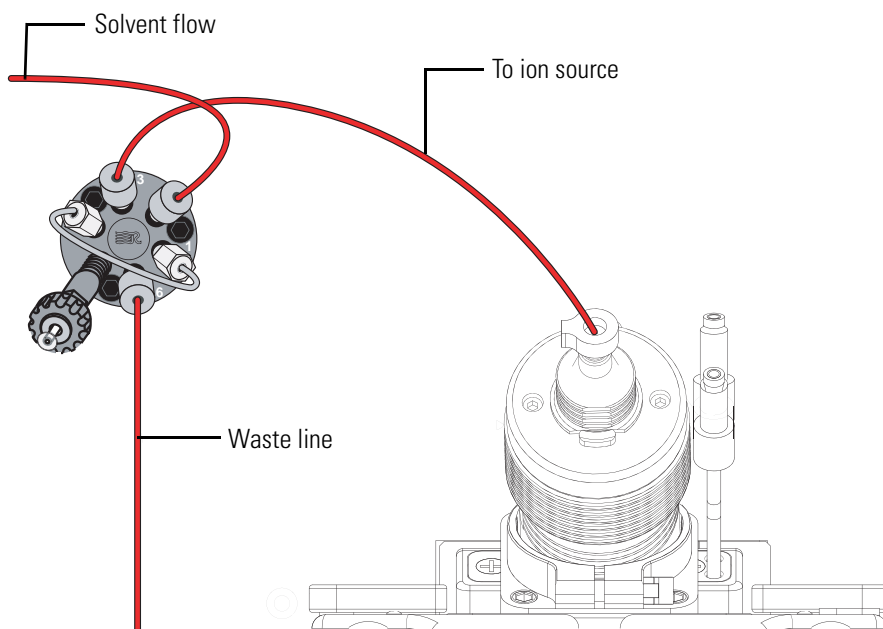


Figure 3-24. Divert valve positions

## Injection Valve Operation

In the loop injection configuration (Figure 3-25), the switching valve is used to switch between load and inject modes. The valve has two positions:

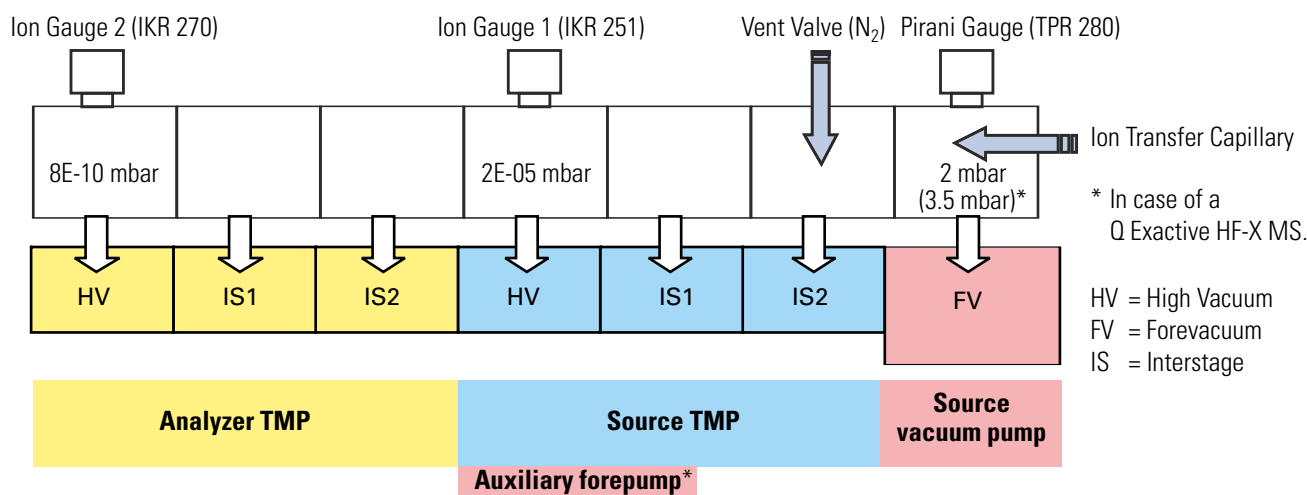
- Load position—Inject the sample solution through port 5. The injected sample enters and exits the sample loop through ports 4 and 1, respectively. As you overfill the sample loop, the sample solution exits the valve through port 6. Solvent flow from the LC pump enters and exits the valve through ports 2 and 3, respectively.
- Inject position—After filling the sample loop, the controls available in the Tune software are used. Solvent flow from the LC pump backflushes sample out of the sample loop and then out of the valve through port 3 toward the detector.



**Figure 3-25.** Load/Inject positions

## Vacuum System

The vacuum manifold encloses the ion source interface, ion guides, C-Trap, and the Orbitrap analyzer. The vacuum manifold consists of thick-walled aluminum chambers with machined flanges on the front, sides, and bottom, and various electrical feedthroughs and gas inlets. The vacuum manifold is divided into three chambers. The region inside the first chamber, called the S-lens region or funnel region, is evacuated by a rotary-vane pump (source vacuum pump). The region inside the second chamber, called the source chamber, is evacuated by a turbomolecular pump (source TMP). The region inside the third chamber, called the analyzer chamber, is evacuated by another turbomolecular pump (analyzer TMP). [Figure 3-26](#) shows a schematic overview of the vacuum system, [Table 3-9](#) shows the vacuum regions of the mass spectrometer. See [page 3-16](#) for information about the vacuum gauges in the Exactive Series mass spectrometer.



**Figure 3-26.** Schematic of vacuum system in Exactive Series MS

**Table 3-9.** Vacuum regions overview

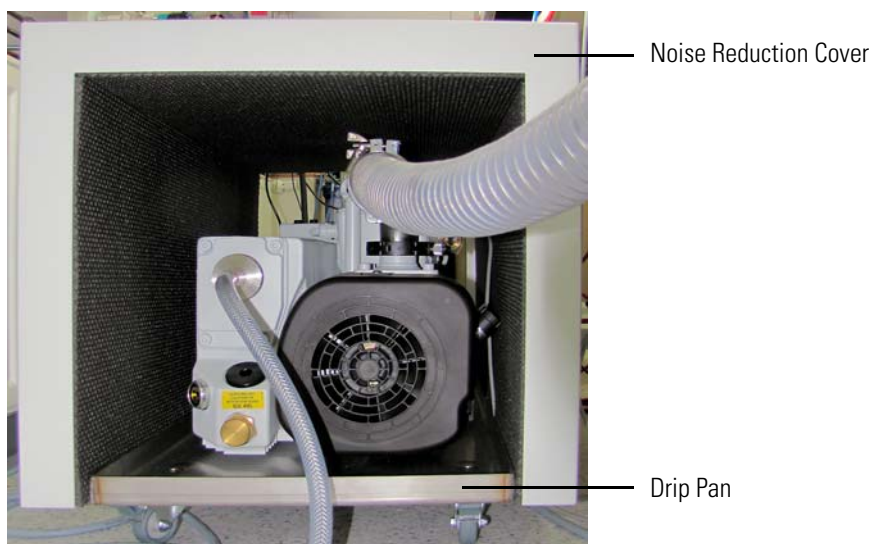
Region in instrument	Vacuum [mbar]	applied by
Ion Max housing	1E+03	Atmosphere
S-lens region (Exactive Plus, Exactive Plus EMR, Q Exactive, Q Exactive Focus, Q Exactive Plus, and Q Exactive HF MS)	2	Source vacuum pump
Funnel region (Q Exactive HF-X MS)	3.5	Source TMP IS2
Injection flatapole		Source TMP IS2
Bent flatapole		Source TMP IS1
Transfer multipole (Exactive Plus MS)	3E-05	
Transfer multipole (Exactive Plus EMR MS)	1E-05 to 1E-04	Source TMP HV
Quadrupole (Q Exactive, Q Exactive Focus, Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X MS)	3E-05	
Z-lens		Analyzer TMP IS2
Region between Z-lens and Orbitrap analyzer		Analyzer TMP IS1
Orbitrap analyzer	< 8E-10	Analyzer TMP HV

## Source Vacuum Pumps

In the Q Exactive HF-X MS, a single-stage rotary vane pump (MS 120, manufacturer: Agilent Technologies) is used as source vacuum pump. It evacuates the funnel region of the vacuum manifold. The pump has a nominal pumping speed of about 110 m<sup>3</sup>/h. This pump has an integrated noise reduction cover and is equipped with wheels.

In all other Exactive Series MS, a single-stage rotary vane pump (SOGEVAC™ SV 65 BI, manufacturer: Oerlikon Leybold Vacuum) is used as source vacuum pump. It establishes the vacuum that is necessary for the proper operation of the source TMP. The pump also evacuates the S-lens region of the vacuum manifold. The pump has a nominal pumping speed of about 60 m<sup>3</sup>/h.

The SOGEVAC forepump is placed on a drip pan with wheels under the workbench immediately behind the mass spectrometer. See [Figure 3-27](#). A noise reduction cover for the forepump is shipped with the instrument.



**Figure 3-27.** Forepump SOGEVAC 65 BI with noise reduction cover and drip pan

## Connections to the Source Vacuum Pump

A section of 4.5 cm (1.8 in.) ID reinforced PVC tubing connects the source vacuum pump to the large vacuum port at the rear side of the mass spectrometer. See [Figure 3-4](#) on [page 3-11](#). An exhaust hose connects the forepump to the exhaust system in the laboratory. The pump is designed to operate at a nominal voltage of 230 V AC, 50/60 Hz. Connect the power cord of the forepump to a wall receptacle that is fused with 15 A or 16 A.

The source vacuum pump is switched on and off by a contact closure signal from the mass spectrometer. The relay control cable of the forepump is plugged into the D-sub port on the power column next to the Ethernet port. See [Figure 3-6](#) on [page 3-14](#).

For a detailed description of the forepump and for instructions on user maintenance, refer to the handbook of the manufacturer. See also “[Maintenance of the Forepumps](#)” on [page 8-8](#).

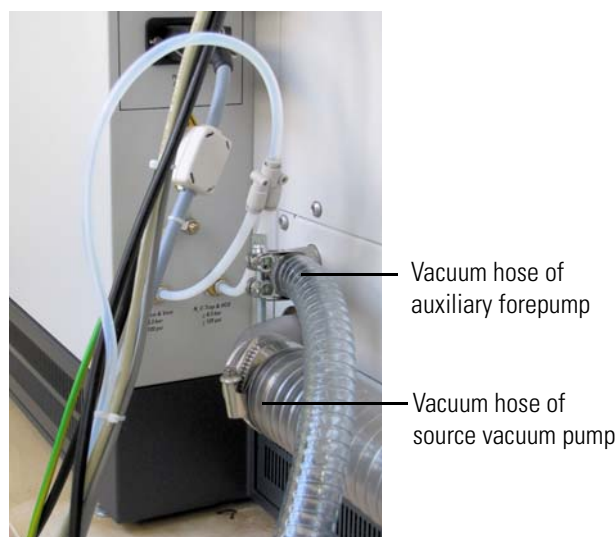
## Auxiliary Forepump

In the Q Exactive HF-X MS, a two-stage rotary vane pump (DUO 11, manufacturer: Pfeiffer Vacuum) supplies as auxiliary forepump the forevacuum for the source TMP. The pump has a nominal pumping speed of about 9 m<sup>3</sup>/h at 50 Hz / 10.5 m<sup>3</sup> at 60 Hz. The auxiliary forevacuum pump is powered over a switchable socket at the instrument. See [Figure 3-6](#) on [page 3-14](#).

A drip pan and a noise reduction cover for the auxiliary forepump are shipped with the instrument.

## Connections to the Auxiliary Forepump

Connect the power supply cord of the auxiliary forepump of the Q Exactive HF-X MS to the outlet labeled *Auxiliary Forepump* on the power column at the rear side of the mass spectrometer. Connect the exhaust hose of the pump to the exhaust system of the laboratory. A T-piece is used to join the exhaust lines of both forepumps.



**Figure 3-28.** Vacuum ports of Q Exactive HF-X MS



The vacuum hose of the auxiliary forepump of the Q Exactive HF-X MS has an inner diameter of 19 mm ( $\frac{3}{4}$  in.). Connect the vacuum hose of the pump to the small vacuum port at the rear side of the MS. See [Figure 3-28](#). Run the auxiliary vacuum hose according to the same instructions as described above for the main vacuum hose.

## Turbomolecular Pumps

Two turbomolecular pumps (TMPs) provide the vacuum for the mass spectrometer. The TMPs are controlled by individual controllers and powered by +24 V DC (480 W) power supplies. Power for the TMPs is turned off by the main power circuit breaker switch, but not by the electronics service switch. The TMPs are air cooled by fans that are mounted in fan inserts on the bottom of the instrument.

Pump controllers supply power to the TMPs and control them. The status of each TMP (such as temperature or rotational speed) is sent from the TMP controller to the vacuum control board. See [page 3-51](#).

### Source TMP

The vacuum in the source chamber is created by a three-stage split flow TMP (SplitFlow 310, manufacturer: Pfeiffer Vacuum). The TMP mounts onto the bottom of the vacuum manifold. The source TMP has three pumping inlets (see [Figure 3-26](#) on [page 3-40](#)):

- A 30 L/s interstage inlet (IS2) in the molecular drag section of the pump, which evacuates the region between S-lens exit lens or ion funnel lens and inter-flatapole lens.
- A 155 L/s interstage inlet (IS1) about half way down the rotor stack, which evacuates the bent flatapole region.
- A 200 L/s high-vacuum (HV) inlet at the top of the rotor stack, which evacuates the transfer multipole/quadrupole region.

In the Q Exactive HF-X MS, the auxiliary forepump provides the forevacuum for the source TMP. In all other Exactive Series instruments, the source vacuum pump provides the forevacuum for the source TMP.

For a detailed description of the source TMP and for instructions on user maintenance, refer to the handbook for the pump. See also [“Maintenance of the Source TMP”](#) on [page 8-11](#).

## **Analyzer TMP**

The vacuum in the analyzer chamber is created by a second three-stage split flow TMP (TURBOVAC 250i, manufacturer: Oerlikon Leybold Vacuum). The pump mounts onto the bottom of the vacuum manifold. The analyzer TMP has three pumping inlets (see [Figure 3-26](#) on [page 3-40](#)):

- A 20 L/s interstage inlet (IS2) in the molecular drag section of the pump, which evacuates the Z-lens region.
- An 20 L/s interstage inlet (IS1) about half way down the rotor stack, which evacuates the region between Z-lens and Orbitrap analyzer.
- A 250 L/s high-vacuum (HV) inlet at the top of the rotor stack, which evacuates the UHV (Orbitrap analyzer) chamber.

The interstage inlet IS1 of the source TMP provides the forevacuum for the analyzer TMP.

For a detailed description of the analyzer TMP and for instructions on user maintenance, refer to the handbook for the pump. See also “[Maintenance of the Analyzer TMP](#)” on [page 8-11](#).

## **Vent Valve**

The vent valve is a solenoid-operated valve that allows the vacuum manifold to be vented. The vent valve is closed when the solenoid is energized. The vacuum control board switches the vent valve.

The vacuum manifold is vented when external power is removed from the instrument. (Power is removed from the instrument by a power failure or by placing the main power circuit breaker in the Off (O) position.) Power is provided to the vent valve for a short time after the external power is removed. If external power is not restored to the instrument in this time, power to the vent valve solenoid is shut off. When power to the vent valve solenoid is shut off, the vent valve opens and the manifold is vented with nitrogen. See [Figure 3-26](#) on [page 3-40](#) and [Figure 3-29](#) on [page 3-46](#). The vent valve closes after power is restored to the instrument.

## System Bakeout

After the system has been open to the atmosphere (for example, during maintenance work or a power outage), the vacuum deteriorates due to contaminations of the inner parts of the vacuum system caused by moisture. These contaminations must be removed by heating the vacuum system: a system bakeout. See [“Baking Out the System”](#) on [page 8-12](#) for instructions on performing a system bakeout.

## Bakeout Devices

To provide the high temperatures required for performing a system bakeout, the mass spectrometer is equipped with two halogen bulbs inside the vacuum chamber. Furthermore, two heating cartridges are built into the block that serves as housing for the analyzer TMP.

## Bakeout Control

For a system bakeout, the instrument software simultaneously switches all heaters by relays. The vacuum control board controls the bakeout procedure. For example, the heaters are switched off in case of a failure of the fan below the analyzer TMP.

**NOTICE** Individual printed circuit boards also have devices for checking the actual temperature. ▲

## Cooling Fans

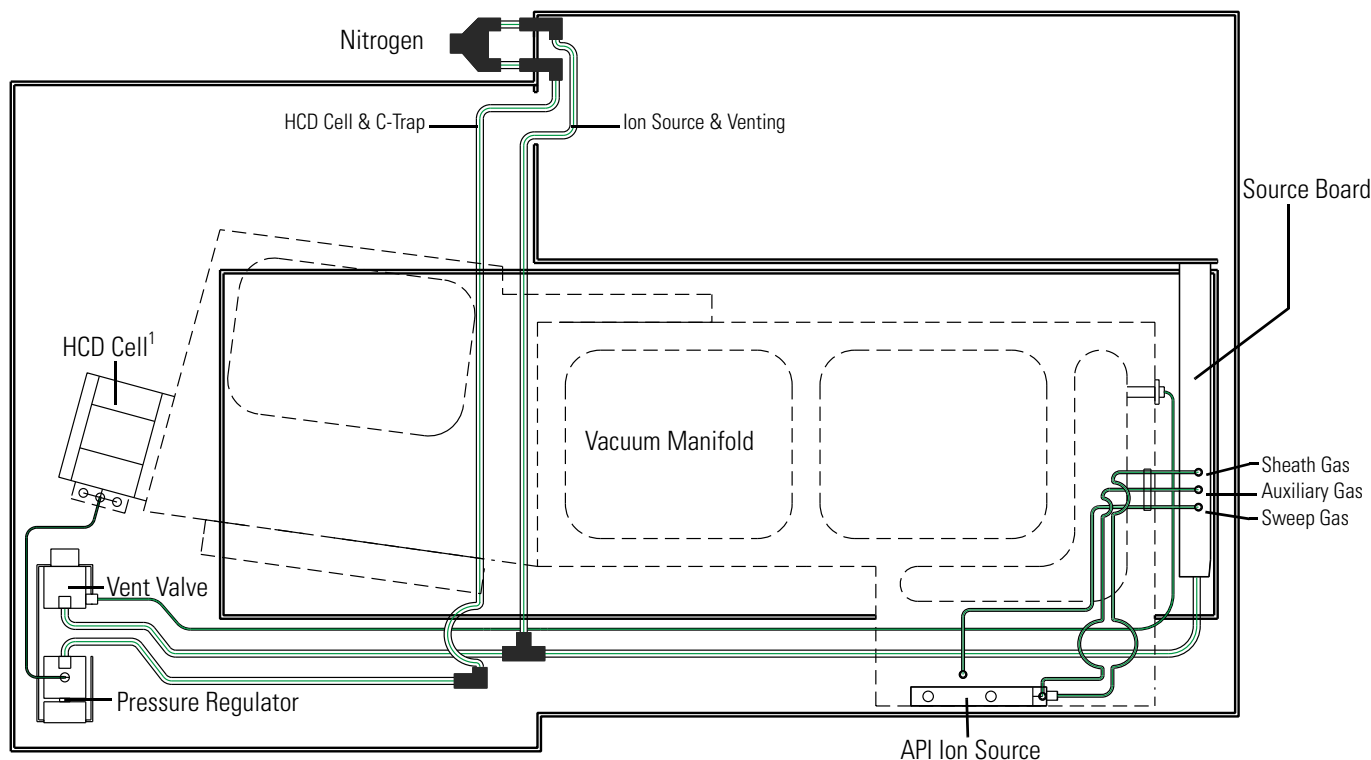
Six fans provide cooling for the Exactive Series mass spectrometers. On the right instrument side, a fan insert with four fans cools the source TMP and the electronic boards. On the left instrument side, a second insert with two fans cools the analyzer chamber and the analyzer TMP. From the rear of the mass spectrometer, air is drawn in through fan filters. The exhaust air is expelled from the ventilation slots on the sides of the mass spectrometer.

The vacuum control board monitors all fans in the instrument. In case of a fan failure, the board triggers an alert in the Tune software. In case of a failure of the fans below the analyzer TMP, no bakeout procedure is possible.

**NOTICE** In addition to the fans described in this topic, various printed circuit boards are equipped with individual fans. ▲

## Gas Supply

Exactive Series mass spectrometers require high-purity (99%) nitrogen for the API source gases (sheath/auxiliary/sweep gas), for the collision gas (bath gas) of the C-Trap, and for the collision gas for the HCD cell (if present<sup>1</sup>). Nitrogen is also used to vent the vacuum manifold with the vent valve if the system is shut down. The required pressure is  $800 \pm 30$  kPa ( $8 \pm 0.3$  bar,  $116 \pm 4$  psi). The vented vacuum manifold is protected against overpressure by pressure relief valves. [Figure 3-29](#) shows a schematic of the gas supply in the instrument.



**Figure 3-29.** Schematic of gas supply

## Gas Distribution in the Instrument

The nitrogen inlet ports are at the bottom of the power column at the rear side of the instrument:

- Source gas & vent gas (left)
- HCD cell & C-Trap (right)

If you use only high-purity nitrogen, the gas that comes from the gas supply in the laboratory enters the instrument through a Y-piece that is connected to both nitrogen ports. See [Figure 3-29](#). For the HCD cell,

<sup>1</sup> This feature may not be present in your Exactive Plus mass spectrometer.

Thermo Fisher Scientific recommends that you use ultra high-purity (99.999%) nitrogen. In this case, the Y-piece is not used. See “[Gas Supply](#)” on [page 5-11](#) for details.

The gas flow from the left nitrogen port is directed through Teflon™ tubing to the source board. On the board, a valve terminal divides the nitrogen flow into three streams (sheath/auxiliary/sweep gas) to the API source. A T-piece diverts part of this nitrogen flow to the vent valve (See [page 3-44](#) for further information.). When the vacuum control board switches the vent valve, the nitrogen is led through stainless steel tubing to the vacuum manifold.

The gas flow from the right nitrogen port is directed through Teflon tubing to a pressure regulator, which keeps the gas pressure to C-Trap and HCD cell constant. From the regulator, the collision gas is led to the HCD cell next to the C-Trap (flow rate: ~0.5 mL/min). In the Exactive Plus EMR, Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X mass spectrometers, an electronic pressure regulator sets the nitrogen pressure according to the operating mode of the instrument and the chosen user setting. The nitrogen gas that leaks from the HCD cell is used for ion trapping and cooling in the C-Trap.

## Printed Circuit Boards

The Exactive Series mass spectrometer is controlled by a PC running the Xcalibur™ software suite. The software controls all aspects of the instrument. The main software elements are the control of ion detection and the control of the Orbitrap analyzer. The following pages contain a short overview of the various electronic boards of the mass spectrometer.

The electronics of the mass spectrometer contains complicated and numerous circuits. Therefore, only qualified and skilled electronics engineers should perform servicing.

A Thermo Fisher Scientific field service engineer should be called if servicing is required. It is further recommended to use Thermo Fisher Scientific spare parts only. Before you call a service engineer, try to find the defect by means of errors indicated in the Tune software. A precise description of the defect will ease the repair and reduce the costs.

## Preamplifier

The preamplifier board is a broadband amplifier with high-resistive differential inputs. It converts the image current, which is induced by the ions oscillating in the Orbitrap analyzer, to a proportional output voltage. The preamplifier interfaces through coaxial cables directly to the data acquisition board, which also provides the electric power for the preamplifier. After analog-to-digital conversion on the data acquisition board, the output voltage undergoes further Fourier transformation on the internal computer.

## Data Acquisition Board (DAQ Board)

The data acquisition (DAQ) board converts detected ion signals coming from the preamplifier to digital form. Then it sends the digital signals through a USB connection to the mainboard of the internal computer. The SPI bus is used for transmitting set commands and readbacks. A trigger input is used for synchronizing the DAQ board with the FT adapter board. By means of a relay, the DAQ board provides the electric power for the preamplifier.

## Internal Computer (Data Acquisition Unit)

The internal computer controls the instrument's electronics and runs software that is downloaded from the data system computer. The internal computer performs the Fast Fourier Transformation (FFT) of the image current after it has been converted by the DAQ board.

The internal computer communicates with the data system computer and LC modules through a 1 Gbit Ethernet switch. Internal USB connections connect it to vacuum control board, data acquisition board, and FT adapter board. An external USB port on the power panel (See [Figure 3-5](#) on [page 3-12](#).) enables the internal computer to communicate with dedicated devices of the LC/MS system.

## Source Board

The source board controls the temperature of the ion source. Each source type is identified by a specific built-in resistor. The board also controls the flow rates of the gases in use. The board controls the 8 kV power supply for the ion sources. By means of a safety relay, it switches off the power supply when the source is removed from the mass spectrometer. The source board controls the heaters for the heated capillary and the APCI heater. It also provides support for the APPI lamp. Communication between the source board and external ion sources is established by an RS232 connection (Serial Source Interface) to the FT adapter board.

In the Exactive Plus EMR mass spectrometer, the source board controls the electronic pressure valve that sets the pressure in the HCD cell.

The source board distributes power to the ion gauges, the switching valves, the syringe pump, and the nitrogen gas valves—including the vent valve. Two connections to the I/O board allow the source board to communicate with other devices of the LC/MS system.

The system status LEDs on the front side of the instrument (See [Figure 3-3](#) on [page 3-10](#).) are controlled by the source board. The displayed status information partially comes from other boards. The board communicates through the SPI bus.

## 8 kV Power Supply

The 8 kV power supply delivers voltage to either the ESI or the HESI needle in the ESI mode or the corona discharge needle in the APCI mode. Typical operating voltages range from  $\pm 3$  to  $\pm 6$  kV. In the ESI mode the voltage is regulated, whereas in the APCI mode the current is regulated. This power supply is controlled by the source board.

## Ion Optic Supply DC Board

With the exception of the quadrupole in the Q Exactive, Q Exactive Focus, Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X MS, the ion optic supply DC board provides the DC voltages for all ion-optical

components in front of the C-Trap as well as the HCD voltages. Additionally, it provides DC voltage supply and control signals for the S-lens RF generator board or the funnel RF generator board.

## **Ion Optic Supply RF Board**

With the exception of the quadrupole in the Q Exactive, Q Exactive Focus, Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X MS, the ion optic supply RF board provides the RF voltages for all ion-optical components in front of the C-Trap as well as the HCD voltages. It has an RF detector for the RF output control. In the Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X MS, the board provides the DC voltages for the split lens and for the injection flatpole.

## **Quadrupole Board**

In the Q Exactive, Q Exactive Focus, Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X MS, the quadrupole board (quad board) supplies RF voltages and DC voltages for the quadrupole. See [“Quadrupole Mass Filter”](#) on [page 3-29](#). Set values and readbacks of voltages, currents, and temperatures are communicated through the SPI bus.

## **FT Adapter Board**

The FT adapter board links the internal computer to the various system components. Its main function is the control of scan events in the instrument. The board contains a micro controller, an FPGA (Field Programmable Gate Array), and serial port connectors.

Through the USB interface, the internal computer transmits set commands for system components to the FT adapter board. By the same interface, the internal computer requests readback values. The FT adapter board converts the set commands during the scan and sends the readback data through USB to the internal computer. The master interface of the Extended Orbitrap SPI bus of the FT adapter board serves for transmitting the set commands and readbacks.

Communication between the FT adapter board and external ion sources is established by an RS232 connection (Serial Source Interface) to the source board. The FT adapter board communicates with the syringe pump by the I/O board.

## **SPI Bus**

Various boards communicate system parameters and monitor readbacks over the Serial Peripheral Interface (SPI) bus. The master interface of the SPI bus is on the FT adapter board.



## Vacuum Control Board

The vacuum control board controls the vacuum system. Depending on the quality of the vacuum and the status of the TMPs, it switches the vacuum gauges, the pumps, and the 230 V relays. When the vacuum measured by the Ion Gauge 2 is better than 1E-8 mbar, the vacuum control board switches on the power supplies of the high voltage electronics and the capillary heater.

On the vacuum control board, analog signals from vacuum gauges are converted to digital signals and passed to the internal computer through a USB connection. TMPs are attached to a serial port connector and this is connected by the signal lines to the vacuum control board. (See “[Vacuum System](#)” on [page 3-40](#).)

The board controls external relays with 24 V DC connections. In addition to the vent valve, the board also switches the valve that controls the flow of the HCD collision gas. The vacuum control board controls the bakeout heaters. It also monitors six fans in the instrument; it switches off the two fans below the analyzer TMP during a system bakeout. In case of a fan failure, the board triggers an alert in the Tune software.

## C-Trap RF Board

The C-Trap RF board operates the C-Trap with four phases of RF voltage (Main RF) and three pulsed DC voltages (PUSH, PULL, and OFFSET). It allows simultaneous switching off the RF and pulsing of each C-Trap electrode. See “[Orbitrap Analyzer](#)” on [page 3-32](#) for further information. The board also provides the entrance voltage and the exit voltage to the C-Trap. The board communicates with the other boards through the SPI bus.

## CE HV Supply Board

The central electrode high-voltage supply board provides five voltages for the ion optics of Exactive Series mass spectrometers:

- Two high voltages supply lenses that follow the C-Trap.
- Two DC voltages and one AC voltage are applied to the RF C-Trap main board to be used as focusing potentials for the C-Trap.

Furthermore, the board supplies six DC voltages to the Orbitrap analyzer:

- Four central electrode (CE) voltages: CE POS, CE NEG, CE LOW+, and CE LOW-
- Two deflector electrode (DE) voltages: DE HIGH and DE LOW

For positive ions, the CE voltages are negative and the DE voltages are positive. The maximum CE voltage is 5 kV and the maximum DE voltage is 1.25 kV. See [“Orbitrap Analyzer”](#) on [page 3-32](#) for further information.

Also, the analog-to-digital (AD) conversion of the PT-100 signal takes place on this board.

The board communicates through the SPI bus. A Peltier element on the rear side of the board serves as means of dissipation.

## CE Pulser Board

The central electrode pulser board switches the injection and measurement voltages for the central electrode and the deflector electrode of the Orbitrap analyzer. Resistor-capacitor circuits on the board convert the switching pulse into a smooth transition between the voltages. Furthermore, the board switches the polarity of the central Orbitrap electrode.

The temperature of the Orbitrap analyzer is measured by the PT-100 temperature probe. The signal of the probe is converted and analyzed on the CE pulser board. Then it is sent to the CE HV supply board where analog-to-digital conversion takes place.

## Power Supply DAQ Board

The power supply DAQ board provides the voltages that are required by the data acquisition board. The board is equipped with a fan for heat dissipation.

## I/O Board

The input/output (I/O) board provides the interfaces for data exchange between the Exactive Series mass spectrometer and other devices of the LC/MS system. It contains a reset switch, four relay outputs, a digital inlet port, two analog inlet ports, and a serial interface for controlling an external syringe pump. (See “[Peripheral Control](#)” on [page 3-12](#).) It is connected to the FT adapter board and to the source board.

## S-Lens RF Generator

In instruments with an S-lens, the S-lens RF generator board provides the RF and DC potentials for the S-lens assembly. Additionally, it provides signal paths for DC offsets to various elements in the S-lens assembly and for the capillary heater and its temperature sensor. The ion optic supply DC board supplies the DC voltage for this board.

## Funnel RF Generator

In the Q Exactive HF-X MS, the funnel RF generator board replaces the S-Lens RF generator board that is present in the other Exactive Series instruments. This board supplies the RF voltages to the ion funnel. It is controlled by the ion optic supply DC board and it supplies appropriate voltages—including several from both the IOS-DC and Source boards—to the inlet stack of the ion optics through the existing feedthrough cable into the instrument’s vacuum.

## Forepump On/Off Board

The forepump on/off board switches on and off the source vacuum pump by a contact closure signal. It is controlled by the vacuum control board.

The relay control cable of the forepump is plugged into the D-sub port on the power column next to the Ethernet port. See [Figure 3-6](#) on [page 3-14](#).

**Functional Description**  
Printed Circuit Boards

## Chapter 4 Safety


This chapter contains information that is important for your own safety or the safety of others, and that prevents damage to the instrument, Read this chapter carefully before you install or operate the instrument and its accessories, or come into contact with it.

### Contents

- [Safety Symbols and Signal Words in this Manual on page 4-2](#)
- [Safety Symbols on the Instrument on page 4-3](#)
- [Intended Use on page 4-6](#)
- [Electric Safety Precautions on page 4-8](#)
- [In Case of Emergency on page 4-9](#)
- [Residual Hazards on page 4-11](#)


## Safety Symbols and Signal Words in this Manual

Notices concerning the safety of the personnel operating the Exactive Series mass spectrometer appear different from the main flow of text. Safety notices include the following:

-  Always be aware of what to do with, and the effect of, safety information.
  
- ▲ CAUTION** Points out a hazardous situation that can lead to minor or medium injury if it is not avoided.
  
- ▲ WARNING** Points out a hazardous situation that can lead to severe injury or death if it is not avoided.
  
- ▲ DANGER** Points out a hazardous situation that will lead to severe injury or death if it is not avoided.

### Observing this Manual

This manual must always be kept near the instrument to be available for quick reference.


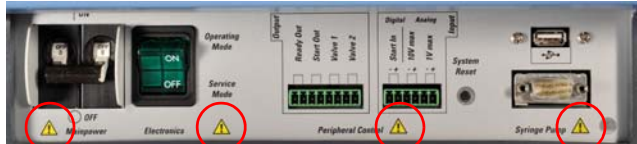

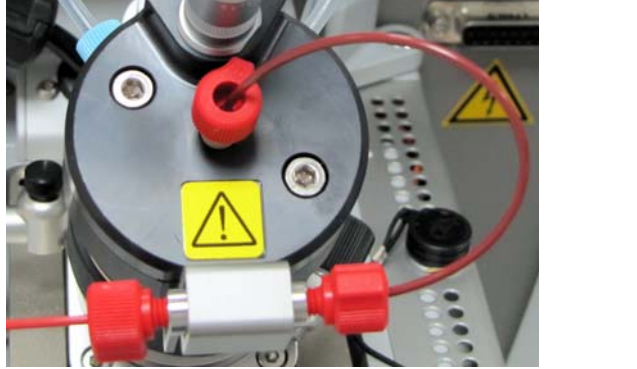


-  Be sure to read and comply with all precautions described in this manual.

System configurations and specifications in this manual supersede all previous information received by the purchaser.






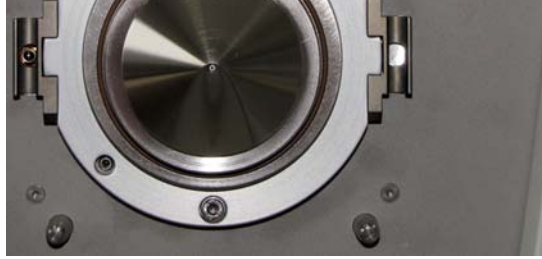


## Safety Symbols on the Instrument

Table 4-1 lists all safety labels on the instrument and their respective positions. See the indicated safety notices to prevent harm to the operator and to protect the instrument against damage. If present, read and follow the instructions on the labels.

**Table 4-1.** Safety labels on the instrument



Label	Label description	Label position
	<p>Four labels of this type are attached to the power panel on the left side of the instrument. See red circles in figure.</p> <p>The label indicates the presence of electric current at the switches or contact ports. See <a href="#">page 5-34</a> for details.</p>	
	<p>This label is attached to the end cover of the HESI probe, near the sample inlet.</p> <p>The label indicates the presence of high voltage and hazardous chemicals at the probe. See <a href="#">page 6-12</a> for details.</p>	
	<p>This label is attached to the right panel on the rear side of the instrument.</p> <p>The label indicates the presence of electric current and moving parts inside the instrument. See <a href="#">page 5-12</a> for details.</p>	

**Table 4-1.** Safety labels on the instrument, continued

Label	Label description	Label position
	<p>This label is attached to the power column at the rear side of the instrument, below the power outlets. See white circle in figure.</p> <p>The label indicates the presence of electric current at the ports at the power column. See <a href="#">page 5-10</a> for details.</p>	
	<p>Two labels of this type are attached to the ion source mount, one next to the D-sub port for APCI/ESI, another one next to the D-sub port for APPI.</p> <p>The labels indicate the presence of high voltage at the ion source. See <a href="#">page 8-31</a> for details.</p>	
	<p>This label is attached to the front side of the instrument, above the ion source mount.</p> <p>The label indicates the presence of hot surfaces at the ion source mount. See <a href="#">page 8-44</a> for details.</p>	
	<p>This label is engraved on top of the ion source housing, next to the micrometer for adjusting the Y-axis probe mount position. See white circle in figure.</p> <p>The label indicates the presence of hot surfaces at the ion source housing. See <a href="#">page 8-39</a> for details.</p>	



**Table 4-1.** Safety labels on the instrument, continued

Label	Label description	Label position
	<p>This label is attached to the front of the ion source housing.</p> <p>The label indicates the presence of hot surfaces at the ion source housing. See <a href="#">page 8-30</a> for details.</p>	

## Rating Plate

To identify the instrument correctly when you contact Thermo Fisher Scientific, always have the information from the rating plate available. The rating plate is attached to the power column at the rear side of the instrument. See [Figure 4-1](#). It contains the serial number, which is important in any type of communication with Thermo Fisher Scientific.



**Figure 4-1.** Rating plate (Exactive Plus MS)

## Intended Use

Exactive Series mass spectrometers are stand-alone Orbitrap™ instruments with an atmospheric pressure ionization (API) source with heated-electrospray ionization (HESI) probe for liquid chromatography (LC) mass spectrometry (MS) high-throughput applications.



Observe the following usage guidelines when you operate the Exactive Series mass spectrometer:

- The instrument is designed to be placed on a bench in the laboratory. It is not designed for use outdoors.
- The instrument is designed to be used exclusively with API sources and probes that are approved by Thermo Fisher Scientific.
- The instrument is designed for laboratory research use only. It is not designed for use in diagnostic or medical therapeutic procedures.

If the Exactive Series mass spectrometer is used in a manner that is not specified by Thermo Fisher Scientific, the protection that is provided by the instrument could be impaired. Thermo Fisher Scientific assumes no responsibility and will not be liable for instrument damage and/or operator injury that might result from using the instrument with other API sources and probes.

### Notice on the Susceptibility to Electromagnetic Transmissions

The instrument is designed to work in a controlled electromagnetic environment. Do not use radio frequency transmitters, such as mobile phones, in close proximity to the instrument.

## Qualification of the Personnel



Personnel that install or operate Exactive Series mass spectrometers must have the following qualifications:

- **Electrical Connections**  
The electrical installation must be made by qualified and skilled personnel (electrician) according to the appropriate regulations (for example, cable cross-sections, fuses, grounding connection). Refer to the *Exactive Series Pre-Installation Requirements Guide* for the specifications.
- **Installation**  
Only employees of Thermo Fisher Scientific or personnel who act on behalf of Thermo Fisher Scientific are allowed to install the Exactive Series mass spectrometer.

- **General Operation**  
Exactive Series mass spectrometers are designed to be operated by qualified laboratory personnel. Before they start, all users must be instructed about the hazards that are presented by the instrument and by the used chemicals. The users must be advised to read the relevant Material Safety Data Sheets (MSDSs).
- **Decommissioning**  
Only employees of Thermo Fisher Scientific or personnel who act on behalf of Thermo Fisher Scientific are allowed to decommission the Exactive Series mass spectrometer. For information about decommissioning third-party components (for example, forepumps), refer to the manuals that came with these components.

## Permitted Materials

Exactive Series mass spectrometers are designed to be operated with the following materials:

- Nitrogen gas: Used for the API sheath gas, API auxiliary/sweep gas, C-Trap bath gas, and HCD collision gas
- Forepump oil: Used for cooling, lubrication, and sealing of the forepump

**NOTICE** Use only the forepump oil that is indicated on the name plate and pump. If other oils are used, the manufacturers reject all responsibility should any trouble occur. See [page 9-4](#) for a specification of the forepump oil. ▲

- Calibration compounds, samples  
Polar or less polar chemical compounds—soluble in water or appropriate organic solvent. Compounds can have different molecular sizes. Compounds derive from environmental specimens of different origins; origin can be from living or non-living matter. Examples are sugars (carbohydrates) from plant material, proteins or peptides from animal or human cell lines, synthetic polymers deriving from an organic synthesis. Small molecules can derive from a honey sample when screening for or quantifying pesticides or from an organic synthesis.
- Solvents, additives  
Typically, mixtures of water and organic solvents are applied. Organic solvents can be methanol, acetonitrile, or isopropanol. Also chloroform or dichloromethane are solvents applied when these are needed to solubilize the compounds of interest and to prepare them ready-to-use for the ion source interface.  
Common additives to the solvent mixtures are acids such as trifluoroacetic acid or formic acid (positive ion mode) or a base such as ammonium hydroxide (negative ion mode).

For information about the material permitted to operate the API source, refer to the *Ion Max and Ion Max-S API Source Hardware Manual*.

## Electric Safety Precautions

### **▲ WARNING**

**High Voltage.** High voltages (up to 8 kV) capable of causing an electric shock are used in the instrument.

Observe the following safety precautions when you operate or perform service on the instrument:

- The instrument is properly grounded in accordance with regulations when it is shipped. You do not need to make any changes to the electrical connections or to the instrument's chassis to ensure safe operation.
- There are no customer serviceable parts inside. Do not remove any housing or protective cover except it is permitted elsewhere in this manual. When you leave the system, make sure that all protective covers and doors are properly connected and closed, and that heated areas are separated and marked to protect unqualified personnel.
- Do not turn on the instrument if you suspect that it has incurred any kind of electrical damage. Instead, disconnect the power cords of *mass spectrometer and source vacuum pump* and contact a Thermo Fisher Scientific field service engineer for a product evaluation. Do not try to use the instrument until it has been evaluated. Electrical damage might have occurred if the system shows visible signs of damage, or has been transported under severe stress.
- Do not place any objects on top of the instrument—especially not containers with liquids—unless it is requested by the user documentation. Leaking liquids might get into contact with electronic components and cause a short circuit.

## In Case of Emergency

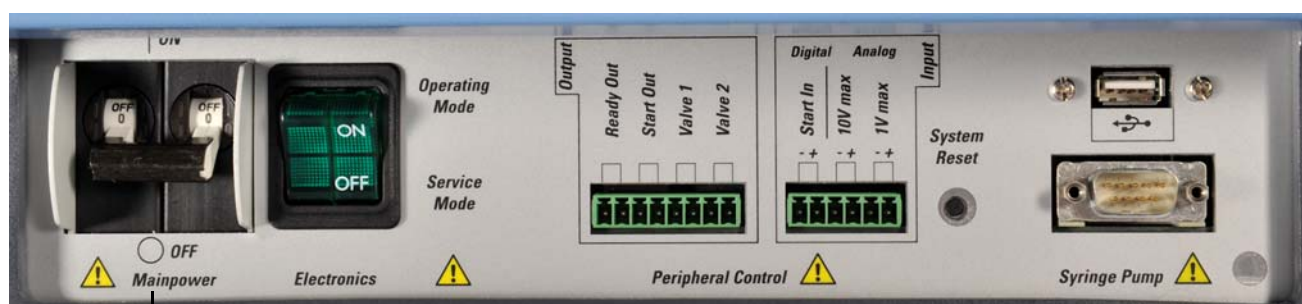
### ❖ To shut down the system in case of emergency

1. Disconnect the power cord of the mass spectrometer to ensure that the instrument is free from all electric current. All power to the MS, including the internal vacuum pumps, is shut off. Also, all power to any devices that are supplied with power by the MS (for example, auxiliary forepump, switching valves, syringe pump) is shut off.

**NOTICE** Placing the main power circuit breaker switch (labeled Mainpower) on the power panel (Figure 4-2) in the Off (O) position may not be sufficient. ▲

### ▲ WARNING

**Electric Current.** Electric shock hazard. Do not use the electronics service switch to shut down the instrument. The electric components of the vacuum system will still be connected to the electric power supply and the pumps will remain running.



Main Power Circuit Breaker Switch

**Figure 4-2.** Power panel, showing main power circuit breaker switch and reset button



Power Panel

**Figure 4-3.** Rear side view of instrument

**Safety**

In Case of Emergency

2. The source vacuum pump is only switched off with the relay control cable. To disconnect a forepump from its electric power supply, unplug the power cord.
3. Turn off the computer with its On/Off switch.

## Residual Hazards

Users of Exactive Series mass spectrometers must pay attention to the following residual hazards.

### **⚠ WARNING**

**High Voltage.** If you touch liquid that leaks from the probe sample inlet while the mass spectrometer is in operation, you might receive an electric shock. Do not tighten the probe sample inlet fitting to eliminate a liquid leak while the mass spectrometer is in operation.

### **⚠ WARNING**

**Suffocation Hazard.** Most of the nitrogen that is introduced into the API source escapes into the laboratory atmosphere. Accumulation of nitrogen gas could displace sufficient oxygen to suffocate personnel in the laboratory. Make sure that the laboratory is well ventilated. Always operate the Exactive Series mass spectrometer and the API source with attached drain tubing assembly that connects the source housing drain to a dedicated exhaust system. Local regulations may require a risk assessment for the workplace.

### **⚠ WARNING**

**Electromagnetic Radiation.** Parts of the forevacuum pump emit electromagnetic radiation. This radiation can interfere with the operation of cardiac pacemakers and implanted heart defibrillators, possibly causing death or serious injury. If you wear these devices, keep at least 30 cm away from the forevacuum pump.

### **⚠ CAUTION**

**Hazardous Chemicals.** Samples and solvents might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle solvents or samples. Also contain waste streams and use proper ventilation. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of a particular compound.

### **⚠ CAUTION**

**Hot Parts.** The forepump in function is hot and some surfaces could reach a temperature higher than 80 °C (176 °F). Touching parts of the forepump might cause burns. Switch off the pump and let it cool down before any intervention. If you need to work on a pump that is “still warm from operation,” then always wear heat protective gloves.

## **▲ CAUTION**

**Hot Parts.** During operation of the mass spectrometer, ion transfer capillary and sweep cone can reach temperatures up to 450 °C. This might cause severe burns upon touching or ignite combustible material. The external surface of the ion source housing can become hot enough to cause skin burns.

Do not touch the ion source housing when the mass spectrometer is in operation. Let the ion source cool down as described in this manual before you remove the ion source housing. Do not touch the ion source mount immediately after you have removed the ion source housing. Keep combustible materials away from the ion source mount. Do not let the instrument stay unattended when the housing is not mounted to the source.

## **Personal Protective Equipment**

Appropriate safety clothing must be worn at all times while you operate the instrument, particularly when you handle hazardous material.

This manual can only give general suggestions for personal protective equipment (PPE), which protects the wearer from hazardous substances. Refer to the Material Safety Data Sheets (MSDSs) of the chemicals handled in your laboratory for advice on specific hazards or additional equipment.

### **Eye Protection**

The type of eye protection required depends on the hazard. For most situations, safety glasses with side shields are adequate. Where there is a risk of splashing chemicals, goggles are required.

### **Protective Clothing**

When the possibility of chemical contamination exists, protective clothing that resists physical and chemical hazards should be worn over street clothes. Lab coats are appropriate for minor chemical splashes and solids contamination, while plastic or rubber aprons are best for protection from corrosive or irritating liquids.

### **Gloves**

For handling chemical compounds and organic solvents, Thermo Fisher Scientific recommends white nitrile clean room gloves from [Fisher Scientific](#) or [Unity Lab Services](#).

For handling hot objects, gloves made of heat-resistant materials (for example, leather) should be available.



## Chapter 5 Installation

This chapter describes the conditions for an operating environment that will ensure continued high performance of your Exactive Series system.

### Contents

- [Safety Guidelines for Installation](#) on page 5-2
- [Placing the Instrument](#) on page 5-3
- [Laboratory Conditions](#) on page 5-9
- [Setting Up Instrument Hardware and Adjusting System Parameters](#) on page 5-15
- [Configuring the Ion Source](#) on page 5-16
- [Connecting Frequently Used Devices](#) on page 5-18
- [Obtaining Calibration Solutions](#) on page 5-39

To be sure that your laboratory is ready for the installation of the Exactive Series system, you have to meet all requirements specified in the *Exactive Series Pre-Installation Requirements Guide*. This guide also provides comprehensive information to assist in planning and preparing your lab site. A printed version of the *Exactive Series Pre-Installation Requirements Guide* is part of the Preinstallation Kit. This kit is sent to your laboratory before the arrival of the Exactive Series mass spectrometer.

## Safety Guidelines for Installation

When you install the Exactive Series system, pay attention to the following general safety guidelines.

### ▲ WARNING

**Suffocation Hazard.** Most of the nitrogen that is introduced into the API source escapes into the laboratory atmosphere. Accumulation of nitrogen gas could displace sufficient oxygen to suffocate personnel in the laboratory. Make sure that the laboratory is well ventilated. Always operate Exactive Series mass spectrometer and API source with attached drain tubing assembly that connects the source housing drain to a dedicated exhaust system. Local regulations may require a risk assessment for the workplace.

### ▲ WARNING

**Hazardous Chemicals.** The forepump eventually exhausts much of what is introduced into the mass spectrometer, including the small amount of oil vapor that mechanical pumps can emit. The effluent of the forepump might contain noxious chemicals. The connection of the forepump to an adequate exhaust system is mandatory!

### ▲ WARNING

**Hazardous Chemicals.** The source exhaust might contain noxious material. It will contain traces of the samples and solvents that you are introducing into the source. Potential health hazards of these compounds include chemical toxicity of solvents, samples, and buffers, as well as biohazards of biological samples. To prevent contamination of the laboratory, always operate the ion source with the drain tubing connected. The drain tubing must lead to a waste container that is connected to a dedicated fume exhaust system.

### ▲ CAUTION

**Hazardous Chemicals.** Samples and solvents might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle solvents or samples. Also contain waste streams and use proper ventilation. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of a particular solvent.

### ▲ CAUTION

**Hot Parts.** During operation of the mass spectrometer, ion transfer capillary and sweep cone can reach temperatures up to 450 °C. This might cause severe burns upon touching or ignite combustible material. The external surface of the ion source housing can become hot enough to cause skin burns.

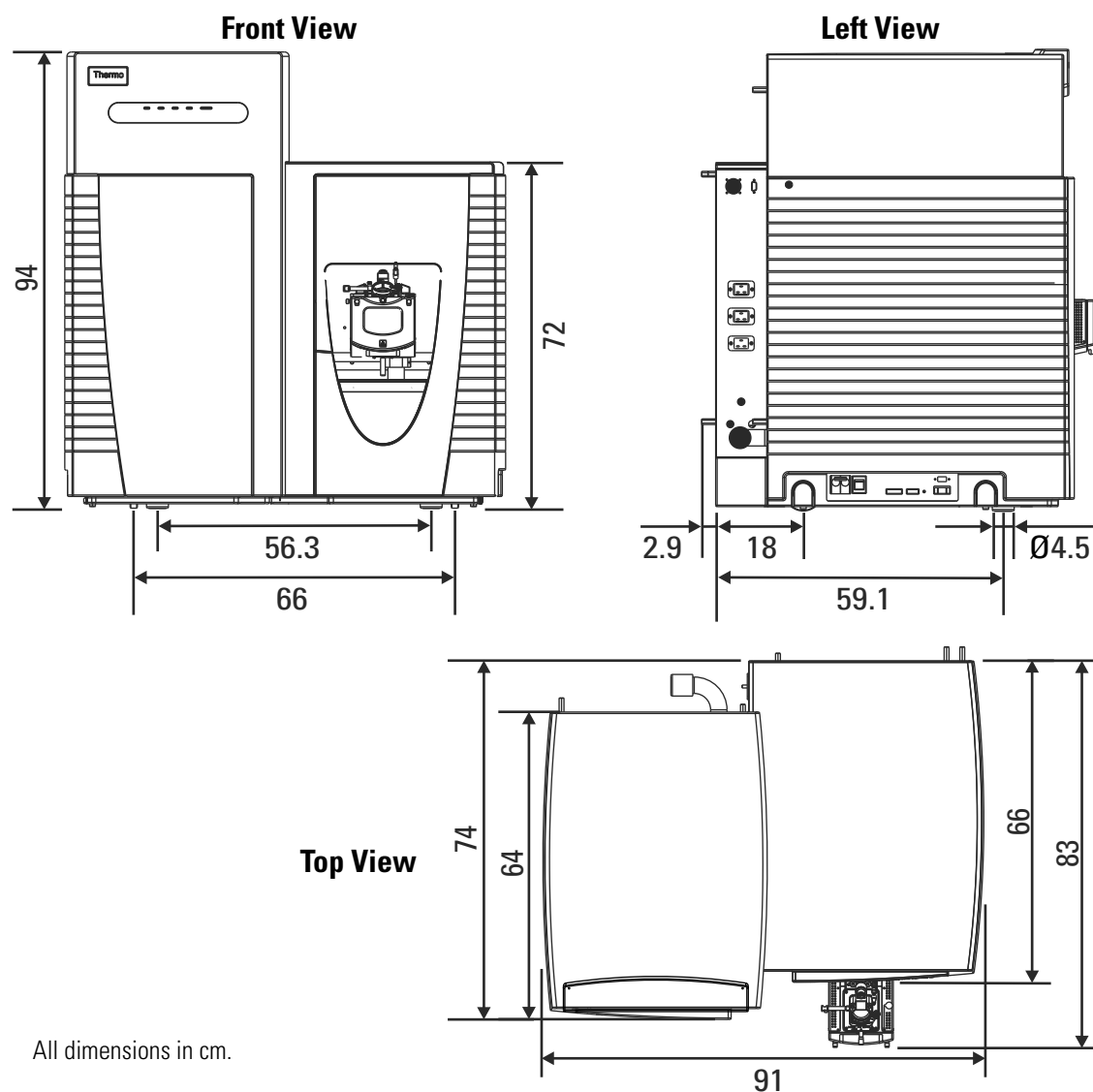
Do not touch the ion source housing when the mass spectrometer is in operation. Let the ion source cool down as described in this manual before you remove the ion source housing. Do not touch the ion source mount immediately after you have removed the ion source housing. Keep combustible materials away from the ion source mount. Do not let the instrument stay unattended when the housing is not mounted to the source.

## Placing the Instrument

This section provides information that helps you positioning the instrument in the laboratory.

### Instrument Dimensions

Exactive Plus and Exactive Plus EMR mass spectrometers have maximum dimensions of  $h$  94 cm (37 in.),  $w$  91 cm (36 in.),  $l$  83 cm (33 in.). [Figure 5-1](#) shows a schematic view of the instrument with important instrument dimensions.

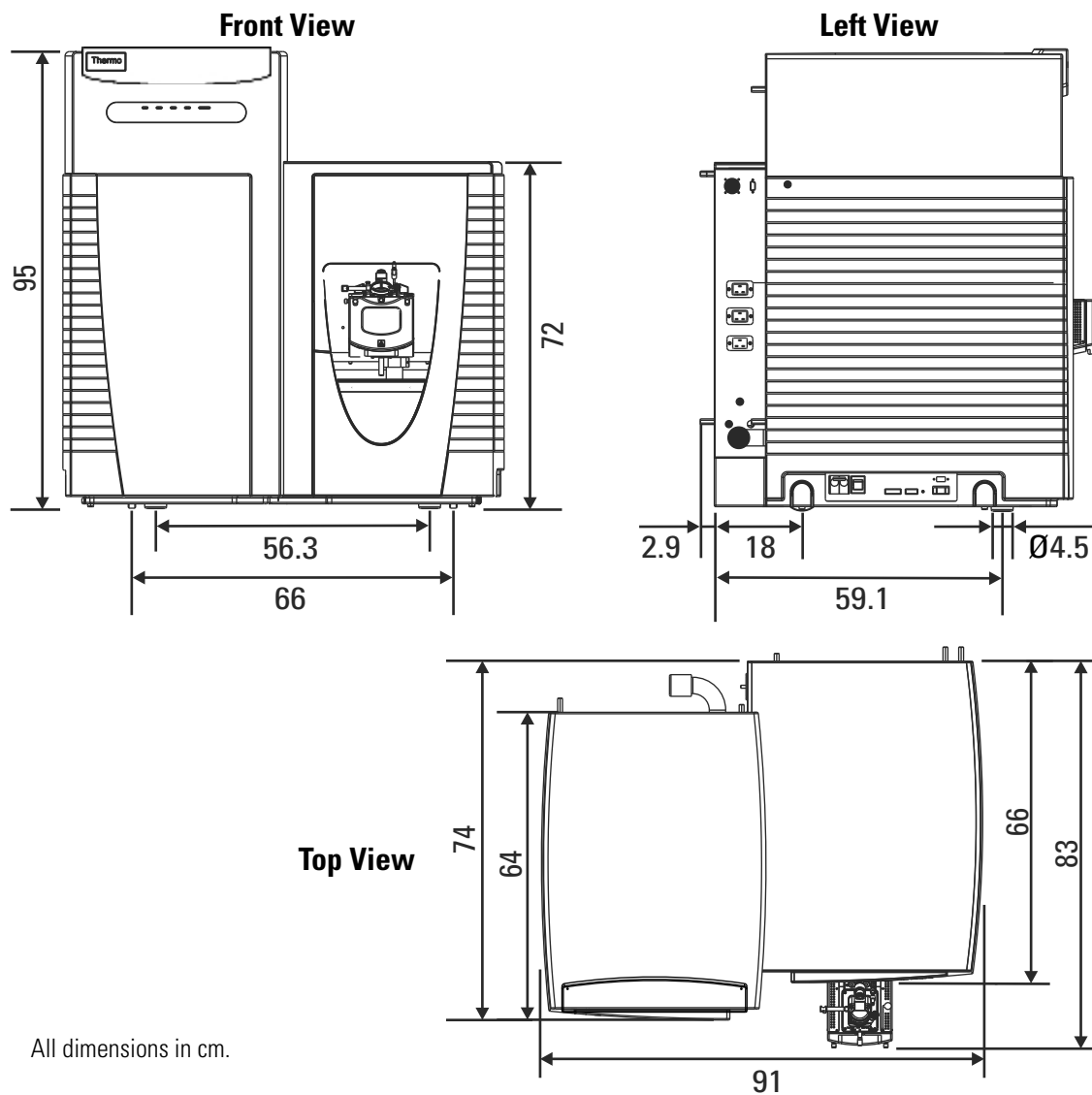


**Figure 5-1.** Dimensions of the Exactive Plus and Exactive Plus EMR MS

## Installation

### Placing the Instrument

Q Exactive, Q Exactive Focus, Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X mass spectrometers have maximum dimensions of  $h$  95 cm (37 in.),  $w$  91 cm (36 in.),  $l$  83 cm (33 in.). Figure 5-2 shows a schematic view of the instrument with important instrument dimensions.



**Figure 5-2.** Dimensions of the Q Exactive, Q Exactive Focus, Q Exactive Plus, Q Exactive HF, and Q Exactive HF-X MS

## Workbench for Instrument

The workbench for the MS system must be capable of supporting the weight of the mass spectrometer (about 180 kg) plus the weight of any option (liquid chromatograph, for example) and stand in a secure and level position.



Only workbenches with four legs provide sufficient stability for the Exactive Series mass spectrometer. The workbench top must be dry and clean (free of grease). Thermo Fisher Scientific recommends that you use a workbench with a skidproof top.

## Minimum Clearance

Allow at least 15 cm (6 in.) of clear space behind the system for proper air circulation and for clearance of the gas lines and electrical connections. This also provides sufficient space for accessing the fan filters on the rear side of the mass spectrometer. In addition, allow at least 92 cm (36 in.) of vertical clearance between the top of the mass spectrometer and any shelves above it.

To allow shutting off the mass spectrometer in an emergency, free access to the power panel on the left side and to the power column on the rear side of the instrument must be possible at any time.

**NOTICE** Do not block the ventilation slots at the rear side of the mass spectrometer. Items might fall behind the instrument, inhibit airflow, and cause the system to overheat. Depending on the circumstances, either the Tune software will switch off the instrument and display an error message or the turbomolecular pump control will shut down the instrument and vent it. ▲

## Moving the Instrument



**NOTICE** Before moving the instrument from one place to another, all participating personnel must carefully read and follow the instructions given in this manual. For information about moving the forepump, see [page 8-10](#). ▲

Exactive Series instruments are provided with four retractable handles. Each instrument is shipped on a pallet with the handles pulled out and fixed on the pallet. See [Figure 5-3](#). Safety catches prevent the handles from unintentionally being retracted after they have been pulled out. Inspect the handles to verify that their safety catches are engaged before you start lifting the instrument. Push down the safety catch on a handle to slide it into the instrument.



**Figure 5-3.** Handles, fixed on the transport pallet

**▲ CAUTION**

**Heavy Load.** Because of its weight of about 180 kg, handling the instrument alone might cause muscle strain and back injury. Lifting and moving the instrument requires the effort of at least *six persons* to keep the individual load below acceptable limits (maximum 40 kg for men or 15 kg for women for a duration of 5 seconds). The carriers must be trained in how to carry loads properly (for example, by rising from the knees with a straight back). Thermo Fisher Scientific recommends that you use a pallet jack to lift the mass spectrometer to the height of the workbench.

**▲ CAUTION**

**Heavy Objects.** Mass spectrometer and forepump might move uncontrollably and cause injuries. Wear steel-reinforced safety shoes and gloves during installation or maintenance.

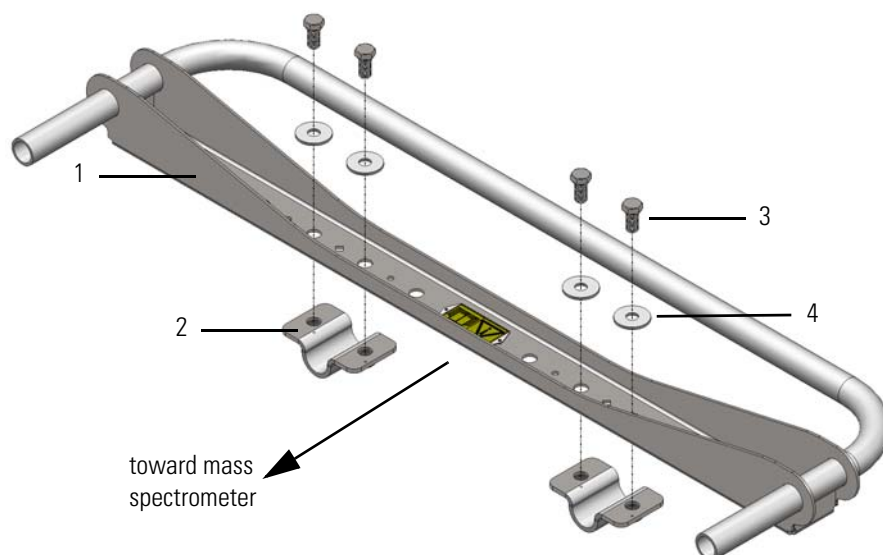
The instrument is shipped with two lifting devices, each providing sufficient space for three persons that are standing side by side. An instrument with attached lifting devices does not fit through a door with a width of 80 cm (32 in.), in contrast to the unpacked instrument alone. Furthermore, the six persons that carry the instrument require considerable space for maneuvering. Therefore, Thermo Fisher Scientific recommends that you use a pallet jack when you move the instrument into another room.

The following instructions assume that the instrument has been moved to the installation site with a pallet jack and the top cover of the transport crate has been removed.

❖ **To move the instrument onto the workbench**

1. Gather six persons and appoint one person that takes command and gives instructions to the remaining people.
2. Lift the instrument to the height of the working bench by using the pallet jack.
3. Remove the four clamps that fix the instrument to the transport pallet. See [Figure 5-3](#).

4. Each lifting device consists of a folded metal sheet with holes and a twice bent tube. It comes with four hexagonal screws, four washers, and two clamps. Mount each device onto the handles at one instrument side:
  - a. Place a clamp (pos. 2 in [Figure 5-4](#)) below each handle.



Labeled Components: 1=Lifting device; 2=clamp; 3=hexagonal screw; 4=washer

**Figure 5-4.** Lifting device

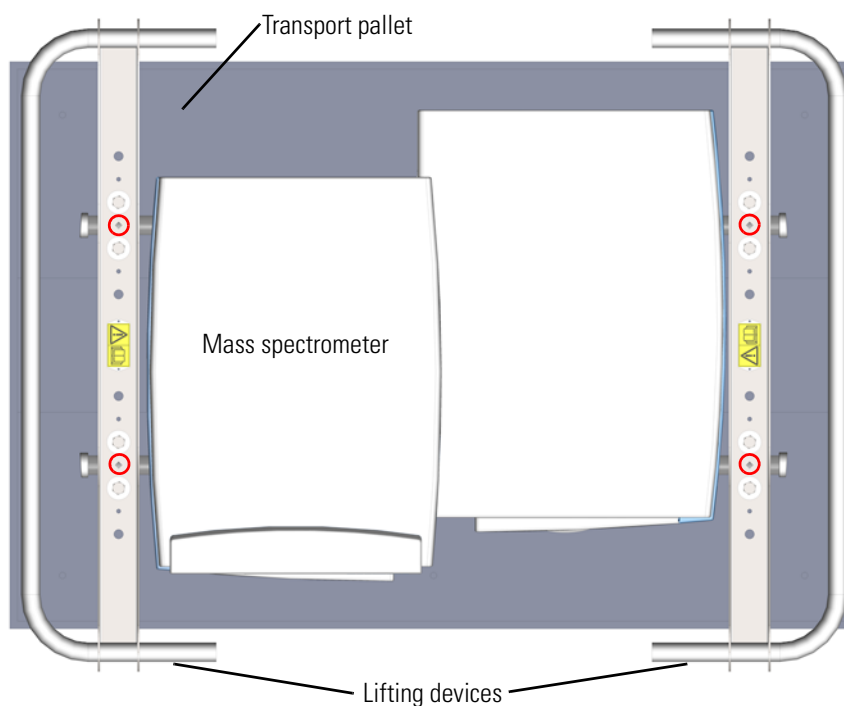
- b. Two diamond-shaped holes in the metal sheet of the lifting device indicate the place where the handles of the instrument shall be mounted to the device. Hold the device so that the yellow label on the lifting device is visible, which advises users to read the manual. Place the device on top of the handles, with the two ends of the twice bent tube pointing toward the instrument.
- c. Insert two screws (pos. 3 in [Figure 5-4](#)) with washers (pos. 4) at each side of a diamond-shaped hole and fasten the clamp with them. Repeat this for the other diamond-shaped hole. Make sure that the device is aligned parallel to the side of the instrument, and not twisted. Check that the lifting device is tightly attached to the handles.
- d. At the opposite side of the instrument, repeat the above steps with the other lifting device. The figure on the right shows a closeup view of a handle that is mounted to the lifting device. Note the diamond-shaped hole between the hexagonal screws.



## Installation

### Placing the Instrument

The ends of the lifting devices must be aligned flush with each other as shown in [Figure 5-5](#). Red circles in the figure indicate the positions of the diamond-shaped holes in the lifting devices.



**Figure 5-5.** Lifting devices attached to instrument (top view)

### **⚠ CAUTION**

**Top Heavy Load.** The mass spectrometer might tip over while being moved in the laboratory and cause bodily injury or instrument damage. The instrument's center of gravity is at the top of the front side: the instrument has a tendency to tilt forward. When lifting the instrument, support the top of the instrument and keep the tilt angle below 5°; do not exceed 10°.

5. On command, all six carriers lift off the instrument simultaneously—to prevent them from experiencing an uneven load distribution. Using the lifting devices, place the instrument onto the bench.
6. Remove the lifting devices from the handles.
7. The rear pair of the four support points for the instrument consists of wheels. Thus, only two persons are necessary for moving the instrument into its final position on a bench, while holding the two front handles. See [Figure 5-2](#) on [page 5-4](#) for information about the position of the support points.

#### ❖ **To store away the handles**

Push down the spring (safety catch) of the handle with a screw driver and shove the handle into its housing.



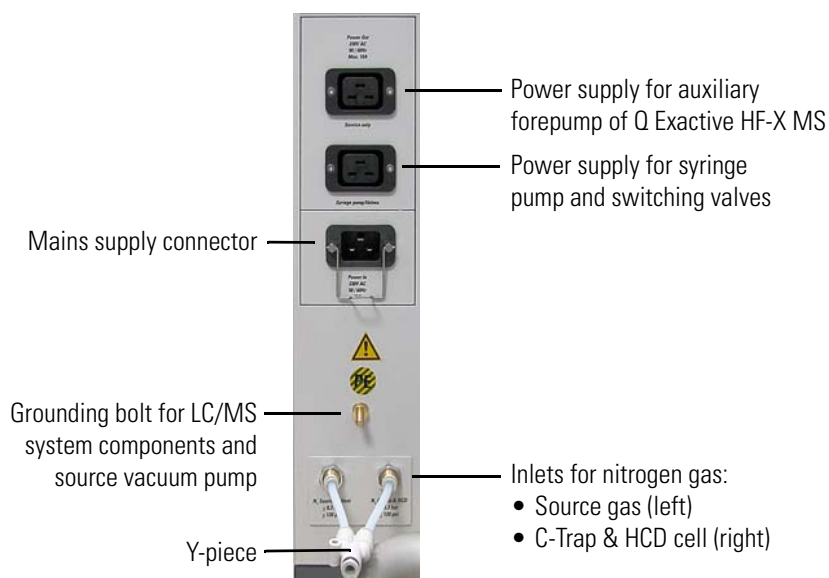
## Laboratory Conditions

This section gives an overview of important requirements for the laboratory where the Exactive Series mass spectrometer is placed. For details, refer to the *Exactive Series Pre-Installation Requirements Guide*.

### Power Supply

The Exactive Series mass spectrometer and the source vacuum pump require dedicated wall outlets providing a nominal voltage of 230 V AC, 50/60 Hz, single phase. Line voltages can vary between a minimum of 207 V AC and a maximum of 253 V AC. Connect the power cords of the instrument and the pump to wall receptacles that are fused with 15 A or 16 A.

**Notice for Customers in North America** Systems installed in areas with 208 V power experience voltage sags during high use periods that might place the line voltage below the operating parameters described in this section. In this case, you must protect the instrument with a buck/boost transformer to make sure that power is within the specified parameters at all times. You need to supply a dedicated single phase 30 amp 208 V AC power line with a good earth ground that terminates in a NEMA L6-30R receptacle located within 6 feet of the desired instrument location. ▲



**Figure 5-6.** Power and gas connections of Exactive Series MS

The components of the data system (computer, monitor, and Ethernet switch) and the devices of the LC system require wall outlets at a nominal voltage of 230 V AC or 120 V AC, 50/60 Hz. Electric power for syringe pump, switch valve, and auxiliary forepump is supplied by the MS. See [Figure 5-6](#).

**▲ WARNING**

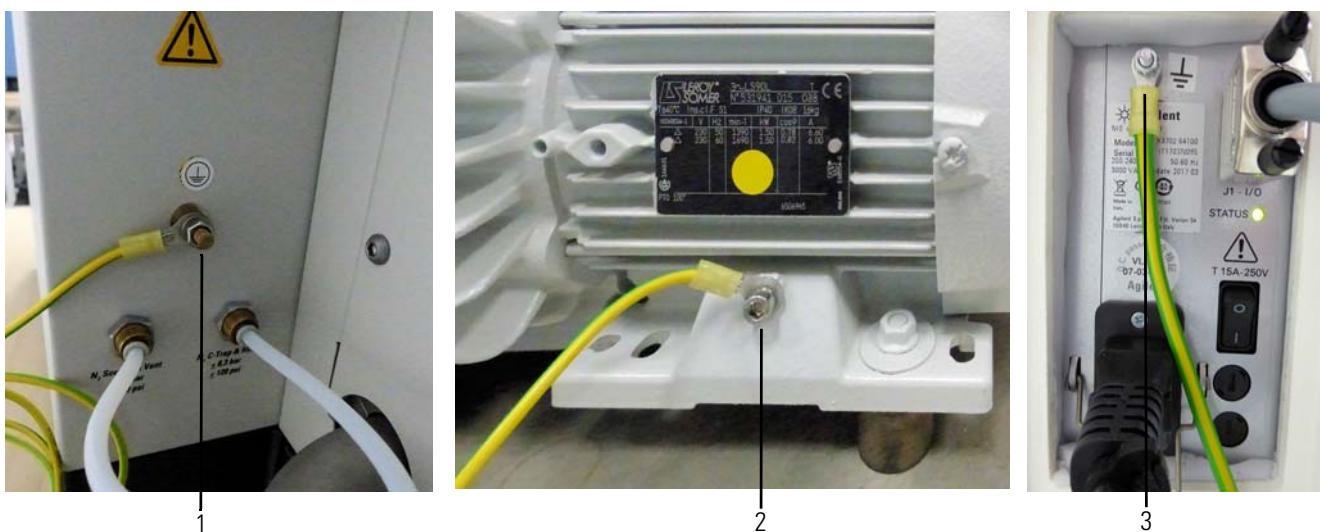
**Electric Current.** Electric shock hazard. Wrong usage of these ports might endanger personnel. Read and understand this manual to prevent harm to the operator and to protect equipment against damage. To make sure that the instrument is free from all electric current, always disconnect the power cords of *mass spectrometer and source vacuum pump* before you try any type of maintenance.

**Grounding of Source Vacuum Pump**

Connect the grounding cable of the pump to the grounding bolt at the rear side of the MS (see [Figure 5-7](#)).

**▲ CAUTION**

**High Leakage Current.** Additional Grounding Required. For safe operation of the instrument and good quality of your measurement, an additional grounding path between the instrument and the source vacuum pump must be established. The green/yellow grounding cable that is delivered with the switch cord for the pump must be connected to the grounding bolt on the instrument and the grounding screw on the pump.



Labeled Components: 1= grounding bolt at power column of MS, 2=grounding screw on SOGEVAC pump, 3=grounding screw on Agilent pump (in case of a Q Exactive HF-X MS)

**Figure 5-7.** Grounding connections for source vacuum pumps

## Gas Supply

Exactive Series mass spectrometers require high-purity (99%) nitrogen. The nitrogen inlet ports are at the bottom of the power column at the rear side of the instrument. See [Figure 5-6](#) on [page 5-9](#).

**NOTICE** Do not connect other gases than nitrogen to the Exactive Series mass spectrometer! This might affect instrument performance. The maximum pressure for the gas inlet is 830 kPa (8.3 bar, 120 psi). ▲

Also consider the information about nitrogen gas consumption in “[Checking the Nitrogen Supply](#)” on [page 6-4](#) and in the Notice on [page 6-7](#).

### ❖ To connect the high-purity nitrogen source to the mass spectrometer

1. Connect an appropriate length of Teflon™ tubing to the nitrogen source in the laboratory. The Installation Kit contains 10 m (33 ft) of suitable Teflon tubing (OD 6 mm, see [Chapter 9, “Replaceable Parts”](#)). The connection for the Teflon hose to the nitrogen gas supply is not provided in the kit; you have to supply this part.
2. Insert the opposite end of the Teflon tubing into the press-in fitting of the Y-piece that is attached to the gas ports at the rear side of the instrument. See [Figure 5-6](#). To connect the tubing, align the Teflon tubing with the opening in the fitting and firmly push the tubing into the fitting until the tubing is secure.

The fragment ions that are generated in the HCD cell are generally quite reactive. High purity nitrogen contains notably more water and oxygen than ultra-high purity nitrogen, which gives rise to gas-phase adducts and related products. These species would deteriorate the MS/MS spectral assignments. For the HCD cell (if present<sup>1</sup>), ultra-high purity (99.999%) nitrogen is therefore recommended.

### ❖ To use ultra high-purity nitrogen for the HCD cell

1. Remove the Y-piece with the two short tubing sections from the instrument.
2. Connect the tubing that comes from the *high-purity nitrogen* source to the *left nitrogen inlet* of the instrument.
3. Connect the tubing that comes from the *ultra-high purity nitrogen* source to the *right nitrogen inlet* of the instrument.

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<sup>1</sup> This feature may not be present in your Exactive Plus mass spectrometer.

**▲ WARNING**

**Moving Parts and High Voltage.** Risk of injury or electric shock. The interior of the instrument contains parts that are moving or that are at high voltages. When opening the instrument housing is necessary, call a Thermo Fisher Scientific field service engineer.

**▲ WARNING**

**Suffocation Hazard.** Most of the nitrogen that is introduced into the API source escapes into the laboratory atmosphere. Accumulation of nitrogen gas could displace sufficient oxygen to suffocate personnel in the laboratory. Make sure that the laboratory is well ventilated. Always operate Exactive Series mass spectrometer and API source with attached drain tubing assembly that connects the source housing drain to a dedicated exhaust system. Local regulations may require a risk assessment for the workplace.

## Laboratory Temperature

The mass spectrometer is designed to operate at a laboratory room temperature between 15 and 26 °C (59 and 78 °F).

**NOTICE** Do not put the mass spectrometer under an air duct, near windows, or near heating and cooling sources. Temperature fluctuations of 1 °C or more over a 10 minutes period can affect instrument performance. ▲

## Humidity

The relative humidity of the operating environment must be between 40 and 70%, with no condensation. It is recommended that your laboratory be equipped with a temperature/humidity monitor. This makes sure that the laboratory is always within the required temperature and humidity specifications.

**NOTICE** Operating the mass spectrometer at very low humidity might cause the accumulation and discharge of static electricity, which can shorten the life of electronic components. Operating the mass spectrometer at high humidity might cause condensation, oxidation, and short circuits, and will also block the filters on the cooling fans.

A significant change of the humidity in the laboratory can affect the mass accuracy. If the humidity in the laboratory has changed significantly since the last mass calibration, Thermo Fisher Scientific recommends that you refresh the mass calibration. ▲

## Ventilation and Fume Exhaust

Consider the following safety guidelines for ventilation and exhaust.

### ▲ WARNING

**Suffocation Hazard.** Most of the nitrogen that is introduced into the API source escapes into the laboratory atmosphere. Accumulation of nitrogen gas could displace sufficient oxygen to suffocate personnel in the laboratory. Make sure that the laboratory is well ventilated. Always operate Exactive Series mass spectrometer and API source with attached drain tubing assembly that connects the source housing drain to a dedicated exhaust system. Local regulations may require a risk assessment for the workplace.

### ▲ WARNING

**Hazardous Chemicals.** The source exhaust might contain noxious material. It will contain traces of the samples and solvents that you are introducing into the source. Potential health hazards of these compounds include chemical toxicity of solvents, samples, and buffers, as well as biohazards of biological samples. To prevent contamination of the laboratory, always operate the ion source with the drain tubing connected. The drain tubing must lead to a waste container that is connected to a dedicated fume exhaust system. Do **not** vent the drain tubing (or any vent tubing connected to the waste container) to the same fume exhaust system to which you have connected the forepumps.

### ▲ WARNING

**Hazardous Chemicals.** The forepumps eventually exhaust much of what is introduced into the mass spectrometer, including the small amount of oil vapor that mechanical pumps can emit. The effluent of the forepumps might contain noxious chemicals. Connect the exhaust ports of the rotary pumps to an exhaust gas line leading out of the building or to an adequate exhaust system.

## Vibration

Floors must be free of vibration caused, for example, by equipment in adjoining locations.

**NOTICE** Because of the natural vibration of a forepump during operation, it must not have any mechanical contact to the mass spectrometer with the exception of the vacuum hose. Otherwise, the vibration might affect instrument performance. Therefore, install the pump on the floor below the mass spectrometer and not near the system on the workbench. ▲

**Installation**

Laboratory Conditions

**Airborne Noise Emission**

The A-weighted emission sound pressure level created by the Exactive Series mass spectrometer at work stations does not exceed 70 dB(A).

## Setting Up Instrument Hardware and Adjusting System Parameters

 Only employees of Thermo Fisher Scientific or personnel who act on behalf of Thermo Fisher Scientific are allowed to install the Exactive Series mass spectrometer.

The Exactive Series mass spectrometer and other devices shipped with it are installed by a Thermo Fisher Scientific field service engineer. During the installation, the service engineer will demonstrate the basics of equipment operation and routine maintenance.

If you wish to connect the mass spectrometer to other LC equipment, see [“Connecting Frequently Used Devices”](#) on [page 5-18](#) for advice. Also refer to the manuals that came with the LC equipment.

The QuickStart Guide for your instrument gives an introduction on setting up and operating the Exactive Series mass spectrometer. For detailed information about changing the instrument parameters and developing experiments for the instrument, refer to the Software Manual or the Tune Help.

## Configuring the Ion Source

The API source can be configured to operate in several API modes, including electrospray ionization (ESI), atmospheric pressure chemical ionization (APCI), and atmospheric pressure photoionization (APPI). A separate nanospray ionization (NSI) probe is necessary to operate in NSI mode.

## Changing the Ion Source Housing

For information about changing the ion source housing, see [“Removing and Reinstalling the Ion Max API Source Housing”](#) on page 8-16. Also refer to the manuals that came with the API source and the API probe. When you change the ion source housing, pay attention to the following general safety guidelines.

### **▲ WARNING**

**Hazardous Chemicals.** The source exhaust might contain noxious material. It will contain traces of the samples and solvents that you are introducing into the source. Potential health hazards of these compounds include chemical toxicity of solvents, samples, and buffers, as well as biohazards of biological samples. To prevent contamination of the laboratory, always operate the ion source with the drain tubing connected. The drain tubing must lead to a waste container that is connected to a dedicated fume exhaust system.

### **▲ CAUTION**

**Hot Parts.** During operation of the mass spectrometer, ion transfer capillary and sweep cone can reach temperatures up to 450 °C. This might cause severe burns upon touching or ignite combustible material. The external surface of the ion source housing can become hot enough to cause skin burns.

Do not touch the ion source housing when the mass spectrometer is in operation. Let the ion source cool down as described in this manual before you remove the ion source housing. Do not touch the ion source mount immediately after you have removed the ion source housing. Keep combustible materials away from the ion source mount. Do not let the instrument stay unattended when the housing is not mounted to the source.



## Changing the API Probe

As default, Exactive Series mass spectrometers are delivered with the HESI-II probe. See “[API Probe Maintenance](#)” on [page 8-29](#) for instructions about installing and removing this API probe. Also refer to the *HESI-II Probe User Guide*.

For information about changing other API probes, refer to the manuals that came with the API source and the API probe. When you change the API probe, pay attention to the following general safety guidelines.

### **CAUTION**

**Hot Parts.** During operation of the mass spectrometer, ion transfer capillary and sweep cone can reach temperatures up to 450 °C. This might cause severe burns upon touching or ignite combustible material. The external surface of the ion source housing can become hot enough to cause skin burns.

Do not touch the ion source housing when the mass spectrometer is in operation. Let the ion source cool down as described in this manual before you remove the ion source housing. Do not touch the ion source mount immediately after you have removed the ion source housing. Keep combustible materials away from the ion source mount. Do not let the instrument stay unattended when the housing is not mounted to the source.



Only qualified laboratory personnel are allowed to change the API probe.

## Connecting Frequently Used Devices

This section provides information on how to connect the Exactive Series mass spectrometer to external devices that are frequently used with the instrument. It also describes the specifications for the peripheral control connections.

### Connecting the API Probe to the Mass Spectrometer

#### ❖ To connect liquid lines to the API probe

1. Install the API source housing and the API probe onto the mass spectrometer as described in the manuals that came with the API source and the API probe.
2. Install liquid lines between switching valve, LC system, syringe pump, and grounding union, as appropriate for your application. For more information, see [“Connecting the Inlet Plumbing”](#) on [page 5-19](#).
3. Connect the 1 inch ID Tygon™ tubing (see [Chapter 9, “Replaceable Parts”](#)) to the source housing drain.
4. Insert the other end of the tubing into a waste container, and vent the waste container to a fume exhaust system.

**NOTICE** Prevent solvent waste from backing up into the API source and mass spectrometer. Always make sure that the drain tubing is above the level of liquid in the waste container.

Do not vent the drain tube connected to the waste container to the same fume exhaust system to which you have connected the forepump. Connecting the API source drain tube and the forepump exhaust to the same fume exhaust system is likely to contaminate the analyzer optics. Equip your laboratory with at least two independent fume exhaust systems. Route the exhaust tubing from the forepump to a dedicated fume exhaust system. Route the drain tube from the API source to the waste container. Vent the waste container to a dedicated fume exhaust system that is independent from that used for exhausting the forepump. ▲

## Connecting the Inlet Plumbing

This section describes how to make the appropriate plumbing connections to introduce sample into the Ion Max API source of the Exactive Series mass spectrometer.

**NOTICE** This manual describes only making plumbing connections for ESI/MS and APCI/MS. For information about making plumbing connections for other probe types (H-ESI probe, for example), refer to the manuals that came with these probes. ▲

### Sample Introduction

With the Exactive Series mass spectrometer, which allows using a switching valve or a syringe pump, you can introduce sample into the API source as follows:

- The syringe pump is often used to introduce calibration solution for automatic tuning and calibrating in ESI mode. You can also use this technique to introduce a solution of pure analyte at a steady rate in ESI mode, for example, for determining the structure of an unknown compound.

For direct infusion, connect the syringe pump directly to the Ion Max API source. To push sample into the ion source, set the rate at which the syringe pump depresses the plunger of the syringe.

- You can also use a union Tee to direct samples from the syringe pump into an LC flow (without a column), which then enters the mass spectrometer. This technique is used to introduce sample at a steady rate and at higher solvent flow rates; it is used especially for tuning in ESI or APCI on an analyte of interest. You can also use this technique to introduce a solution of pure analyte at a steady rate in ESI or APCI.

For high-flow infusion, connect the syringe pump and the outlet of an LC pump to two legs of a union Tee, and then connect the third leg of the union Tee to the ion source. To introduce sample into the ion source, set the rate at which the syringe pump depresses the plunger of the syringe and the flow rate of the solvent stream produced by the LC pump.

- You can introduce samples from a syringe into the loop of the injector valve. You can then use the switching valve to introduce the sample into an LC flow, which then enters the mass spectrometer. This technique is used in ESI or APCI to introduce pure analytes into the mass spectrometer in a slug. It is useful when you have a limited quantity of pure analyte.

For loop injection (flow injection analyses), connect the solvent flow from an LC pump to port 2 of the switching valve, a sample loop to ports 1 and 4 of the valve, and a loop filler to port 5 of the valve. To introduce sample into the ion source, load sample into the sample loop through the loop filler, and then switch the position of the injection valve, allowing the solvent stream to backflush the contents of the sample loop into the ion source.

- You can also use an LC autosampler to introduce samples into an LC flow. This technique is also used in ESI or APCI to introduce a slug of *pure analyte* into the LC flow and then into the mass spectrometer.

Furthermore, you can perform LC/MS experiments with an LC autosampler to introduce a *mixture* onto an LC column. This technique is used with ESI or APCI to separate the analytes before they are introduced sequentially into the mass spectrometer.

For automated injections with an autosampler, connect the outlet from a liquid chromatography system that contains an autosampler to port 2 of the switching valve. Then set up an autosampler to make automated injections into the solvent flow produced by the LC pump.

Table 5-1 summarizes the sample introduction and analytical techniques for ESI/MS and APCI/MS.

**Table 5-1.** Sample introduction and analytical techniques for ESI/MS and APCI/MS

Sample introduction into the mass spectrometer	ESI analytical technique	APCI analytical technique	Procedure for connecting the plumbing
Direct infusion	Analysis of a pure analyte Automatic calibration and tuning		“Setting Up the Inlet for Direct Infusion” on page 5-22
High-flow infusion (syringe pump injection into LC solvent flow)	Analysis of a pure analyte	Analysis of a pure analyte	“Setting Up the Inlet for High-Flow Infusion” on page 5-24
Loop injection into LC solvent flow	Analysis of a pure analyte Automatic optimization of tuning with an analyte	Analysis of a pure analyte Automatic optimization of tuning with an analyte	“Setting Up the Inlet for Loop Injections (Flow Injection Analyses)” on page 5-30
LC system with autosampler (without chromatographic separation)	Analysis of one or more pure analytes	Analysis of one or more pure analytes	“Setting Up the Inlet for an LC/MS System with an Autosampler” on page 5-32
LC system with autosampler (with LC column for chromatographic separations)	Analysis of a mixture	Analysis of a mixture	“Setting Up the Inlet for an LC/MS System with an Autosampler” on page 5-32








## Fittings, Tubing, Unions, and Sample Loops

The Exactive Series mass spectrometer allows connecting up to two external switching valves (Rheodyne MX Series II™, for example). These valves are 6-port, two-position injection valves. The six ports use standard 10-32 fittings for high-pressure 1/16 inch OD tubing. The LC union and the union Tee that you use to connect the syringe pump to the ion source also use standard 10-32 fittings for 1/16 inch OD tubing.

**NOTICE** When you cut PEEK™ tubing, always make square cuts. Thermo Fisher Scientific recommends that you use a tubing cutter to cut the PEEK™ tubing used to make the inlet plumbing connections. ▲

Table 5-2 lists the frequently used parts for making plumbing connections for ESI/MS and APCI/MS.







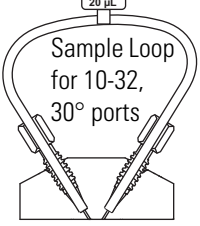
**Table 5-2.** Frequently used parts for making plumbing connections for ESI/MS and APCI/MS

Part	Part Description	Part Number
	Tubing, fused-silica, 0.1-mm ID × 0.4-mm OD (infusion line)	00106-10504
	Tubing, fused-silica, 0.1-mm ID × 0.190-mm OD (fused-silica sample tube and fused-silica capillary tube)	00106-10499
	Tubing, PEEK™, 0.005-in ID × 1/16-in. OD (red)	00301-22912
	Tube, Teflon, 0.03-in ID × 1/16-in. OD (for use with syringe needle and LC union)	00301-22915
	Tubing, PVC, unreinforced, 3/8-in. ID (clear) (API probe drain tube)	00301-22895
	Fitting, adapter, Kel-F™, Upchurch Scientific™ (connects directly to ESI probe inlet)	00101-18080
	Fitting, fingertight, Upchurch Scientific (natural) (used with (red) PEEK™ tubing)	00101-18081
	Ferrule, Kel-F, 0.008-in. ID, Upchurch Scientific (clear) (used with fused-silica tubing and the blunt-tip, 34-gauge stainless steel needle included in Metal Needle Kit)	00101-18114
	Ferrule, Kel-F, 0.012-in. ID, Upchurch Scientific (clear) (used with blunt-tip, 32-gauge stainless steel needle included in Metal Needle Kit)	00101-18116
	Ferrule, 0.016-in. ID, PEEK™, Upchurch Scientific (natural) (for use with fused-silica infusion line)	00101-18120
	Ferrule, LC, 1/16-in., stainless steel (used to connect tubing and the sample loop to the switching valve)	2522-3830
	Fitting, grounding union, 1/16-in. orifice, stainless steel	00101-18182

## Installation

Connecting Frequently Used Devices

**Table 5-2.** Frequently used parts for making plumbing connections for ESI/MS and APCI/MS, continued

Part	Part Description	Part Number
	Fitting, fingertight, Upchurch Scientific (used with red PEEK™ tubing)	00101-18195
	Ferrule, Fingertight 2, Upchurch Scientific (natural) (used with the Teflon tubing and red PEEK™ tubing)	00101-18196
	Fitting, LC union, 0.010-in. orifice, PEEK™ (black)	00101-18202
	Fitting, union Tee, 0.020-in. orifice, PEEK™ (black)	00101-18204
	Fitting, adapter union, PEEK™, Upchurch Scientific (natural) (used with blunt-tip 32- or 34-gauge stainless steel needle, included in Metal Needle Kit)	00101-18206
	Nut, LC for 1/16-in. stainless steel, Rheodyne	2522-0066
	5 µL sample loop, stainless steel, Rheodyne	00110-22026
	10 µL sample loop, stainless steel, Rheodyne	00110-22012
	20 µL sample loop, stainless steel, Rheodyne	00110-22028
	100 µL sample loop, stainless steel, Rheodyne	00110-22018

## Setting Up the Inlet for Direct Infusion

To tune and calibrate the Exactive Series mass spectrometer, use the syringe pump to infuse a sample solution into the ion source that is set up for ESI mode. A suitable syringe pump (Chemyx Fusion 100, see [Chapter 9, “Replaceable Parts”](#)) is shipped with the instrument. For instructions about establishing power supply and communication between syringe pump and mass spectrometer, see [page 5-33](#).

To introduce sample solution with the syringe pump, you must connect an infusion line between the syringe pump and the grounding union that is held by the grounding bar of the Ion Max API source.

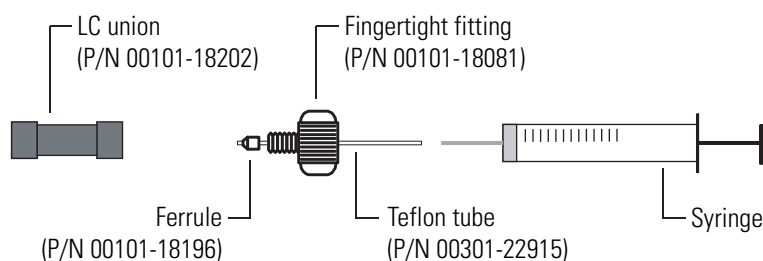
To connect the syringe to the grounding union, follow these procedures:

1. [Setting Up the Syringe](#)
2. [Connecting an Infusion Line to the Grounding Union](#)

## Setting Up the Syringe

### ❖ To fill the syringe, connect it to the LC union, and insert it into the syringe pump

1. Fill a clean, 500- $\mu$ L Unimetrics syringe with your sample solution.
2. Connect a 4-cm (1.5-in.) length of Teflon™ tubing (0.03-in. ID  $\times$  1/16-in. OD) with a fingertight fitting (for a 10-32 receiving port and 1/16-in. OD tubing) and a ferrule to the LC union. See [Figure 5-8](#).
3. Insert the needle of the syringe into the segment of Teflon tube. Make sure that the needle tip of the syringe fits readily into the opening in the free end of the Teflon tubing. If necessary, you can enlarge the opening at the end of the tubing slightly.



**Figure 5-8.** Connecting the syringe and the LC union

4. Place the syringe into the syringe holder of the syringe pump.
5. While squeezing the release buttons on the syringe pump handle, push the handle forward until it just contacts the syringe plunger.

## Connecting an Infusion Line to the Grounding Union

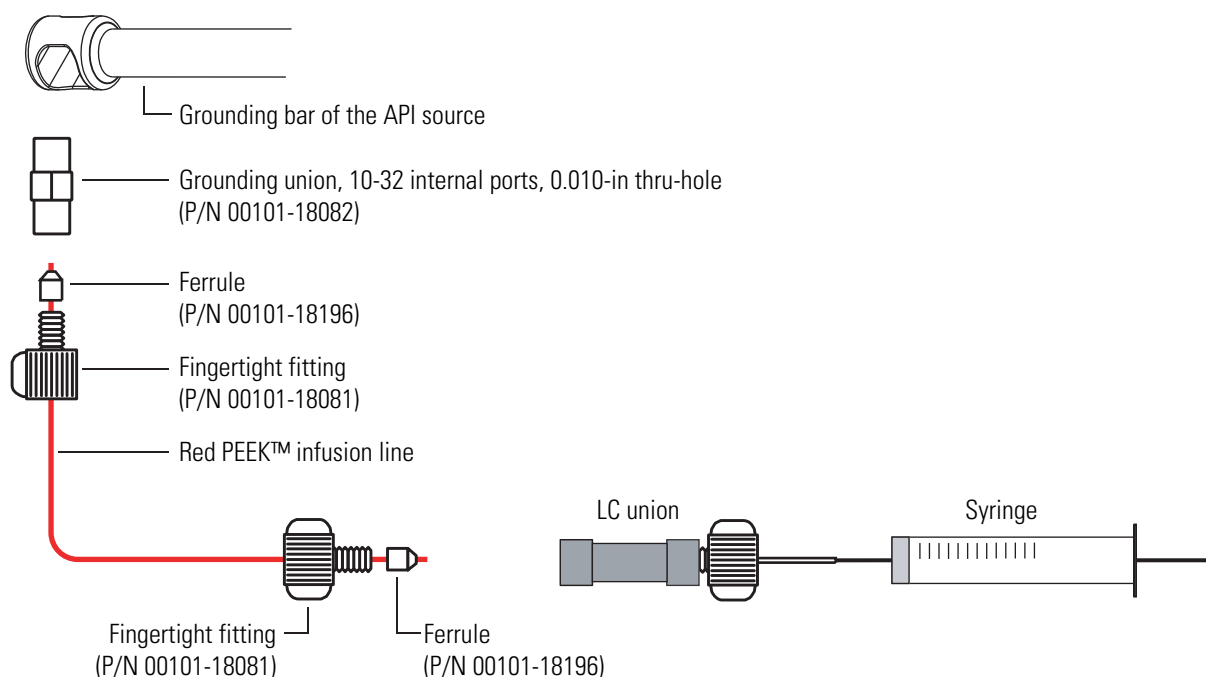
### ❖ To connect an infusion line between the LC union and the grounding union

1. Connect a section of red PEEK™ tubing (infusion line) with a fingertight fitting and ferrule (for a 10-32 conical receiving port and 1/16-in. OD tubing) to the free end of the LC union.
2. Connect the other end of the infusion line with a fingertight fitting (for a 10-32 port and 1/16-in. OD tubing) and a ferrule to the grounding union.

## Installation

### Connecting Frequently Used Devices

Figure 5-9 shows the connection between the grounding union and the LC union made with red PEEK™ tubing and fingertight fittings.



**Figure 5-9.** Connecting the infusion line to the LC union and the grounding union

## Setting Up the Inlet for High-Flow Infusion

You can configure (plumb) a switching valve as a loop injector (for flow injection analysis) or as a divert valve. You can also use the switching valve to divert the LC flow between the mass spectrometer and waste when the valve is in the divert valve configuration, or switch between load and inject modes when the valve is in the loop injector configuration.

The Exactive Series mass spectrometer allows connecting up to two external switching valves (Rheodyne MX Series II™, for example). The valves are controlled by the instrument software by means of contact closures. For instructions about establishing power supply and communication between switching valve(s) and mass spectrometer, see [page 5-34](#).

For high-flow infusion analyses, connect the syringe pump and the outlet of an LC pump to two legs of a union Tee. Connect the third leg of the union Tee to the ion source.

To make the plumbing connections for sample introduction from the syringe pump into solvent flow from an LC pump, perform these procedures in any order:

- [Connecting the Syringe to the Union Tee](#)
- [Connecting the Union Tee to the Switching Valve](#)



- [Connecting the LC Pump to the Switching Valve](#)
- [Connecting the Switching Valve to a Waste Container](#)
- [Connecting the Union Tee to the Ion Source](#)

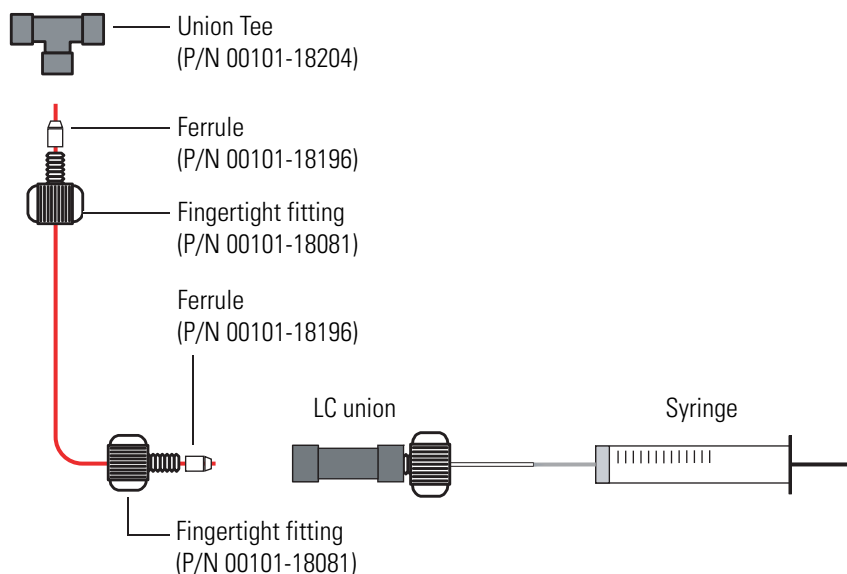
### Connecting the Syringe to the Union Tee

Use red PEEK™ tubing and fingertight fittings with ferrules to connect the syringe to the LC union Tee.

#### ❖ To connect the syringe to the LC union Tee

1. Set up the syringe as described in “[Setting Up the Syringe](#)” on [page 5-23](#).
2. With a fingertight fitting and a ferrule, connect a red PEEK™ infusion line to the free end of the LC union that is connected to the syringe.
3. With a fingertight fitting and a ferrule, connect the other end of the red PEEK™ infusion line to the union Tee.

[Figure 5-10](#) shows the fittings required to connect the LC union to the union Tee.



**Figure 5-10.** Connecting the LC union to the union Tee

### Connecting the Union Tee to the Switching Valve

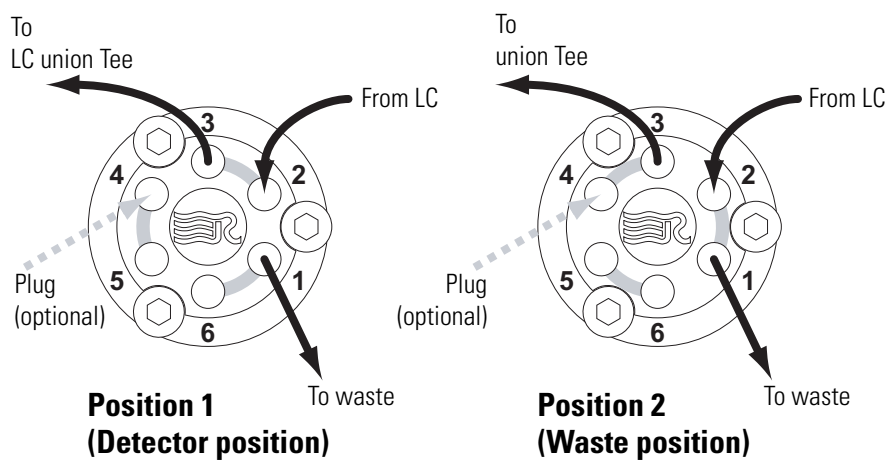
#### ❖ To connect the union Tee to the switching valve

1. With a fingertight fitting and a ferrule, connect a length of red PEEK™ tubing to port 3 of the switching valve. Or, use a stainless steel nut and ferrule to connect the tubing to the switching valve.

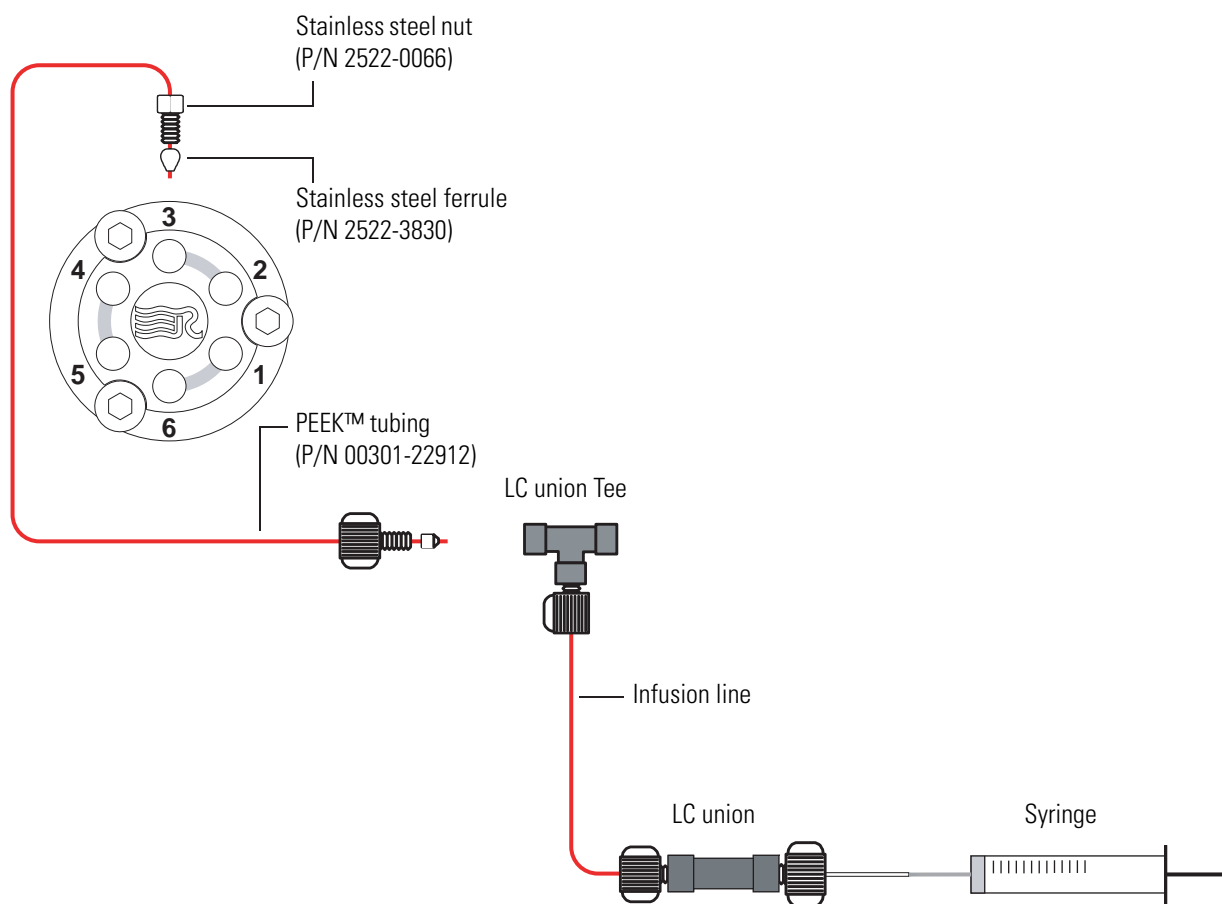
## Installation

### Connecting Frequently Used Devices

2. With a fingertight fitting and a ferrule, connect the other end of the tubing to the free end of the union Tee. See [Figure 5-11](#) and [Figure 5-12](#).



**Figure 5-11.** Six-port switching valve connections



**Figure 5-12.** Connecting the LC union to the union Tee

## Connecting the LC Pump to the Switching Valve

### ❖ To connect the LC pump to the switching valve

1. With a fingertight fitting and a ferrule, connect a length of PEEK™ tubing to port 2 of the switching valve. [Figure 5-11](#) on [page 5-26](#) shows the ports of the switching valve.
2. With an appropriate fitting and ferrule, connect the other end of the tubing to the outlet of the LC.

## Connecting the Switching Valve to a Waste Container

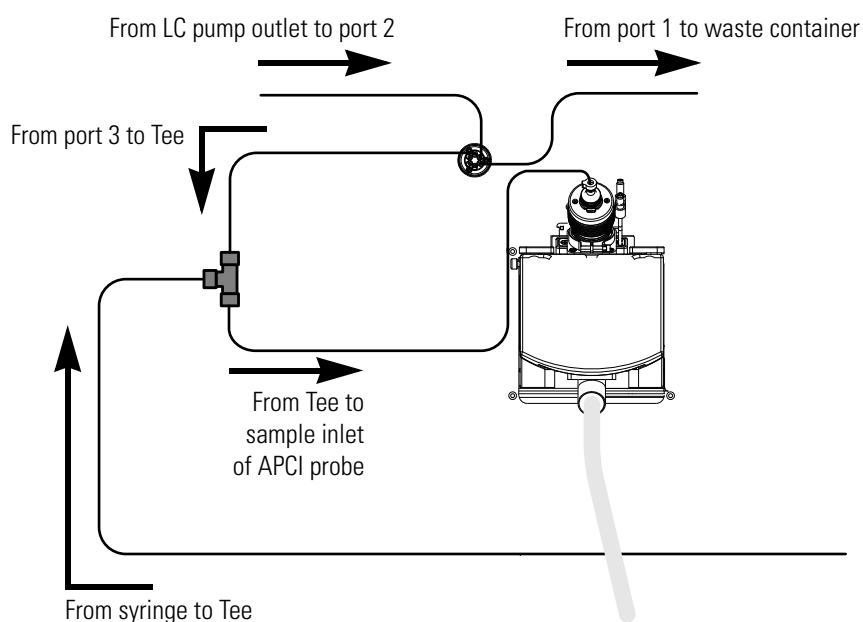
### ❖ To connect the switching valve to a waste container

1. With a fingertight fitting and a ferrule, connect a length of red PEEK™ tubing to port 1 of the switching valve. [Figure 5-11](#) on [page 5-26](#) shows the ports of the switching valve.
2. Insert the other end of the tubing into a suitable waste container.

## Connecting the Union Tee to the Ion Source

### ❖ To connect the union Tee to the ion source

1. With a fingertight fitting and a ferrule, connect one end of a length of red PEEK™ tubing to the union Tee. [Figure 5-13](#) shows the connections to the union Tee.

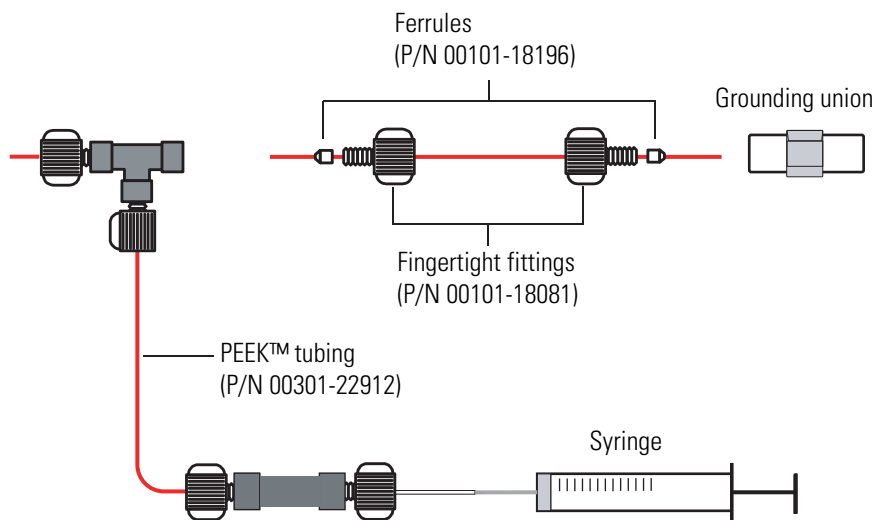


**Figure 5-13.** Plumbing diagram showing APCI/MS sample introduction with high-flow infusion

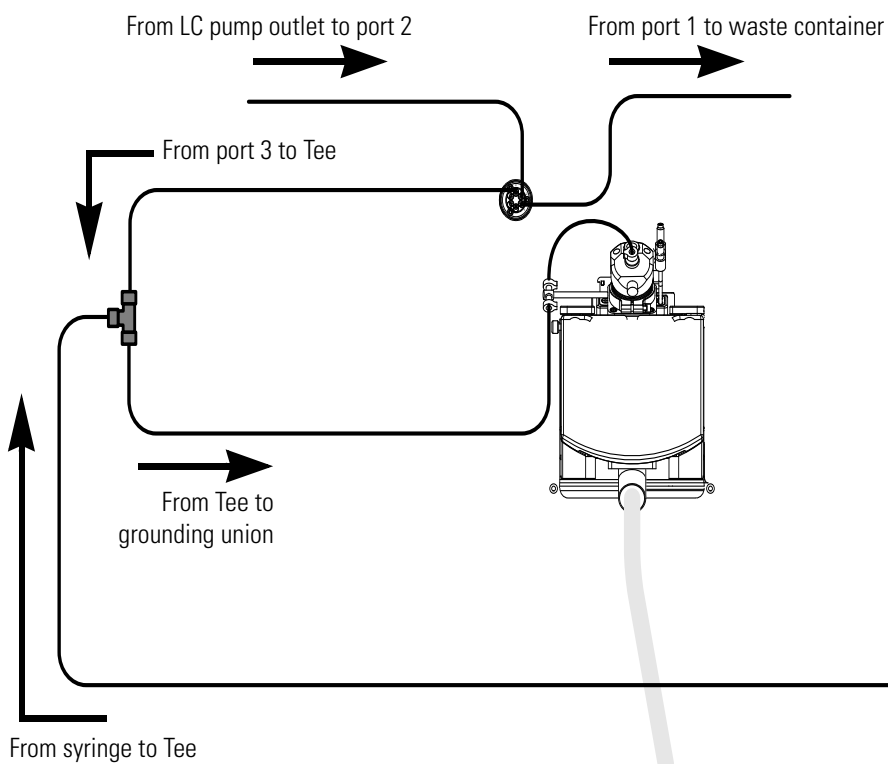
2. Depending on whether you are using the ESI probe or the APCI probe, do one of the following:
  - For the APCI probe, use a fingertight fitting and a ferrule to connect the other end of the tubing directly to the sample inlet of the APCI probe. [Figure 5-13](#) shows the connection between the union Tee and the sample inlet of the APCI probe.

**NOTICE** Do not use the grounding bar of the Ion Max API source for the APCI probe. A knurled nut secures the grounding bar to the Ion Max API source. You do not need to remove the grounding bar to run the system in the APCI mode. ▲

- For the ESI probe, use a fingertight fitting and a ferrule to connect the other end of the tubing to the grounding union that is held by the grounding bar of the Ion Max API source. See [Figure 5-14](#) and [Figure 5-15](#).  
The grounding union slides into the grounding bar on the Ion Max API source as shown in [Figure 5-19](#) on [page 5-33](#). For instructions on connecting the grounding union to the ESI probe sample inlet, refer to the *Ion Max and Ion Max-S API Source Hardware Manual*.



**Figure 5-14.** Connecting the union Tee to the grounding union used for the ESI probe

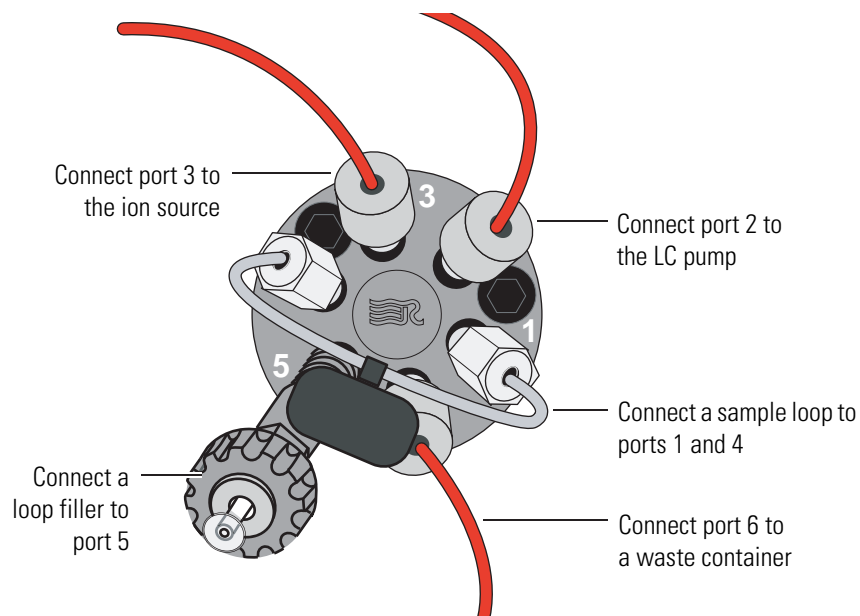


**Figure 5-15.** Plumbing diagram showing ESI/MS sample introduction with high-flow infusion

## Setting Up the Inlet for Loop Injections (Flow Injection Analyses)

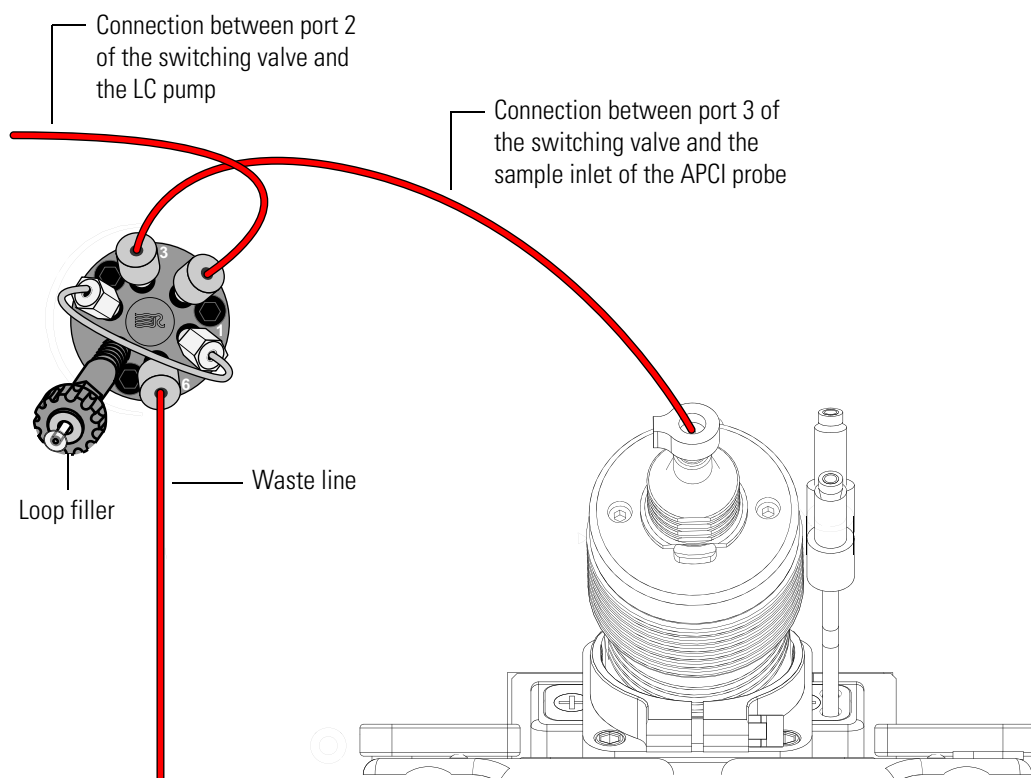
### ❖ To set up the inlet for loop injections

1. Connect a loop filler to port 5 of the switching valve. See [Figure 5-16](#).

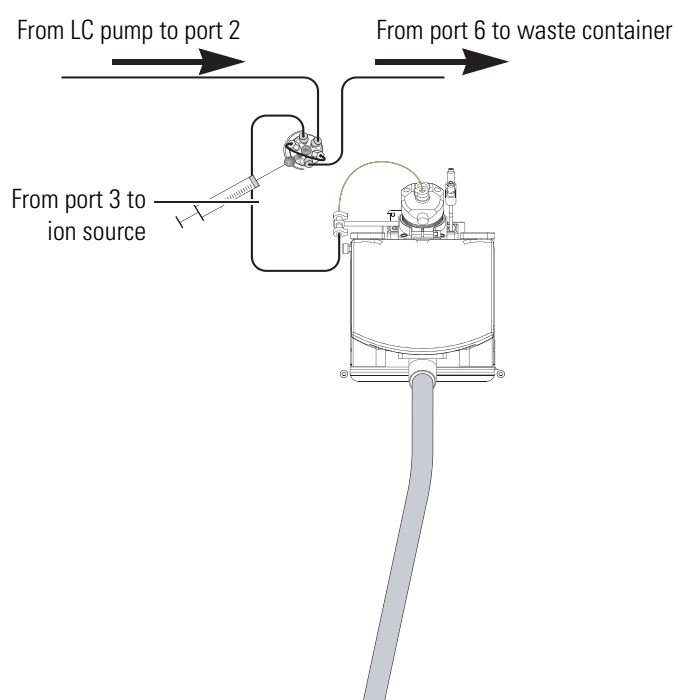


**Figure 5-16.** Switching valve set up for loop injections

2. Connect a sample loop to ports 1 and 4.
3. To connect the LC pump to port 2 of the switching valve:
  - a. With an appropriate fitting and ferrule, connect one end of a length of red PEEK™ tubing to the outlet of the LC pump.
  - b. Using a fingertight fitting and a ferrule, connect the other end of the tubing to port 2 of the switching valve.
4. Depending on whether you are using the APCI probe or the ESI probe, do one of the following to connect port 3 of the switching valve to the ion source:
  - For the APCI probe, use two fingertight fittings and two ferrules to connect a length of red PEEK™ tubing between port 3 of the switching valve and the sample inlet of the APCI probe. See [Figure 5-17](#).
  - For the ESI probe, use two fingertight fittings and two ferrules to connect a length of red PEEK™ tubing between port 3 of the switching valve and the grounding union. See [Figure 5-18](#). To connect the other end of the grounding union to the ESI probe sample inlet, follow the instructions in the *Ion Max and Ion Max-S API Source Hardware Manual*.



**Figure 5-17.** Plumbing diagram for loop injection into the solvent flow from an LC into an APCI probe



**Figure 5-18.** Plumbing diagram for loop injection into the solvent flow from an LC into an ESI probe

5. To connect the switching valve to a waste container:
  - a. Use a fingertight fitting and a ferrule to connect one end of a length of red PEEK™ tubing to port 6 of the switching valve.
  - b. Place the other end of the tubing to an appropriate waste container.

### **Setting Up the Inlet for an LC/MS System with an Autosampler**

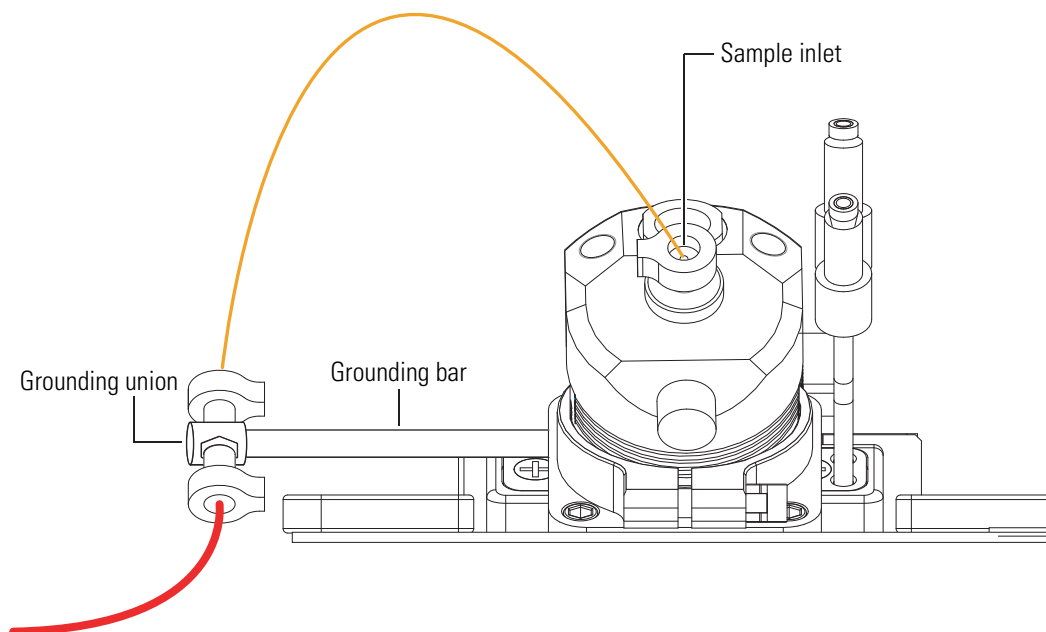
❖ **To connect the inlet plumbing for an LC/MS system with an autosampler**

1. Using an appropriate fitting and ferrule, connect one end of a length of red PEEK™ tubing to the outlet of the LC system.
2. Using a fingertight fitting and a ferrule, connect the other end of the tubing to port 2 of the switching valve.
3. To connect port 3 of the switching valve to the ion source, depending on the probe type, do one of the following:
  - For the ESI probe, use two fingertight fittings and two ferrules to connect a length of red PEEK™ tubing between port 3 of the switching valve and the grounding union. To connect the other end of the grounding union to the ESI probe sample inlet, follow the instructions in the *Ion Max and Ion Max-S API Source Hardware Manual*.
  - For the APCI probe, use two fingertight fittings and two ferrules to connect a length of red PEEK™ tubing between port 3 of the switching valve and the APCI probe sample inlet.
4. To connect the switching valve to a waste container:
  - a. Using a fingertight fitting and a ferrule, connect one end of a length of red PEEK™ tubing to port 1 of the switching valve.
  - b. Place the other end of the tubing to an appropriate waste container.



## Connecting the Grounding Union to the ESI Probe Sample Inlet

For instruction on connecting the PEEK™ safety sleeve and fused-silica sample tube from the grounding union to the ESI probe sample inlet, refer to the *Ion Max and Ion Max-S API Source Hardware Manual*.



**Figure 5-19.** Connecting the grounding union to the sample inlet of the ESI probe

## Establishing Power Supply and Communication for the Syringe Pump

Before you start connecting the syringe pump, make sure that it is mounted to the holder that is attached to the right side of the mass spectrometer.

**NOTICE** To prevent the holder from getting out of place, make sure that the top of the instrument housing is dry and free of dust before you put the holder in its position. ▲

### ❖ To establish power supply and communication between syringe pump and mass spectrometer

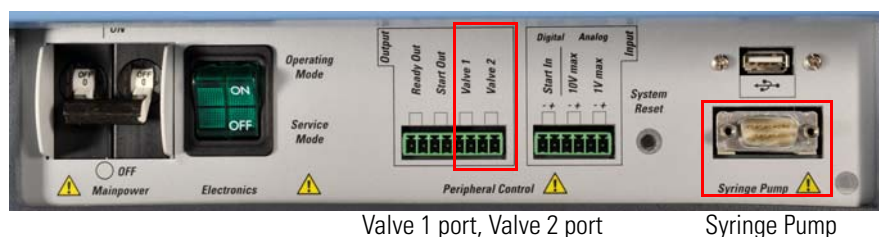
1. Use the RS232 interface cable to connect the syringe contact on the power panel of the Exactive Series mass spectrometer to the RS232 serial port at the rear side of the syringe pump. See [Figure 5-20](#). The syringe contact allows controlling the syringe pump by the instrument software.
2. Connect the power strip that is shipped with the mass spectrometer to the outlet labeled Syringe pump / Valves of the power column at the rear side of the mass spectrometer. See [Figure 3-6](#) on [page 3-14](#).

## Installation

### Connecting Frequently Used Devices

3. Connect the power cord of the syringe pump to an outlet on the power strip. To switch on the syringe pump, use the power switch at the rear side of the syringe pump.

**NOTICE** Keep the power switch in the On position; this way electric power to the syringe pump is controlled by the mass spectrometer. ▲



**Figure 5-20.** Power panel with peripherals ports



**Electric Current.** Electric shock hazard. Wrong usage of switches or contact ports might endanger personnel. Read and understand this manual to prevent harm to the operator and to protect the equipment against damage.

Refer to the Software Manual or the Help for details about controlling the syringe pump with the Tune software. Refer also to the manual that came with the syringe pump for further information.

## Establishing Power Supply and Communication for the Switching Valve(s)

Before you start connecting the switching valve(s), make sure that they are mounted to the holder that is attached to the right side of the mass spectrometer.

**NOTICE** To prevent the holder from getting out of place, make sure that the top of the instrument housing is dry and free of dust before you put the holder in its position. ▲

### ❖ To establish power supply and communication between switching valve(s) and mass spectrometer

1. Contact closure signals from the Exactive Series mass spectrometer to a switching valve are transmitted by an interface cable:
  - a. Connect the interface cable to the mating connector on the back of the MX Series II Module. The Valve 1 port and the Valve 2 port of the mass spectrometer are located on the power panel of the mass spectrometer. See [Figure 5-20](#).

- b. Connect the interface cable of each switching valve to a port: connect wire #1 of the interface cable to one terminal and wire #6 to the other terminal. The Exactive Series mass spectrometer does not differentiate between the terminals. A suitable plug connector (P/N 2087270) for the peripheral control output connection is provided with the Installation Kit.
2. The Exactive Series mass spectrometer provides electric power for the switching valve(s):
  - a. Plug the Universal Power Supply male barrel connector into the MX Module female port at the rear side of the switching valve.
  - b. Plug the female connector of the power cord into the Universal Power Supply.
  - c. Connect the power strip that is shipped with the mass spectrometer to the outlet labeled Syringe pump / Valves of the power column at the rear side of the mass spectrometer. See [Figure 3-6 on page 3-14](#).
  - d. Plug the opposite end of the power cord into an outlet on the power strip.

**NOTICE** Electric power to the switching valve(s) is controlled by the mass spectrometer. ▲

Refer to the Software Manual or the Help for details about controlling a switching valve with the Tune software. Refer also to the manual that came with the switching valve for further information.

## User I/O Connections

This section describes the specifications for the peripheral control connections. It contains the following topics:

- [Output Specifications](#)
- [Input Specifications](#)

Location and function of the peripheral control connections are described in “[Peripheral Control](#)” on [page 3-12](#).

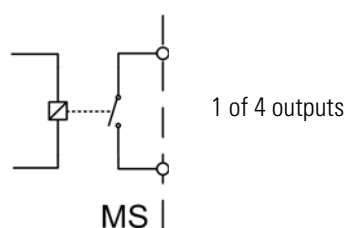
### Output Specifications

The Exactive Series mass spectrometer outputs correspond to the status functions listed below. The outputs are potential-free relay contacts, which are closed when the status indicated by the name is true.

The following outputs are available:

- Ready Out (Pins 1 and 2)
- Start Out (Pins 3 and 4)
- Valve 1 (Pins 5 and 6)
- Valve 2 (Pins 7 and 8)

Location and function of the peripheral control outputs are described on [page 3-12](#). [Figure 5-21](#) shows the circuit diagram and [Table 5-3](#) lists the specifications of the peripheral control output.



**Figure 5-21.** Output equivalent schematic

**Table 5-3.** Output circuit specifications

Contact closed	$R_{\text{on}} < 0.2 \Omega$
Contact open	$R_{\text{off}} > 1 \text{ G}\Omega$
Current	$I_{\text{max}} = 0.5 \text{ A}$
Voltage	$V_{\text{max}} = 30 \text{ V}$
Power	$P_{\text{max}} = 10 \text{ W}$

## Input Specifications

The Exactive Series mass spectrometer provides one digital and two analog inputs to connect external devices.

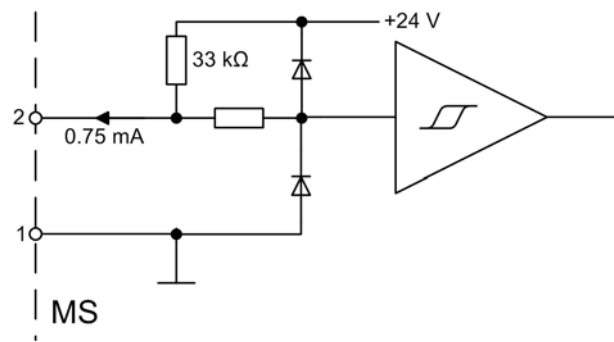
The following inputs are available:

- Start In port (Pins 1 and 2)
- Analog Input ports (10 V: Pins 3 and 4), (1 V: Pins 5 and 6)

### Start In Input Specification

The Start In input is an input with internal pull-up resistor for connecting external relays contacts or open collector transistors. Start is triggered with the falling edge of input voltage.

Location and function of the Start In input are described on [page 3-13](#). [Figure 5-22](#) shows the circuit diagram and [Table 5-4](#) lists the specifications of the peripheral control output.



**Figure 5-22.** Start In input equivalent schematic

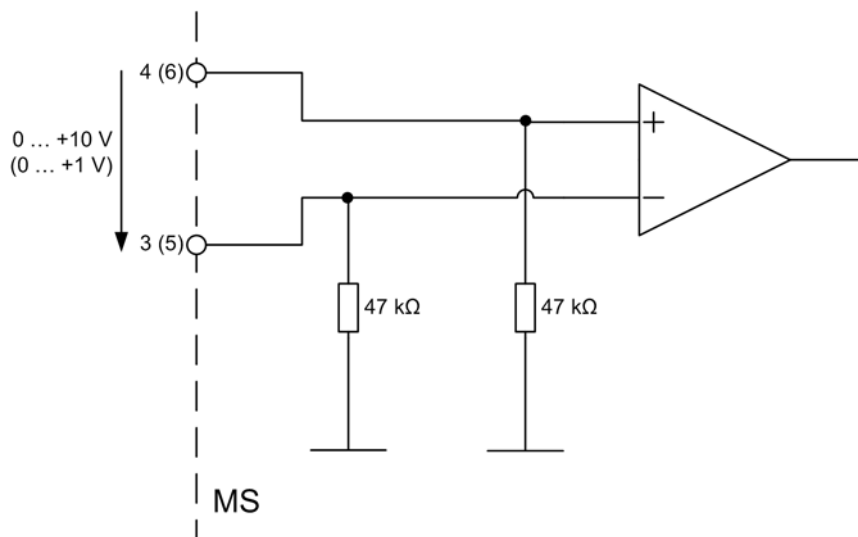
**Table 5-4.** Start In input circuit specifications

Low level input voltage	$U_{in} < 0.8 \text{ V @ } 0.75 \text{ mA}$
High level input voltage	$U_{in} > 2.0 \text{ V}$

### Analog Inputs Specifications

The analog inputs are differential inputs without isolation for connecting external analog voltages. Both inputs reference to the same analog ground.

Location and function of the analog inputs are described on [page 3-13](#). [Figure 5-23](#) shows the circuit diagram and [Table 5-5](#) lists the specifications of the peripheral control output.



**Figure 5-23.** Analog inputs equivalent schematic

**Table 5-5.** Analog inputs circuit specifications

Input Voltage	$U_{in}$	0 ... +10 V / 0 ... +1 V
Input Resistor	$R_{in}$	47 k $\Omega$ to Ground

## Obtaining Calibration Solutions

This section describes how to obtain ready-to-use calibration solutions and how to prepare calibration solutions from the chemicals.

### About Calibration Solutions

The *positive ion mode calibration solution* allows calibrating Thermo Scientific mass spectrometers with the ESI or HESI II probe in positive ion mode. Supported instruments are the Thermo Scientific Exactive Series mass spectrometers, the Thermo Scientific LTQ Velos Series mass spectrometers, and the Thermo Scientific LTQ Orbitrap Velos Series mass spectrometers. The positive ion mode calibration solution covers a mass range from  $m/z$  74 to  $m/z$  1822 and is therefore usable for calibrations between  $m/z$  50 and  $m/z$  2000.

The *negative ion mode calibration solution* allows calibrating Thermo Scientific mass spectrometers with the ESI or HESI II probe in negative ion mode. Supported instruments are the Exactive Series mass spectrometers and LTQ based hybrid instruments (LTQ FT, LTQ FT Ultra, and LTQ Orbitrap Series). The negative ion mode calibration solution covers a mass range from  $m/z$  265 to  $m/z$  1880 and is therefore usable for calibrations between  $m/z$  50 and  $m/z$  2000.

To calibrate the extended mass range of the Exactive Plus EMR mass spectrometer, use a solution of cesium iodide. For instructions about preparing the calibration solution, see [page 5-46](#).

### Obtaining Ready-to-Use Calibration Solutions

To free users from time-consuming mixing and dilution steps and to allow them to focus on data acquisition, Thermo Fisher Scientific provides ready-to-use calibration solutions. [Table 5-6](#) shows the available calibration solution packages.

**Table 5-6.** Available calibration solutions packages

Calibration Solution	Product Name	Product Number
Positive ion mode	Pierce LTQ Velos ESI Positive Ion Calibration Solution, 10 mL	88323
Negative ion mode	Pierce ESI Negative Ion Calibration Solution, 10 mL	88324

You can order ready-to-use calibration solutions from [www.thermofisher.com](http://www.thermofisher.com) or [www.fishersci.com](http://www.fishersci.com). The prepared calibration solutions are shipped at ambient temperature and stable at 2–8 °C for 1.5 years.

## Preparing Calibration Solutions

This section provides information about calibration compounds, solvents, and modifiers used for preparing the calibration solutions.

### CAUTION

**Hazardous Chemicals.** Potentially hazardous chemicals, solvents, and modifiers are used in procedures throughout this chapter. For a description of the specific hazards of a compound, read the Material Safety Data Sheet (MSDS). Avoid exposure to potentially harmful materials. Always wear protective gloves and safety glasses when you handle solvents or corrosives. Store and handle all chemicals in accordance with standard safety procedures. Also contain waste streams and use proper ventilation.

Material Safety Data Sheets provide summarized information on the hazards and toxicity of specific chemical compounds. The MSDS also provides information on the proper handling of compounds, first aid for accidental exposure, and procedures for the remedy of spills or leaks.

The Material Safety Data Sheets describing the chemicals being used are to be freely available to lab personnel for them to examine at any time. Producers and suppliers of chemical compounds are required by law to provide their customers with the most current health and safety information in the form of an MSDS. Read the MSDS for each chemical you use.



## Calibration Compounds

The *n*-butylamine, caffeine, MRFA, Ultramark™ 1621, sodium dodecyl sulfate, and sodium taurocholate that are needed to make the calibration solutions are supplied with the chemical accessory kit. When you order replacements, use the information listed in [Table 5-7](#).

**Table 5-7.** Calibration- and Test-Chemicals

Description	Quantity	Supplier Product Number
<b>Supplier: Sigma™ Chemical Company, see below.</b>		
<i>n</i> -Butylamine <sup>a</sup>	25 mL	471305-25ML
Sodium Dodecyl Sulfate	10 g	L4509-10G
Sodium Taurocholate Hydrate	250 mg	T4009-250MG
Caffeine Methanol Solution	1 mL	C6035-1ML
<b>Supplier: ABCR GmbH &amp; Co. KG, see below.</b>		
Ultramark™ 1621 Mass Spec. Standard	250 mg	AB172435
<b>Supplier: Thermo Fisher Scientific</b>		
Met-Arg-Phe-Ala acetate salt	1 mg	1305050

<sup>a</sup> If ordering elsewhere, use only mass spec grade.

To order more of these compounds, contact:

Sigma Chemical Company  
P. O. Box 14508  
St. Louis, Missouri, USA 63178-9916  
Phone (800) 325-3010 (in the USA or Canada)  
(314) 771-3750 (outside the USA or Canada)  
Web site [www.sigma-aldrich.com](http://www.sigma-aldrich.com)

or

ABCR GmbH & Co. KG  
Im Schleht 10  
D-76187 Karlsruhe, Germany  
Phone +49 (0)721 950 61-0  
Fax +49 (0)721 950 61-80  
Email [info@abcr.de](mailto:info@abcr.de)  
Web site [www.abcr.de](http://www.abcr.de)

**Solvents and Modifiers**

Installation of the instrument requires LC/MS grade methanol and water. Solvent modifiers might also be required during the installation of some systems. The following solvents are useful in operating and maintaining your instrument:

- Methanol
- Acetonitrile
- Water
- Isopropyl alcohol
- Acetic acid (modifier)
- Formic acid (modifier)

Some solvent impurities are transparent to UV/VIS detectors. Therefore, some LC/MS grade solvents might contain contaminants that interfere with the performance of the mass spectrometer. To operate your instrument, choose high purity solvents with minimum contamination.

You can order LC/MS grade consumables from Thermo Fisher Scientific, which are sold under its Fisher Scientific brand. Visit [www.fishersci.com](http://www.fishersci.com). Use only Optima™ LC/MS grade chemicals for operating your system.

**NOTICE** Consider the following cautions when you prepare calibration solutions:

- Do not filter solvents. Filtering solvents can introduce contamination.
- Do not use plastic pipettes to prepare the tuning and calibration standards. Plastic products can release phthalates that can interfere with your analyses. ▲

## Preparing Stock Solutions

Use the chemicals described in the previous section to prepare the calibration solutions from the following stock solutions:

- [Caffeine Stock Solution](#)
- [MRFA Stock Solution](#)
- [Ultramark 1621 Stock Solution](#)
- [N-Butylamine Stock Solution](#)
- [Sodium Dodecyl Sulfate Stock Solution](#)
- [Sodium Taurocholate Stock Solution](#)

For an instruction about preparing the cesium iodide calibration solution for the Exactive Plus EMR mass spectrometer, see [page 5-46](#).

### Caffeine Stock Solution

A 1 mg/mL stock solution of caffeine in 100% methanol is provided with the Exactive Series mass spectrometer. You can also order this solution through Sigma. The Sigma product number for this solution is C6035.

### MRFA Stock Solution

#### ❖ To prepare the MRFA stock solution

1. Obtain the vial of L-methionyl-arginyl-phenylalanyl-alanine acetate × H<sub>2</sub>O (MRFA) in the accessory kit. In this form, the MRFA sample has an average molecular weight of 523.7 u. Carefully weigh 1.0 mg of the MRFA sample.
2. Dissolve the MRFA sample in a total volume of 330 µL of 50:50 methanol:water. Mix the solution (5.0 nmol/µL) thoroughly.
3. Transfer 50 µL of the 5 nmol/µL solution into a clean polypropylene tube.
4. Add 1.45 mL of 50:50 methanol:water to the tube. Mix this solution (166.7 pmol/µL) thoroughly.
5. Label the tube *MRFA stock solution* and store it in a freezer until it is needed.

### Ultramark 1621 Stock Solution

#### ❖ To prepare the Ultramark 1621 stock solution

1. Obtain the vial of Ultramark 1621 in the accessory kit.

2. Using a syringe, measure out 10  $\mu\text{L}$  of Ultramark 1621, and dissolve it in 10 mL of acetonitrile.
3. Mix the solution thoroughly.
4. Label the vial *Ultramark 1621 stock solution* and store it in a freezer until it is needed.

### ***N*-Butylamine Stock Solution**

#### **❖ To prepare the *n*-butylamine stock solution**

1. Using a syringe, transfer 5  $\mu\text{L}$  of *n*-butylamine to a 10 mL (minimum) volumetric glass flask.
2. Add 9995  $\mu\text{L}$  of 50:50 methanol/water to the flask.
3. Mix the solution thoroughly.
4. Transfer the solution to a vial.
5. Label the vial *N-butylamine stock solution*.

### **Sodium Dodecyl Sulfate Stock Solution**

#### **❖ To prepare the sodium dodecyl sulfate stock solution**

1. Obtain the vial of sodium dodecyl sulfate. In this form, the sample has an average molecular weight of 288.4 u.
2. Prepare the stock solution of sodium dodecyl sulfate by dissolving 2.88 mg in 10 mL of 50:50 methanol:water.
3. Mix the solution (1.0 nmol/ $\mu\text{L}$ ) thoroughly.
4. Label the vial *Sodium Dodecyl Sulfate stock solution (1 nmol/ $\mu\text{L}$ )*.

### **Sodium Taurocholate Stock Solution**

#### **❖ To prepare the sodium taurocholate stock solution**

1. Obtain the vial of sodium taurocholate. In this form, the sample has an average molecular weight of 537.7 u.
2. Prepare the stock solution of sodium taurocholate by dissolving 5.38 mg in 10 mL of 50:50 methanol:water.
3. Mix the solution (1.0 nmol/ $\mu\text{L}$ ) thoroughly.
4. Label the vial *Sodium Taurocholate stock solution (1 nmol/ $\mu\text{L}$ )*.

## Preparing the Positive Ion Mode Calibration Solution

The positive ion mode calibration solution consists of caffeine, MRFA, Ultramark 1621, and *n*-butylamine in an acetonitrile:methanol:water solution that contains 1% acetic acid.

### ❖ To prepare the positive ion mode calibration solution

1. Pipet 20 µL of the caffeine stock solution into a light-protected, clean, dry 10 mL volumetric flask.
2. Pipet 100 µL of the MRFA stock solution into the flask.
3. Pipet 100 µL of the Ultramark 1621 stock solution into the flask.
4. Pipet 100 µL of the stock solution of *n*-butylamine into the flask.

**NOTICE** Use only glass pipets or stainless steel syringes when you measure glacial acetic acid. Using plastic pipet tips causes contamination of acid stock solutions that can introduce contaminants in the calibration solution. ▲

5. Pipet 100 µL of glacial acetic acid into the flask.
6. Pipet 5 mL of acetonitrile into the flask.
7. Bring the volume of the solution up to the 10 mL-mark on the flask with 50:50 methanol:water.
8. Mix the calibration solution thoroughly.
9. Transfer the solution to a light-protected, clean, dry vial.
10. Label the vial *Positive Ion Mode Calibration Solution* and store it in a freezer until it is needed.

## Preparing the Negative Ion Mode Calibration Solution

The negative ion mode calibration solution consists of sodium dodecyl sulfate, sodium taurocholate, and Ultramark 1621 in an acetonitrile:methanol:water solution that contains 1% acetic acid.

### ❖ To prepare the negative ion mode calibration solution

1. Pipet 100 µL of the sodium dodecyl sulfate stock solution into a light-protected, clean, dry 10 mL volumetric flask.
2. Pipet 100 µL of the sodium taurocholate stock solution into the flask.

## Installation

### Obtaining Calibration Solutions

3. Pipet 100  $\mu\text{L}$  of the Ultramark 1621 stock solution into the flask.

**NOTICE** Use only glass pipets or stainless steel syringes when measuring glacial acetic acid. Using plastic pipet tips causes contamination of acid stock solutions that can introduce contaminants in the calibration solution. ▲

4. Pipet 100  $\mu\text{L}$  of glacial acetic acid into the flask.
5. Pipet 5 mL of acetonitrile into the flask.
6. Bring the volume of the solution up to the 10 mL-mark on the flask with 50:50 methanol:water.
7. Mix the solution thoroughly.
8. Transfer the solution to a light-protected, clean, dry vial.
9. Label the vial *Negative Ion Mode Calibration Solution* and store it in a freezer until it is needed.

## Preparing the Cesium Iodide Calibration Solution

To calibrate the extended mass range of the Exactive Plus EMR mass spectrometer, use a solution of cesium iodide. A glass bottle with 1 g of this compound in powder form is shipped with the instrument. The Fisher Scientific catalog number is AC19282-0010.

### ❖ To prepare the cesium iodide calibration solution

1. Obtain the bottle of cesium iodide that is shipped with the mass spectrometer.
2. Prepare the stock solution of cesium iodide by dissolving 2.0 mg CsI in 1 mL of acetonitrile:methanol:water, 30:30:40.
3. Mix the solution (2 mg/mL) thoroughly.
4. Label the vial *Cesium Iodide calibration solution (2 mg/mL)*.

## Chapter 6 Operation

This chapter outlines the checks and cleaning procedures of the Exactive Series system that should be performed every day to ensure the proper operation of your system.

### Contents

- [Safety Guidelines for Operation](#) on page 6-2
- [Before Operating the System](#) on page 6-4
- [Setting the System in Standby Condition](#) on page 6-7
- [Shutting Down the System](#) on page 6-8
- [Starting Up the System after a Shutdown](#) on page 6-10
- [Resetting the System](#) on page 6-14
- [After Operating the System](#) on page 6-15

## Safety Guidelines for Operation

When you operate the Exactive Series system, pay attention to the following general safety guidelines.

### ▲ WARNING

**High Voltage.** If you touch liquid that leaks from the probe sample inlet while the mass spectrometer is in operation, you might receive an electric shock. Do not tighten the probe sample inlet fitting to eliminate a liquid leak while the mass spectrometer is in operation.

### ▲ WARNING

**Suffocation Hazard.** Most of the nitrogen that is introduced into the API source escapes into the laboratory atmosphere. Accumulation of nitrogen gas could displace sufficient oxygen to suffocate personnel in the laboratory. Make sure that the laboratory is well ventilated. Always operate Exactive Series mass spectrometer and API source with attached drain tubing assembly that connects the source housing drain to a dedicated exhaust system. Local regulations may require a risk assessment for the workplace.

### ▲ WARNING

**Electromagnetic Radiation.** Parts of the forevacuum pump emit electromagnetic radiation. This radiation can interfere with the operation of cardiac pacemakers and implanted heart defibrillators, possibly causing death or serious injury. If you wear these devices, keep at least 30 cm away from the forevacuum pump.

### ▲ WARNING

**Hazardous Chemicals.** The forepump eventually exhausts much of what is introduced into the mass spectrometer, including the small amount of oil vapor that mechanical pumps can emit. The effluent of the forepump might contain noxious chemicals. The connection to an adequate exhaust system is mandatory!

### ▲ WARNING

**Hazardous Chemicals.** The source exhaust might contain noxious material. It will contain traces of the samples and solvents that you are introducing into the source. Potential health hazards of these compounds include chemical toxicity of solvents, samples, and buffers, as well as biohazards of biological samples. To prevent contamination of the laboratory, always operate the ion source with the drain tubing connected. The drain tubing must lead to a waste container that is connected to a dedicated fume exhaust system.



**⚠ CAUTION**

**Hazardous Chemicals.** Samples and solvents might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle solvents or samples. Also contain waste streams and use proper ventilation. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of a particular compound.

**⚠ CAUTION**

**Hot Parts.** During operation of the mass spectrometer, ion transfer capillary and sweep cone can reach temperatures up to 450 °C. This might cause severe burns upon touching or ignite combustible material. The external surface of the ion source housing can become hot enough to cause skin burns.

Do not touch the ion source housing when the mass spectrometer is in operation. Let the ion source cool down as described in this manual before you remove the ion source housing. Do not touch the ion source mount immediately after you have removed the ion source housing. Keep combustible materials away from the ion source mount. Do not let the instrument stay unattended when the housing is not mounted to the source.

**⚠ CAUTION**

**Risk of Eye Injury.** The thin, sharp, flexible capillaries are difficult to see against the light. There is a risk of being stabbed or cut when working with the capillaries. Wear safety glasses to prevent eye injuries!

## Before Operating the System

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

- [Checking the Forepumps](#)
- [Checking the Nitrogen Supply](#)
- [Checking the System Vacuum Levels](#)
- [Checking the Disk Space on the Data System](#)
- [Checking the Mass Accuracy of the Instrument](#)

**NOTICE** Accurate results can be obtained only if the system is properly calibrated. ▲

### Checking the Forepumps

❖ **To check each forepump before use**

Make sure that the following conditions are met:

- The forepump is filled with oil.
- It is connected to the power supply.
- The gas ballast is shut.

### Checking the Nitrogen Supply

Check the nitrogen supply on the regulator of the nitrogen gas tank or the liquid nitrogen boil-off tank. Make sure that you have sufficient gas for your analysis. If necessary, replace the tank. Verify that the pressure of nitrogen that reaches the mass spectrometer is at  $800 \pm 30$  kPa ( $8 \pm 0.3$  bar,  $116 \pm 4$  psi). If necessary, adjust the pressure with the tank pressure regulator.

**▲ WARNING**

**Fire Hazard.** Air or oxygen in the ion source could produce a fire when it is combined with volatile solvents and high voltages. Introduce combustible samples and solvents into the instrument only with the nitrogen supply connected to the ion source. Make sure that the nitrogen supply is sufficient for daily operation.

When they operate continuously, Exactive Series mass spectrometers can consume up to 72000 L (2540 ft<sup>3</sup>) of API source gas per day. The gas consumption strongly depends on the type of analysis the instrument is used for. See [Table 6-1](#). A typical consumption of HCD collision gas is 3 L per day.

**Table 6-1.** Typical high purity nitrogen consumption of LC/MS applications

Application	LC Flow Rate (approximate)	Source Settings [psi] <sup>a</sup>	Consumption [L/min] <sup>a</sup>
Nano-Spray		sheath gas = 0, aux gas = 0, sweep gas = 0	0.002
Low flow	5 µL/min	sheath gas = 5, aux gas = 0, sweep gas = 0	1
Medium flow	200 µL/min	sheath gas = 35, aux gas = 10, sweep gas = 0	15
High flow	1 mL/min	sheath gas = 75, aux gas = 20, sweep gas = 5	35

<sup>a</sup> For a Q Exactive HF-X MS with (H)ESI source in Standby condition, the sweep gas flow is set to a default value of 4 psi. This corresponds to a nitrogen consumption of about 8500 L per day.

Continue with [“Checking the System Vacuum Levels.”](#)

## Checking the System Vacuum Levels

For proper performance, the Exactive Series system must operate at the acceptable vacuum levels. Operating the system at poor vacuum levels can cause reduced sensitivity and tuning problems. Check your system for air leaks by checking the system vacuum levels before you begin the first acquisition.



You can check the current pressure values in the Vacuum / Bakeout window of the Tune software. To display the Tune software window, choose **Start > Programs > Thermo Exactive Series > Tune**. The Instrument status LED in the toolbar (see image in margin) turns green when the vacuum levels are sufficient for operating the Exactive Series system. If the LED is not green, you might have an air leak; see [“Vacuum Leak”](#) on [page 7-5](#) for instructions.

Continue with [“Checking the Disk Space on the Data System.”](#)

## Checking the Disk Space on the Data System

Periodically verify that your hard disk drive has enough free space for data acquisition. The amount of available disk space is shown in the Disk Space dialog box.

### ❖ To determine the amount of available disk space

1. From the Home Page window (which is available by choosing **Start > Programs > Thermo Xcalibur > Xcalibur**), choose **Actions > Check Disk Space** to open the Disk Space dialog box. The Disk Space dialog box lists the following:

- Current drive and directory (for example, C:\Xcalibur\system\programs)
- Number of Mb that are available (free) on the current drive

- Percentage of the current drive that is available
  - Total capacity of the current drive
2. To select another disk drive so that you can determine its disk space, click **Directory**.
  3. When you have completed this procedure, choose **OK** to close the dialog box.

If necessary, you can free space on the hard disk by deleting obsolete files and by moving files from the hard disk drive to a backup medium. First, copy files to the backup medium. After you have copied the files, you can delete them from the hard disk.

Continue with “[Checking the Mass Accuracy of the Instrument.](#)”

## Checking the Mass Accuracy of the Instrument

Thermo Fisher Scientific recommends that you check the mass accuracy before you start working. Follow the procedure described in the QuickStart Guide for your instrument.

If the instrument indicates that the tune parameters and calibration parameters are not optimal, Thermo Fisher Scientific recommends that you tune and calibrate the Exactive Series mass spectrometer. Follow the procedure described in the QuickStart Guide.

**NOTICE** *Calibration parameters* are instrument parameters that affect the mass accuracy and resolution. *Tune parameters* are instrument parameters that affect the intensity of the ion signal. ▲

You need to optimize the tune parameters (or change the Tune Method) when you change the type of experiment. Refer to the QuickStart Guide for a procedure for optimizing the tune parameters for your experiment.

## Setting the System in Standby Condition

The Exactive Series system should not be shut down completely if you are not going to use it for a short period of time, such as overnight or over the weekend. In that case, you can keep the system in Standby condition.

Thermo Fisher Scientific recommends that you keep the mass spectrometer in Standby overnight to provide the best mass accuracy next day.

### ❖ To place the Exactive Series system in the Standby condition

1. Wait until data acquisition, if any, is complete.
2. Turn off the flow of sample solution from the LC (or other sample introduction device).

For instructions on how to operate the LC from the front panel, refer to the manual that came with the LC.



3. In the Tune software window, click the **On/Standby** button to put the instrument in Standby condition. The System LED on the front panel of the mass spectrometer turns yellow when the system is in Standby condition.
4. Keep the LC power On.
5. Keep the autosampler power On.
6. Keep the data system power On.
7. Keep the Exactive Series main power circuit breaker switch in the On position.

**NOTICE** When you place a Q Exactive HF-X MS with (H)ESI source in Standby condition, do not switch off the nitrogen supply of the laboratory. To avoid back streaming from the drain, the sweep gas flow is set to a default value of 4 psi. This corresponds to a nitrogen consumption of about 8500 L (300 ft<sup>3</sup>) per day. ▲

## Shutting Down the System

The Exactive Series system does not need to be shut down completely if you are not going to use it for a short period of time, such as overnight or over a weekend. See “[Setting the System in Standby Condition](#)” on [page 6-7](#). This section describes how to shut down the system for a maintenance or service procedure.

**NOTICE** Power is removed abruptly when you place the main power circuit breaker switch (see [Figure 3-5](#) on [page 3-12](#)) in the Off (O) position. Although no component in the system is harmed, this not the recommended shutdown procedure to follow. ▲

### ❖ To shut down the Exactive Series system

1. Wait until data acquisition, if any, is complete.
2. Turn off the flow of sample solution from the LC (or other sample introduction device).

For instructions on how to operate the LC from the front panel, refer to the manual that came with the LC.



3. In the Tune software window, click the **On/Standby** button to put the instrument in Off condition. (See image in margin.) All high voltages are shut off, as are the sheath and auxiliary gas.
4. Put the main power circuit breaker switch of the mass spectrometer in the Off position.

### ▲ WARNING

**High Voltage.** Hazardous electric voltage capable of causing an electric shock is used in the instrument. To make sure that the instrument is free from all electric current, always disconnect the power cords of *mass spectrometer and source vacuum pump* before you try any type of maintenance.

### ▲ CAUTION

**Hot Parts.** During operation of the mass spectrometer, ion transfer capillary and sweep cone can reach temperatures up to 450 °C. This might cause severe burns upon touching or ignite combustible material. The external surface of the ion source housing can become hot enough to cause skin burns.

Do not touch the ion source housing when the mass spectrometer is in operation. Let the ion source cool down as described in this manual before you remove the ion source housing. Do not touch the ion source mount immediately after you have removed the ion source housing. Keep combustible materials away from the ion source mount. Do not let the instrument stay unattended when the housing is not mounted to the source.

If you plan to perform routine or preventive system maintenance on the mass spectrometer only, you do not need to turn off the LC, autosampler, or data system. In this case, the shutdown procedure is completed. However, if you do not plan to operate the system for an extended period of time, you might want to turn off the LC, autosampler, and data system.

**NOTICE** An instrument that is shut down still consumes nitrogen because the vent valve is connected to the nitrogen supply of the laboratory. Keeping on the nitrogen flow prevents humidity from contaminating the vacuum system of the mass spectrometer. You may however switch off the nitrogen if your supply is limited. ▲

## Starting Up the System after a Shutdown

To start up the Exactive Series mass spectrometer after it has been shut down (and vented), you need to do the following:

1. Start up the instrument
2. Set up conditions for operation

## Starting Up the Instrument

### ❖ To start up the Exactive Series system

1. Make sure that the main power circuit breaker switch of the MS is in the Off (O) position.
2. Start up the (optional) LC and autosampler as is described in the manuals that came with the LC and autosampler.
3. Switch on data system and monitor as described in the manuals that came with them. Wait until the operating system of the computer is completely loaded.
4. To start the Tune software on the data system computer, choose **Start > Programs > Thermo Exactive Series > Tune**.

**NOTICE** The data system must be running before you start up the instrument. The instrument will not operate until software is received from the data system. ▲

5. Turn on the nitrogen flow at the tank, if it is off.
6. Place the main power circuit breaker switch of the MS in the On (I) position. When you place the main power circuit breaker switch in the On (I) position, the forepumps and the turbomolecular pumps are started. All LEDs on the mass spectrometer front panel are off.

When the vacuum system is switched on, the following occurs:

- a. After the main switch is switched On, the pumps of the mass spectrometer are run up. The Pirani gauge (see “[Vacuum Gauges](#)” on [page 3-16](#)) monitors the pressure at the forepump. In a short time, a significant pressure decrease must be observed. The quality of the vacuum can be estimated by means of the rotation speed of the TMPs (for example, 80% after 15 minutes).



- b. If the working pressure is not reached after a preset time, the complete system is switched off.

**NOTICE** The vacuum control board triggers an alert in the Tune software when a vacuum failure has occurred. ▲

- c. The Ion Gauge 1 (IKR 251) is switched on only after the source TMP has exceeded 90% of its maximum rotation speed for five minutes. To extend its life time, this ion gauge is switched off automatically after 30 minutes.

**NOTICE** For diagnostic purposes, the ion gauge can be switched on manually in the instrument status view of the Tune software. ▲

If the pressure exceeds  $1\text{E-}4$  mbar for more than 10 seconds, the ion gauge is switched off. After five minutes, the ion gauge is switched on again. After three failed tries, it is only possible to switch on Ion Gauge 1 manually in the Tune software.

- d. The Ion Gauge 2 (IKR 270) is switched on only after both TMPs have exceeded 90% of their maximum rotation speed for five minutes. It is then used to monitor the vacuum in the Orbitrap analyzer.

If the pressure exceeds  $1\text{E-}4$  mbar for more than 10 seconds, the ion gauge is switched off. After five minutes, the ion gauge is switched on again. After three failed tries, it is only possible to switch on Ion Gauge 2 manually in the Tune software.

- e. The Vacuum LED on the system panel turns green when all the following conditions are met:
- In the Tune software, all LEDs are green. (The Ion Gauge 1 is allowed to be off).
  - Analyzer temperature is below  $45\text{ }^{\circ}\text{C}$ .
  - Both TMP frequencies have exceeded 90% of their maximum rotation speed.
- f. When the vacuum measured by the Ion Gauge 2 is better than  $1\text{E-}8$  mbar, the power supplies of the high voltage electronics and the capillary heater are switched on.

**NOTICE** If both ion gauges are defective, it is not possible to switch on the RF voltage and the high voltages. ▲

If you have an LC or autosampler, start it as is described in the manual that came with the LC or autosampler. If you do not have either, go to [“Setting Up Conditions for Operation”](#) below.

## Setting Up Conditions for Operation

### ❖ To set up your Exactive Series mass spectrometer for operation

1. Operation of the system with excessive air and water in the vacuum manifold can cause reduced sensitivity and tuning problems. Before you begin data acquisition with your Exactive Series system, you need to bake out the system for at least twelve hours plus a cooling period of three hours. See [“Baking Out the System”](#) on [page 8-12](#).
2. After having performed a system bakeout, make sure in the Vacuum/Bakeout window of the Tune software that the UHV pressure is  $\leq 1\text{E-}8$  mbar. Also make sure that the FV pressure is in the 1–2 mbar region. Compare the values of the other parameters in the instrument status window with values that you recorded previously.
3. Make sure that the gas pressure is within the operational limits:  
Nitrogen:  $800 \pm 30$  kPa ( $8 \pm 0.3$  bar,  $116 \pm 4$  psi)
4. Continue to set up for H-ESI, ESI, or APCI operation as described in the QuickStart Guide for your instrument.

See also [“Before Operating the System”](#) on [page 6-4](#) for additional information.

## Introducing Sample into the Exactive Series Mass Spectrometer

The Exactive Series mass spectrometer and the equipment for introducing sample solution and/or calibration solution (LC or syringe pump) have been installed by a Thermo Fisher Scientific field service engineer.

If you wish to connect the mass spectrometer to other LC equipment, see [“Connecting Frequently Used Devices”](#) on [page 5-18](#) for advice. Also refer to the manuals that came with the LC equipment.

The QuickStart Guide for your instrument gives an introduction on setting up and operating the Exactive Series mass spectrometer.

Consider the following safety guidelines when you introduce sample into the Exactive Series mass spectrometer.

### **WARNING**

**High Voltage.** If you touch liquid that leaks from the probe sample inlet while the mass spectrometer is in operation, you might receive an electric shock. Do not tighten the probe sample inlet fitting to eliminate a liquid leak while the mass spectrometer is in operation.

**⚠ WARNING**

**Hazardous Chemicals.** Sample solution that contains noxious compounds might drip out of the ion source housing. Always operate Exactive Series mass spectrometer and API source with the drain tubing assembly mounted to the source housing drain. The drain tubing must lead to a waste container that is connected to a dedicated exhaust system.

**⚠ CAUTION**

**Hazardous Chemicals.** Samples and solvents might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle solvents or samples. Also contain waste streams and use proper ventilation. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of a particular compound.

## Performing Mass Spectrum Measurements

The QuickStart Guide for your instrument gives an introduction on performing mass spectrum measurements with the Exactive Series mass spectrometer.

Consider the following safety guidelines when performing measurements with the Exactive Series mass spectrometer.

**⚠ WARNING**

**Suffocation Hazard.** Most of the nitrogen that is introduced into the API source escapes into the laboratory atmosphere. Accumulation of nitrogen gas could displace sufficient oxygen to suffocate personnel in the laboratory. Make sure that the laboratory is well ventilated. Always operate Exactive Series mass spectrometer and API source with attached drain tubing assembly that connects the source housing drain to a dedicated exhaust system. Local regulations may require a risk assessment for the workplace.

**⚠ WARNING**

**Fire Hazard.** Air or oxygen in the ion source could produce a fire when combined with volatile solvents and high voltages. Introduce combustible samples and solvents into the instrument only with the nitrogen supply connected to the ion source. Make sure that the nitrogen supply is sufficient for daily operation.

## Resetting the System

If communication between the mass spectrometer and data system computer is lost, it may be necessary to reset the system using the Reset button of the Exactive Series mass spectrometer.

### ❖ To reset the system

1. Make sure that mass spectrometer and data system computer are both powered on and the mass spectrometer is in Standby condition. See [page 6-7](#) for instructions about placing the instrument to Standby condition.
2. To reset the mass spectrometer, press the Reset button located on the power panel. See [Figure 3-5](#) on [page 3-12](#). Make sure that the Status LED is off before you release the Reset button. When you press the Reset button, the following occurs:
  - a. An interruption of the embedded computer causes the CPU to reboot. All LEDs on the front panel are off except the Power LED.
  - b. After several seconds, the Status LED turns yellow to indicate that the data system and the instrument are starting to establish a communication link.
  - c. After several more seconds, the Status LED turns green to indicate that the data system and the instrument have established a communication link. Software for the operation of the instrument is then transferred from the data system to the instrument.

After 3 minutes, the software transfer is complete. The System LED turns either green to indicate that the instrument is functional and the high voltages are on, or yellow to indicate that the instrument is functional and it is in Standby condition.

**NOTICE** If resetting the system does not resolve the failure: Put the electronics switch in the Service Mode position for about one minute. Afterwards, place the electronics service switch back in the Operating Mode position. ▲

## After Operating the System

After operating the Exactive Series mass spectrometer, perform the following steps in sequence:

1. [Flushing Sample Transfer Line, Sample Tube, and API Probe](#)
2. [Flushing Ion Sweep Cone and Ion Transfer Capillary](#)
3. [Purging the Oil in the Source Vacuum Pump](#)
4. [Emptying the Solvent Waste Container](#)

**NOTICE** Thermo Fisher Scientific recommends that you keep the mass spectrometer in Standby overnight to provide the best mass accuracy next day. ▲

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

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

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

1. Wait until the data acquisition, if any, is complete.
2. Make sure that the door to the API chamber is closed and secured.
3. Choose **Start > Programs > Thermo Exactive Series > Tune** to open the Tune software window.
4. From the Tune software window, click the **On/Standby** button to toggle it from Standby to On. The voltages and gas flows to the API source are switched on.
5. Set up the HESI probe as follows:
  - a. In the Tune software window, display the HESI Source window.
  - b. In the HESI Source window, enter **30** in the Sheath Gas Flow Rate text box.
  - c. In the HESI Source window, enter **5** in the Aux Gas Flow Rate text box.
  - d. In the HESI Source window, enter **0** in the Sweep Gas Flow Rate text box.
  - e. In the HESI Source window, enter **0** in the Spray Voltage text box.



- f. Click **Apply**.
6. Set up and start a flow of 50:50 methanol:water solution from the LC to the API source:
    - Set the Flow Rate to a value that is typical for your experiments.
    - Set the solvent proportions to 50% methanol and water.

**▲ CAUTION**

**Hazardous Substance.** Methanol is highly flammable and noxious. Keep away from heat, sparks, and flame. Avoid accidental exposure. Use with adequate ventilation. When possible, dilute it with 50% water. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of methanol.

7. Let the solution flow through sample transfer line, sample tube, and API probe for 15 minutes. After 15 minutes, switch off the flow of liquid from the LC to the API source. Keep the API source (including APCI vaporizer, sheath gas, and auxiliary gas) on for additional 5 minutes. Stop the LC pump.
8. After 5 minutes, place the system in Standby condition as described in “[Setting the System in Standby Condition](#)” on [page 6-7](#).



Continue with “[Flushing Ion Sweep Cone and Ion Transfer Capillary](#).”

## Flushing Ion Sweep Cone and Ion Transfer Capillary

Clean the ion sweep cone (or spray cone) and the ion transfer capillary on a regular basis to prevent corrosion and to maintain optimum performance of your API source. A good practice is to flush ion sweep cone and ion transfer capillary at the end of each operating day—after you have flushed the sample transfer line, sample tube, and API probe with a 50:50 methanol:water solution from the LC. (See “[Flushing Sample Transfer Line, Sample Tube, and API Probe](#)” on [page 6-15](#).) If you are operating the system with nonvolatile buffers in your solvent system or high concentrations of sample, you might need to clean the ion sweep cone and the ion transfer capillary more often. It is not necessary to vent the system to flush the ion sweep cone and the ion transfer capillary.

### ❖ To clean ion sweep cone and ion transfer capillary

1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source.



**CAUTION**

2. From the Tune software window, click the **On/Standby** button to turn off the mass spectrometer.

**Hot Parts.** The APCI vaporizer typically operates at 350 to 450 °C and the ion transfer capillary typically operates at 250 to 400 °C. This might cause severe burns upon touching. Let the ion source cool down as described in this manual before you touch or remove the vaporizer or the ion transfer capillary.

3. Remove the Ion Max API source from the front of the mass spectrometer, as described in “[Removing the Ion Max API Source Housing](#)” on page 8-17.
4. Use a spray bottle filled with 50:50 solution of methanol/water and a lint-free industrial tissue (Kimwipes™, for example) to clean contaminants from the accessible surfaces of the ion source chamber.

**NOTICE** To prevent contaminating the ion optical elements, do not clean sweep cone or ion transfer capillary with solvent when they are attached to the system. ▲

5. Remove the ion sweep cone (if it is installed):
  - a. Put on a new pair of lint- and powder-free gloves.
  - b. Grasp the outer ridges of the ion sweep cone and pull the cone straight off of the API cone seal. See [Figure 6-1](#). You might need to loosen the set screws on the ion sweep cone in order to remove it.

**NOTICE** This is a good point to remove and clean the ion transfer capillary. See “[Removing, Cleaning, and Reinstalling the Ion Transfer Capillary](#)” on page 8-22. ▲

6. Clean ion transfer capillary and ion sweep cone (if it is installed):
  - a. Place ion sweep cone and ion transfer capillary in a beaker of 50:50 methanol/water.
  - b. Place the beaker in an ultrasonic bath, and sonicate these components for 15 minutes.
  - c. Dry the ion sweep cone.
7. Reinstall the ion sweep cone:
  - a. Carefully align the gas inlet ([Figure 6-2](#)) on the ion sweep cone with the sweep gas supply port ([Figure 6-1](#)) in the API cone seal. Firmly press the ion sweep cone into position.

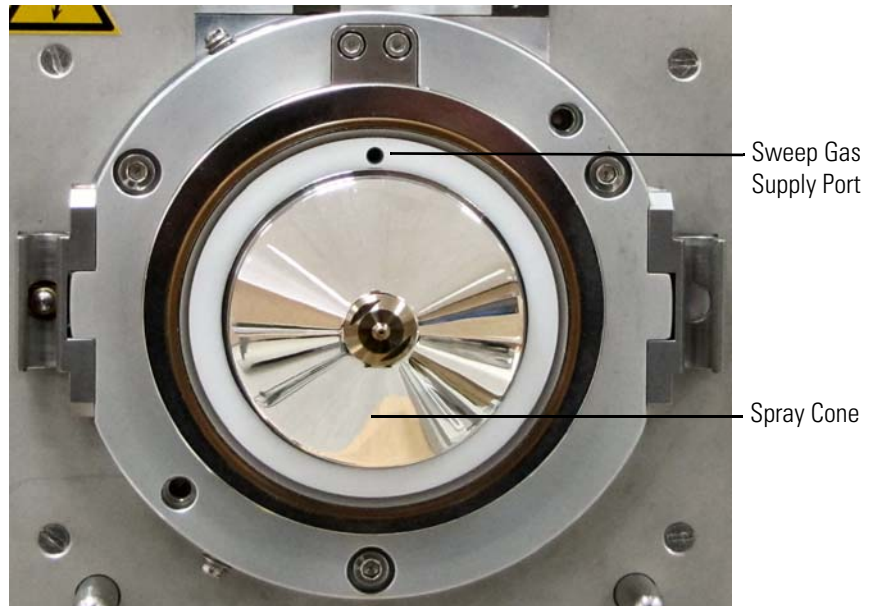


## Operation

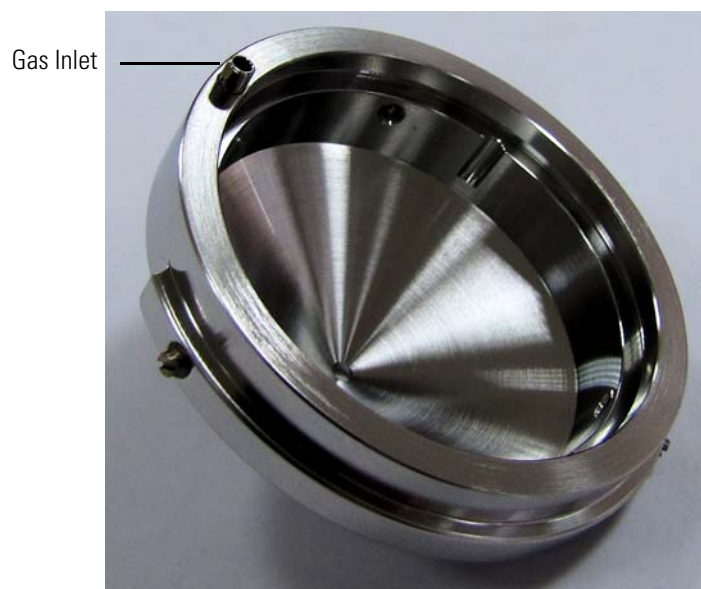
After Operating the System

Note the location of the sweep gas supply port in the API cone seal. The gas inlet on the ion sweep cone is placed in this port. See [Figure 6-1](#) and [Figure 6-2](#).

- b. If necessary, adjust the set screws around the perimeter of the ion sweep cone.



**Figure 6-1.** Sweep gas supply port in the API cone seal



**Figure 6-2.** Ion sweep cone, showing the gas inlet

8. Reinstall the Ion Max API source as described in [“Installing the Ion Max API Source Housing”](#) on [page 8-18](#).

Continue with [“Purging the Oil in the Source Vacuum Pump.”](#)



## Purging the Oil in the Source Vacuum Pump

Purge (decontaminate) the oil in the source vacuum pump on a regular basis to remove water and other dissolved chemicals from the pump oil. Water and other chemicals in the pump can cause corrosion and decrease the lifetime of the pump. A good time to purge the oil is at the end of the working day after you flush API probe, ion sweep cone, and ion transfer capillary.

**NOTICE** Thermo Fisher Scientific recommends that you occasionally purge the oil in the auxiliary forepump of the Q Exactive HF-X MS, too. ▲

### ❖ To purge the oil in the source vacuum pump

1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source.
2. From the Tune software window, click the **On/Standby** button to put the mass spectrometer in Standby. (See image in margin.) Make sure that a septum seals the entrance to the ion transfer capillary.
3. Open the gas ballast valve on the source vacuum pump. Refer to the manual that came with the pump for the location and handling of the gas ballast valve.
4. Let the pump run for 30 minutes with the gas ballast valve open.
5. After 30 minutes, close the gas ballast valve.



Continue with [“Emptying the Solvent Waste Container.”](#)

## Emptying the Solvent Waste Container

### ❖ To empty the solvent waste container

1. Check the solvent level in the solvent waste container on a daily basis.
2. Empty the solvent waste container if necessary. Dispose of the solvent waste in accordance with national and local regulations.

## **Operation**

After Operating the System

## Chapter 7 Troubleshooting

This chapter provides information about identifying and solving common problems with Exactive Series mass spectrometers.

### Contents

- [Safety Guidelines for Troubleshooting](#) on page 7-2
- [Fault Table](#) on page 7-3
- [Main Power Failure](#) on page 7-4
- [Vacuum Leak](#) on page 7-5
- [Failure of UHV Chamber Heating Control](#) on page 7-7
- [Turbomolecular Pump is not Running](#) on page 7-8
- [Failure of Source Heaters / Capillary Heaters](#) on page 7-9

## Safety Guidelines for Troubleshooting

When you perform troubleshooting on the Exactive Series system, pay attention to the following general safety guidelines.

### **WARNING**

**High Voltage.** High voltages capable of creating an electric shock are used in the instrument. Do not remove protective covers from PCBs. Opening the instrument housing is only allowed for maintenance purposes by Thermo Fisher Scientific personnel. To make sure that the instrument is free from all electric current, always disconnect the power cords of *mass spectrometer and source vacuum pump* before you try any type of maintenance.

### **CAUTION**

**Hot Parts.** During operation of the mass spectrometer, ion transfer capillary and sweep cone can reach temperatures up to 450 °C. This might cause severe burns upon touching or ignite combustible material. The external surface of the ion source housing can become hot enough to cause skin burns.

Do not touch the ion source housing when the mass spectrometer is in operation. Let the ion source cool down as described in this manual before you remove the ion source housing. Do not touch the ion source mount immediately after you have removed the ion source housing. Keep combustible materials away from the ion source mount. Do not let the instrument stay unattended when the housing is not mounted to the source.

### **CAUTION**

**Hot Parts.** The forepump in function is hot and some surfaces could reach a temperature higher than 80 °C (176 °F). Touching parts of the forepump might cause burns. Switch off the pump and let it cool down before any intervention. If you need to work on a pump that is “still warm from operation,” then always wear heat protective gloves.



Service by the customer must be performed by trained qualified personnel only and is restricted to servicing mechanical parts. Service on electronic parts must be performed by Thermo Fisher Scientific field service engineers only.

Do not try to repair or replace any component of the system that is not described in this manual without the assistance of your Thermo Fisher Scientific field service engineer.

## Fault Table

If malfunctions on the mass spectrometer occur, you will find possible causes and instructions for repair in [Table 7-1](#).

**Table 7-1.** Troubleshooting

Problem	Possible Causes	Remedy
Tune software shows bad vacuum	System was vented because of a mains failure	<a href="#">page 7-4</a>
	Vacuum leak	<a href="#">page 7-5</a>
Temperature of UHV chamber is higher than expected	UHV chamber heating control has failed	<a href="#">page 7-7</a>
Turbomolecular pump is not running	TMP is switched off because of overheating	<a href="#">page 7-8</a>
Temperature of ion source components is higher than expected	Capillary heating control or ion source heater control has failed	<a href="#">page 7-9</a>

## Main Power Failure

A main power failure has the same consequence as switching off with the main power circuit breaker switch. If the power is available again, the system is started up automatically: the pumps are switched on and the vacuum is created. If the system has been vented during the mains failure, it is necessary to bake out the system to obtain the operating vacuum. See [“Baking Out the System”](#) on [page 8-12](#).

If the log file of the data system shows a reboot of the system and the pressure reading in the Tune software shows a bad vacuum, this indicates that the system was vented. In case of frequent but short power failures we recommend that you install an uninterruptible power supply (UPS). If main power failures occur frequently while the system is not attended (for example, in the night), we recommend that you install a power fail detector.

## Vacuum Leak

For proper performance, the Exactive Series system must operate at acceptable vacuum levels. You can check the current pressure values in the Vacuum / Bakeout window of the Tune software window.

### ❖ To check the vacuum levels

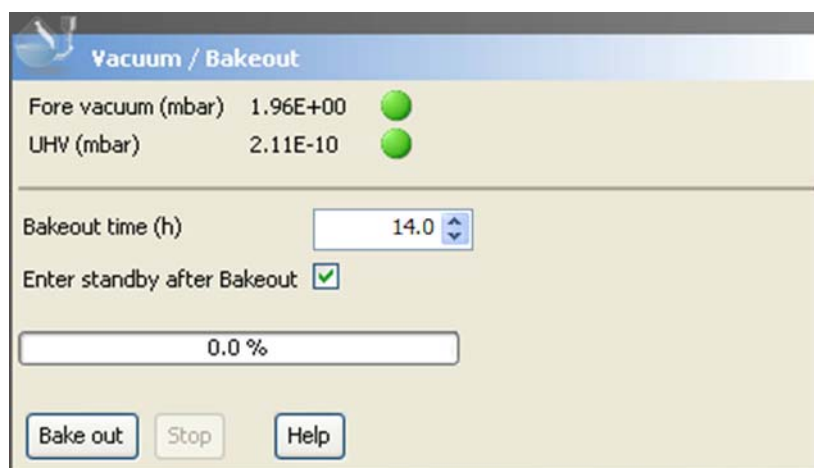
1. To display the Tune software window, choose **Start > Programs > Thermo Exactive Series > Tune**. The Instrument status LED in the toolbar (see image in margin) turns green when the vacuum levels of the instrument are sufficient to operate the Exactive Series system.



2. In the Tasks panel of the Tune software window, click



to display the Vacuum / Bakeout window. See Figure 7-1. Green LEDs indicate that the readback values are sufficient to operate the Exactive Series mass spectrometer.



**Figure 7-1.** Vacuum / Bakeout window

3. Compare the current values of the pressures in the vacuum manifold with the values listed in Table 7-2. If the current values are higher than normal, there might be an air leak.

**Table 7-2.** Typical pressure readings

Gauge type	Name in Tune software	Typical values
Pirani	Forevacuum	about 2 mbar (3.5 mbar) <sup>a</sup> , depends on temperature of heated capillary)
Cold cathode	High Vacuum <sup>b</sup>	about 3E-05 mbar
Cold cathode	Ultra High Vacuum	< 8E-10 mbar

<sup>a</sup> In case of a Q Exactive HF-X MS.

<sup>b</sup> This parameter is visible only when the ion gauge in the high-vacuum chamber is switched on. Refer to the Tune Help for details.

4. If the pressure in the Ultra High Vacuum region is high (above 1E-9 mbar), the instrument needs to be baked out for about

10 hours or more. See [“Baking Out the System”](#) on [page 8-12](#) for instructions on performing a system bakeout.

If the pressure remains high, the system might have an air leak. See below for instructions.

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

Listen for a rush of air or a hissing sound inside the mass spectrometer.

Possible causes of a major leak might be a loose or disconnected fitting, an improperly positioned O-ring, or an open valve. If you suspect an air leak in the forevacuum region, check the vacuum tube for holes. Also check the clamp that fixes the vacuum tube to the forevacuum port (elbow) of the mass spectrometer. See [Figure 3-6](#) on [page 3-14](#). It might be loose because the forepump was shifted or the vacuum tube is twisted.

❖ **To fix an air leak**

1. Shut down the system; see [“Shutting Down the System”](#) on [page 6-8](#).
2. Make a visual inspection of the vacuum system and vacuum lines for leaks.
3. Check each fitting and flange on the system for tightness, and tighten the fittings or flanges that are loose.

Do not tighten fittings indiscriminately. Pay particular attention to fittings that have been changed recently or to fittings that have been subjected to heating and cooling.

4. Make sure that the O-rings and the cover plates of the vacuum manifold are properly positioned.

If you cannot find the location of the leak or tighten the leak yourself, contact your Thermo Fisher Scientific field service engineer.



## Failure of UHV Chamber Heating Control

During general operation of the mass spectrometer, the temperature of the UHV chamber is not regulated. Only during a system bakeout, electric power is supplied to the heating elements of the UHV chamber. The heating always operates at maximum power. Thus, failure of the heating control does not lead to a dangerous overheating of the mass spectrometer.

If the Exactive Series mass spectrometer does not work as expected, use the Tune software for error diagnosis:

- The messages window displays real-time information about the statuses of the instrument, the control service, or other programs. If the heating was terminated, the window displays a corresponding error message.

In case of a failure of the UHV chamber heating control, shut down the mass spectrometer as described on [page 6-8](#). To prevent permanent damage to components of the Exactive Series mass spectrometer, Thermo Fisher Scientific recommends that you call a Thermo Fisher Scientific field service engineer.

## Turbomolecular Pump is not Running

A turbomolecular pump may be switched off because of one of the following reasons:

- Turbomolecular pump is blocked
- Failure of fans in turbomolecular pump

Each of the above reasons might lead to an overheating of the pump. When overheated, a turbomolecular pump switches off automatically to prevent its destruction. This overheating protection prevents the outbreak of a fire and minimizes the risk of destructing the pump.

If the Exactive Series mass spectrometer does not work as expected, use the Tune software for error diagnosis:

- The instrument status window displays real-time status information for the instrument components. All parameters are arranged in a tree view. In addition to showing numerical values of parameters (for example, pump speeds or component temperatures), the instrument status window uses icons to indicate the statuses of system components.
- The messages window displays real-time information about the statuses of the instrument, the control service, or other programs. It might display additional information.

In case of an overheated turbomolecular pump, shut down the mass spectrometer as described on [page 6-8](#). To prevent permanent damage to components of the Exactive Series mass spectrometer, Thermo Fisher Scientific recommends that you call a Thermo Fisher Scientific field service engineer.

## Failure of Source Heaters / Capillary Heaters

A failure of the source heater control or capillary heater control might lead to an overheating of ion source parts. Non-metallic parts of the ion source (gaskets, for example) are made of non-flammable materials, thus preventing any ignition.

If the Exactive Series mass spectrometer does not work as expected, use the Tune software for error diagnosis:

- The API source window (for example, HESI source window) displays the values for capillary temperature and vaporizer temperature.
- The instrument status window displays real-time status information for the instrument components. All parameters are arranged in a tree view. In addition to showing numerical values of parameters (for example, pump speeds or component temperatures), the instrument status window uses icons to indicate the statuses of system components.

A contrast between the temperatures displayed in the Tune software and the observed temperature of hardware components indicates a failure of the heater control.

In case of a failure of the source heater control or capillary heater control, shut down the mass spectrometer as described on [page 6-8](#). To prevent permanent damage to components of the Exactive Series mass spectrometer, Thermo Fisher Scientific recommends that you call a Thermo Fisher Scientific field service engineer.

## **Troubleshooting**

Failure of Source Heaters / Capillary Heaters

## Chapter 8 Maintenance

This chapter describes routine maintenance procedures that must be performed to ensure optimum performance of the Exactive Series mass spectrometer.

### Contents

- [Safety Guidelines for Maintenance on page 8-2](#)
- [General Advice for Maintenance on page 8-4](#)
- [Inspection- and Servicing Plan on page 8-5](#)
- [Maintaining the Vacuum System on page 8-8](#)
- [Maintenance of the Fan Filters on page 8-14](#)
- [API Source Maintenance on page 8-16](#)
- [Maintaining LCs or Autosamplers on page 8-51](#)
- [Consumables on page 8-51](#)
- [Thermo Fisher Scientific Service on page 8-52](#)

## Safety Guidelines for Maintenance

When you perform maintenance on the Exactive Series system, pay attention to the following general safety guidelines.

### ▲ WARNING

**High Voltage.** High voltages capable of causing an electric shock are used in the instrument. Do not remove protective covers from PCBs. Opening the instrument housing is only allowed for maintenance purposes by Thermo Fisher Scientific personnel. To make sure that the instrument is free from all electric current, always disconnect the power cords of *mass spectrometer and source vacuum pump* before you try any type of maintenance.

### ▲ WARNING

**Electromagnetic Radiation.** Parts of the forevacuum pump emit electromagnetic radiation. This radiation can interfere with the operation of cardiac pacemakers and implanted heart defibrillators, possibly causing death or serious injury. If you wear these devices, keep at least 30 cm away from the forevacuum pump.

### ▲ CAUTION

**Hot Parts.** The forepump in function is hot and some surfaces could reach a temperature higher than 80 °C (176 °F). Touching parts of the forepump might cause burns. Switch off the pump and let it cool down before any intervention. If you need to work on a pump that is “still warm from operation,” then always wear heat protective gloves. Take note of the warning labels on the pump.

### ▲ CAUTION

**Hot Parts.** During operation of the mass spectrometer, ion transfer capillary and sweep cone can reach temperatures up to 450 °C. This might cause severe burns upon touching or ignite combustible material. The external surface of the ion source housing can become hot enough to cause skin burns.

Do not touch the ion source housing when the mass spectrometer is in operation. Let the ion source cool down as described in this manual before you remove the ion source housing. Do not touch the ion source mount immediately after you have removed the ion source housing. Keep combustible materials away from the ion source mount. Do not let the instrument stay unattended when the housing is not mounted to the source.

**⚠ CAUTION**

**Hazardous Chemicals.** Samples and solvents might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle solvents or samples. Also contain waste streams and use proper ventilation. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of a particular compound.

**⚠ CAUTION**

**Risk of Eye Injury.** The thin, sharp, flexible capillaries are difficult to see against the light. There is a risk of being stabbed or cut when working with the capillaries. Wear safety glasses to prevent eye injuries!



It is the user's responsibility to maintain the system properly by performing the system maintenance procedures on a regular basis. Service by the customer must be performed by trained qualified personnel only and is restricted to servicing mechanical parts. Service on electronic parts must be performed by Thermo Fisher Scientific field service engineers only.

Do not try to repair or replace any component of the system that is not described in this manual without the assistance of your Thermo Fisher Scientific field service engineer.

Only use fuses of the type and current rating specified. Do not use repaired fuses and do not short-circuit the fuse holder.

## General Advice for Maintenance

When you perform maintenance on the Exactive Series mass spectrometer, observe the following advice:

- Accurate results can be obtained only if the system is in good condition and properly calibrated.
- Preventive maintenance must commence with installation, and must continue during the warranty period to maintain the warranty. Thermo Fisher Scientific offers maintenance and service contracts. Contact your local Thermo Fisher Scientific representative for more information. Routine and infrequent maintenance procedures are listed in [Table 8-1](#).
- The user maintenance procedures described in this manual do not require removing the instrument housing. Thermo Fisher Scientific assumes no responsibility and will not be liable for instrument damage and/or operator injury that might result from using the instrument without the housing attached. Therefore, a Thermo Fisher Scientific field service engineer must be called if removal of the instrument housing is required.
- To successfully carry out the procedures listed in this chapter, observe the following rules:
  - Proceed methodically.
  - Always wear clean, talc-free, and lint-free gloves when you handle the components of the API source, ion optics, mass analyzer, and ion detection system. See “[Personal Protective Equipment](#)” on [page 4-12](#) for a specification for the required gloves.
  - Always place the components on a clean, lint-free surface.
  - Do not overtighten a screw or use excessive force.
  - Dirty tools can contaminate your system. Keep the tools clean and use them exclusively for maintenance and service work at the mass spectrometer.
  - Do not insert a test probe (for example, an oscilloscope probe) into the sockets of female cable connectors on PCBs.



## Inspection- and Servicing Plan

Routine and infrequent maintenance procedures to be performed by the user are listed in [Table 8-1](#).

**Table 8-1.** User maintenance procedures

MS Component	Procedure	Frequency	Procedure Location
Instrument	System bakeout	If necessary (for example, after performing maintenance work on the vacuum system)	<a href="#">page 8-12</a>
	Check warning labels on instrument	Annually	<a href="#">page 8-6</a>
	Leak check gas lines	Annually	<a href="#">page 8-7</a>
	Check condition of tubings and hoses	Annually	<a href="#">page 8-7</a>
Cooling fans	Check fan filters	Every 4 weeks	<a href="#">page 8-14</a>
	Clean fan filters	If necessary	
Forepump	Purge (decontaminate) oil	Daily	<a href="#">page 6-19</a> , see also manufacturer's documentation
	Check oil level	Daily	<a href="#">page 8-8</a> , see also manufacturer's documentation
	Check oil condition	Depends on process	
	Add oil	If oil level is low	
	Check gas ballast valve	Monthly	
	Change oil	Every 8000 h (-one year) of operation	
	Replace exhaust filter	If oil mist appears at exhaust or annually	
	Check anti-suckback valve	Annually	
	Clean fan guard	Annually	
API source	Flush (clean) sample transfer line, sample tube, and API probe	Daily	<a href="#">page 6-15</a>
	Remove and clean ion transfer capillary	Weekly, or if ion transfer capillary bore is contaminated or obstructed	<a href="#">page 8-22</a>
	Replace ion transfer capillary	If ion transfer capillary bore is corroded	<a href="#">page 8-22</a>
	Clean exit lens and S-lens (ion funnel) <sup>a</sup>	As needed <sup>b</sup>	<a href="#">page 8-45</a>

**Table 8-1.** User maintenance procedures, continued

MS Component	Procedure	Frequency	Procedure Location
HESI-II probe	Replace needle insert	If metal needle is blocked	page 8-40
APCI, ESI, or H-ESI probe	Replace fused-silica sample tube	If sample tube is broken or obstructed	<i>Ion Max and Ion Max-S API Source Hardware Manual</i> or <i>HESI-II Probe User Guide</i>
ESI or H-ESI probe	Trim fused-silica sample tube	If polyimide coating on the end of the sample tube has elongated	<i>HESI-II Probe User Guide</i>

<sup>a</sup> In case of a Q Exactive HF-X MS

<sup>b</sup> The frequency of cleaning the components of the mass spectrometer depends on the types and amounts of samples and solvents that are introduced into the instrument.

## Cleaning the Surface of the Instrument

Clean the outside of the instrument with a dry cloth. For removing stains or fingerprints on the surface of the instrument (panels, for example), slightly dampen the cloth (preferably made of microfiber) with distilled water.

**NOTICE** Prevent any liquids from entering the inside of the instrument. Leaking liquids might get into contact with electronic components and cause a short circuit. ▲

## Checking Warning Labels

Safety warnings on mass spectrometer and other devices of the LC/MS system must always be complete, clearly visible and legible.

In addition to the safety instructions that can be found throughout this manual, various warning labels on the instrument inform the user about possible hazards (for example, caused by hot surfaces or high voltage). See “[Safety Symbols on the Instrument](#)” on [page 4-3](#) for an overview. To protect all personnel coming near the instrument, annually make sure that all warning labels on the instrument are still present. If warning labels are missing or unreadable, contact a Thermo Fisher Scientific field service engineer for replacements. Also check the warning labels on forepump and other devices of the LC/MS system.

## Leak-Checking Gas Lines

Regularly leak check each gas line from the gas supply in the laboratory to the instrument.

### ❖ To perform a leak check for a gas line

1. After you have closed all valves in the instrument, monitor the manometer of the gas regulator for some minutes.
2. If the pressure falls significantly (for example, the nitrogen pressure falls by more than 10 psi / 690 mbar in two minutes), then you should search for leaks in the gas line.
3. Search for leaks in the gas line (for example, with a conventional thermal conductivity-based leak detector, such as is widely used to check leaks in gas chromatography equipment).
4. If you detect a leak (which is usually at a connection), then verify the tightness of the connection. In case of doubt, replace it.
5. When you cannot find a leak in the gas line, we recommend that you call a Thermo Fisher Scientific field service engineer to check for gas leaks in the instrument.

## Checking Condition of Tubings and Hoses

Regularly inspect all tubings and hoses that are connected to the mass spectrometer for damage.

### ❖ To check the condition of tubings and hoses

1. Make sure that the gas lines are securely connected, free from kinks, and not trapped.
2. Make sure that the liquid must be able to run freely down the drain tube, which must not contain kinks or liquid traps.
3. Visually inspect all tubing for leaks or signs of deterioration.
4. Visually inspect the surfaces below all liquid lines for signs of liquid.

If you detect a leak or other damage to any tubing or hose, then you must replace it.

## Maintaining the Vacuum System

This section describes user maintenance procedures for the vacuum pumps and the vacuum manifold of the Exactive Series mass spectrometer.

### Pumps Maintenance

This section only outlines the user maintenance procedures for the forepump and the turbomolecular pumps (TMPs) of the mass spectrometer. The manuals of the pump manufacturers give detailed advice regarding safety, operation, maintenance, and installation. Note the warnings and precautions contained in these manuals!

#### Maintenance of the Forepumps

The forepumps require several maintenance procedures to be performed by the user. To simplify the maintenance work, the pump manufacturers recommend that you combine several jobs. For maintenance instructions, refer to the manual that came with the forepump.

Table 8-2 outlines the maintenance schedule for the SOGEVAC™ SV 65 BI forepump as recommended by the pump manufacturer.

**Table 8-2.** Maintenance schedule of the SOGEVAC™ SV 65 BI forepump

Activity	Frequency
Check oil level	Daily
Check oil condition	Depends on process
Check gas ballast valve	Monthly
Change oil	Every 8000 h (~ one year) of operation
Replace exhaust filter	If oil mist appears at exhaust or annually
Check anti-suckback valve	Annually
Clean fan cover	Annually

Table 8-3 outlines the maintenance schedule for the Agilent MS120 forepump as recommended by the pump manufacturer.

**Table 8-3.** Maintenance schedule of the Agilent MS120 forepump

Activity	Frequency
Check oil level before starting.	24 h / daily
Clean with soft cloth surfaces of the pump. If necessary, use a neutral detergent.	100 h / every week
Change the lubricating oil.	7000 h <sup>a</sup> / every year
Replace the exhaust filter.	
Check the electrical connections.	14000 h / every 2 years
Check and, if necessary, replace the coupling elastic insert.	

<sup>a</sup> The first oil change has to be done after 1000 hours of operation. If any polluting substances are found in the oil, the next oil change could take place within 7000 hours.

Table 8-4 outlines the maintenance schedule for the Pfeiffer DUO 11 forepump as recommended by the pump manufacturer.

**Table 8-4.** Maintenance schedule of the Pfeiffer DUO 11 forepump

Activity	Frequency
Check operating fluid level	daily
Visual inspection (leak-tightness/oil leaks)	daily
Check filter insert of external oil mist filter (if existent)	daily
Change filter insert of external oil mist filter (if existent)	as required; at least every 2 years
Change operating fluid	as required; at least every 2 years
Cleaning the pump and renew the seals	as required; at least every 2 years
Clean gas ballast valve and silencer nozzle	as required; at least every 2 years
Clean the motor fan cap	as required; at least every 2 years

**⚠ CAUTION**

**Hot Parts.** The forepump in function is hot and some surfaces could reach a temperature higher than 80 °C (176 °F). Touching parts of the forepump might cause burns. Switch off the pump and let it cool down before any intervention. If you need to work on a pump that is “still warm from operation,” then always wear heat protective gloves. Take note of the warning labels on the pump.

**⚠ CAUTION**

**Hot Liquid.** Touching hot forepump oil might cause burns. Always wear protective gloves and protective goggles when you handle the forepump oil.

**⚠ CAUTION**

**Hazardous Chemicals.** The forepump oil might cause skin or eye irritation and it might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle the forepump oil.



When you dispose used oil, observe the relevant environmental regulations! For instructions about proper handling, refer to the Material Safety Data Sheet (MSDS) for the forepump oil.

Forepump oil and exhaust filters are available from Thermo Fisher Scientific (see Chapter 9, “Replaceable Parts”). If you wish to order other spare parts, contact the pump manufacturer.

## Moving the SOGEVAC Forepump

For easy and effortless transportation of the SOGEVAC 65 BI forevacuum pump, Thermo Fisher Scientific provides a mobile base (drip pan with casters) with the Exactive Series mass spectrometer.

### CAUTION

**Heavy Objects.** Mass spectrometer and forepump might move uncontrollably and cause injuries. Wear steel-reinforced safety shoes and gloves during installation or maintenance.

If lifting of the pump becomes necessary, only a suitable lifting device shall be used to lift the pump at the lifting lug due to the forevacuum pump's weight of about 62 kg.



**A lifting device is the only officially recommended way of handling the pump!**

Should people lift the pump, at least two persons should lift it. Pay attention to the persons' positions when lifting! Straight back, flexed knees, and adapted large back belts, etc. are recommended.

When you move the pump, pay attention to the following guidelines:

- 1 person stands on the left side, one hand under the oil casing and one hand under the pump stator.
- 1 person stands on the right side, one hand under the oil casing and one hand under the motor fan cover.
- Pay attention to your hands when you set down the pump into the drip pan to avoid squashing them!

**NOTICE** Do not lift or pull the pump at the frequency converter or the cables! ▲

## Moving the Forepumps of the Q Exactive HF-X MS

For advice on moving the source vacuum pump (Agilent MS 120) and the auxiliary forepump (Pfeiffer DUO 11) of the Q Exactive HF-X MS, refer to the manuals that are provided by the pump manufacturers.

## **Maintenance of the Turbomolecular Pumps**

This topic outlines the maintenance work for the TMPs. These procedures require removing the housing of the instrument and partially disassembling it. Therefore, a Thermo Fisher Scientific field service engineer must be called if servicing is required. See also [page 8-53](#).

### **Maintenance of the Source TMP**

The pump manufacturer (Pfeiffer Vacuum) recommends that you change the operating fluid reservoir every three years at the latest. Depending on the operating conditions, changing in two-year intervals might be necessary. Changing of the TMP bearing is recommended every four years, at least.

### **Maintenance of the Analyzer TMP**

The pump manufacturer (Oerlikon Leybold Vacuum) recommends that you exchange the standard bearing every 45 000 operating hours at the latest, and that you exchange the rotor assembly every 80 000 operating hours.

## Baking Out the System

The system bakeout of the mass spectrometer removes unwanted gases or molecules (collected or remaining) from the high-vacuum region of the instrument. Ions can collide with those gases or molecules resulting in lower overall sensitivity. Therefore, Thermo Fisher Scientific recommends that you bake out the instrument if the high vacuum decreases noticeable during routine operation.

Bakeout is mandatory after the system has been vented for maintenance or service work in the analyzer region. You should bake out an instrument that has been vented for at least twelve hours (12 hours) before you can start using it again.

If the system has been vented during a power failure, then it is necessary to bake out the system to attain the operating vacuum. See “Starting Up the System after a Shutdown” on page 6-10.

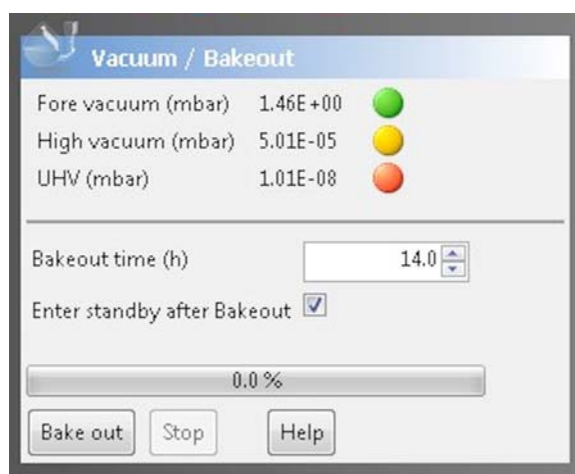
**NOTICE** Before you start the bakeout, make sure that the pumps are up and running at their operating speed. If you have just switched on the mass spectrometer, this will take about 10 minutes. See “Starting Up the Instrument” on page 6-10. To check the pump speed, open the Instrument Status window of the Tune software and expand the Vacuum System node of the Instrument tree. ▲

### ❖ To perform a system bakeout



1. In the Tune software window, click the **On/Standby** button to put the instrument in Off condition. (See image in margin.)
2. In the Tasks panel of the Tune software window, click

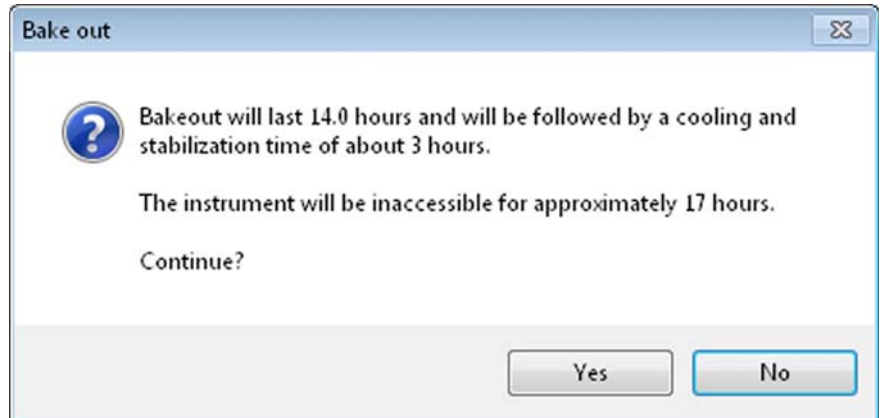
 to display the Vacuum / Bakeout window. See Figure 8-1.



**Figure 8-1.** Vacuum / Bakeout window

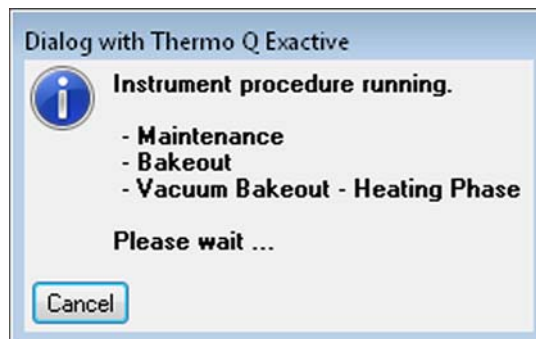


3. Enter the desired baking duration (in hours) into the spin box. The available range is 4 to 30 hours.
4. Click **Bake out**. A dialog box shows the duration of the baking procedure. See [Figure 8-2](#). Click **Yes** to confirm the message.



**Figure 8-2.** Bakeout dialog box

5. The dialog box disappears and the baking procedure starts. The instrument indicates the active bakeout procedure by a flashing Vacuum LED. (See [Figure 3-3](#) on [page 3-10](#).) Additionally, the Tune software displays a corresponding message box. See [Figure 8-3](#).



**Figure 8-3.** Message box: Vacuum Bakeout active

6. The baking of the instrument stops after the preset duration. The Vacuum LED keeps flashing until the cooling and stabilization time (of about 3 hours) is finished.

Click **Stop** in the Vacuum / Bakeout window to abort the baking routine before the preset time.

**CAUTION**

**Hot Parts.** If you abort a system bakeout, parts of the instrument can be hot. Touching hot parts of the instrument immediately after a bakeout might cause burns. Let the instrument cool for at least three hours before you start operating it again.

## Maintenance of the Fan Filters

Each of the two ventilation slots at the rear side of the mass spectrometer is equipped with a fan filter. See [Figure 8-4](#).



**Figure 8-4.** Ventilation slots at the rear side of the instrument

**NOTICE** Do not block the ventilation slots at the rear of the mass spectrometer. Items might fall behind the instrument, inhibit airflow, and cause the system to overheat. Depending on the circumstances, either the Tune software will switch off the instrument and display an error message or the turbomolecular pump control will shut down the instrument and vent it. ▲

### Checking the Fan Filters

Check the fan filters every four weeks.

#### ❖ To check the fan filters

1. Each fan filter bracket is mounted on hinges. Insert a finger into the recess in the instrument frame and pull at the fan filter bracket to open it. See [Figure 8-4](#) and [Figure 8-5](#).
2. Remove each fan filter from the rear of the mass spectrometer by pulling it out of the filter bracket. See [Figure 8-5](#).



**Figure 8-5.** Removing fan filters from the filter bracket

If the fan filters are covered with dust, proceed as described in [“Cleaning the Fan Filters”](#) below. Replacements for the fan filters are available from Thermo Fisher Scientific (see [Chapter 9, “Replaceable Parts”](#)).

## **Cleaning the Fan Filters**

### **❖ To clean the fan filters**

1. Remove the fan filters as described in [“Checking the Fan Filters”](#) above.
2. Wash the fan filters in a solution of soap and water.
3. Rinse the fan filters with tap water.
4. Squeeze the water from the fan filters and let them air dry.
5. Reinstall the fan filters in the fan filter brackets.

## API Source Maintenance

Various routine maintenance procedures must be performed to ensure optimum performance of the Atmospheric Pressure Ionization (API) source. Most of the procedures involve cleaning. This section also describes procedures for replacing the ion transfer capillary.

Refer also to the *Ion Max and Ion Max-S API Source Hardware Manual* and the *HESI-II Probe User Guide* for information about maintenance procedures for the API source.

### Frequency of Cleaning

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

- Sample transfer line, sample tube, and API probe should be cleaned at the end of each operating day to remove any residual salts from buffered mobile phases or other contamination that might have accumulated during normal operation. See [“Flushing Sample Transfer Line, Sample Tube, and API Probe”](#) on page 6-15.
- Ion transfer capillary and ion sweep cone of the API source need to be removed and cleaned periodically. See [“Removing, Cleaning, and Reinstalling the Ion Transfer Capillary”](#) on page 8-22.
- Exit lens and S-lens or ion funnel become dirty at a slower rate than the API probe, ion sweep cone, and ion transfer capillary. See [“Removing, Cleaning, and Reinstalling the Exit Lens and the S-Lens”](#) on page 8-45 or [“Removing, Cleaning, and Reinstalling the Exit Lens and the Ion Funnel”](#) on page 8-48.

**NOTICE** Generally, you must not open the vacuum manifold. Cleaning of the components therein is rarely (if ever) required. If you believe that cleaning of these components is required, you should contact Thermo Fisher Scientific and schedule a visit by a Thermo Fisher Scientific field service engineer. ▲

### Removing and Reinstalling the Ion Max API Source Housing

You need to remove the Ion Max API source housing before you perform maintenance on the ion optics and the ion source interface.

This section contains the following topics:

- [Removing the Ion Max API Source Housing](#)

- [Installing the Ion Max API Source Housing](#)
- [Connecting the Source Housing Drain to the Waste Container](#)

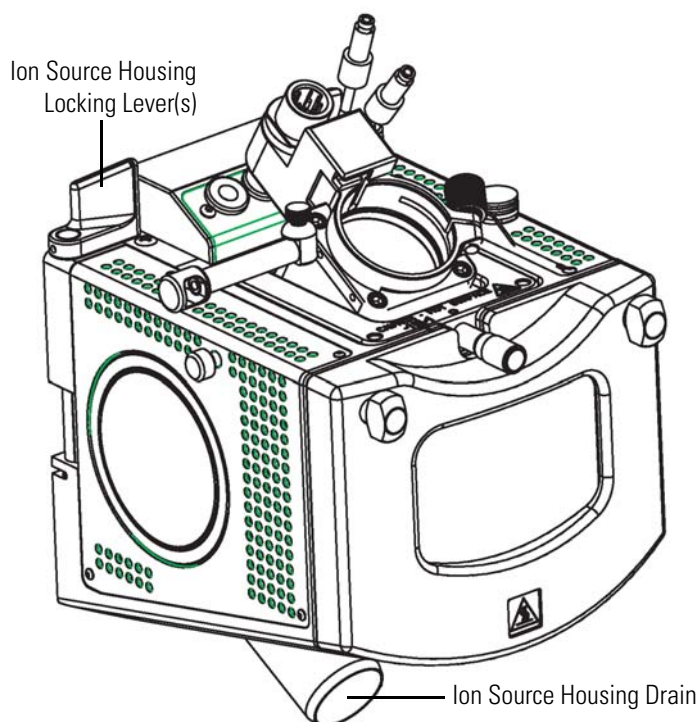
## Removing the Ion Max API Source Housing

You need to remove the Ion Max API source housing to access the ion sweep cone.

### **⚠ CAUTION**

**Hot Parts.** During operation of the mass spectrometer, ion transfer capillary and sweep cone can reach temperatures up to 450 °C. This might cause severe burns upon touching or ignite combustible material. The external surface of the ion source housing can become hot enough to cause skin burns.

Do not touch the ion source housing when the mass spectrometer is in operation. Let the ion source cool down as described in this manual before you remove the ion source housing. Do not touch the ion source mount immediately after you have removed the ion source housing. Keep combustible materials away from the ion source mount. Do not let the instrument stay unattended when the housing is not mounted to the source.



**Figure 8-6.** Ion Max API source housing, showing detail of components

❖ **To remove the ion source housing**

1. If the mass spectrometer was recently in operation, let the ion source housing cool down before you touch its external metal surface.

Set the capillary temperature to 65 °C or place the electronics service switch in the Service Mode position. Wait until the ion source has cooled down (approximately 30 minutes) before you begin working on it.

2. If a probe is connected to the source housing, disconnect the external liquid lines before you remove the source housing from the mass spectrometer.
3. Remove the drain tube from the ion source housing drain. See [Figure 8-6](#).
4. Rotate the ion source housing locking levers 90 degrees to release the ion source housing from the ion source mount assembly.
5. Remove the ion source housing by pulling it straight off the ion source mount assembly, and place the housing in a safe location for temporary storage.

**NOTICE** When the source housing is removed, the Tune software displays a message box to indicate that the ion source is open. When the source is open for more than 60 minutes, the system automatically switches into Off mode. ▲

## Installing the Ion Max API Source Housing

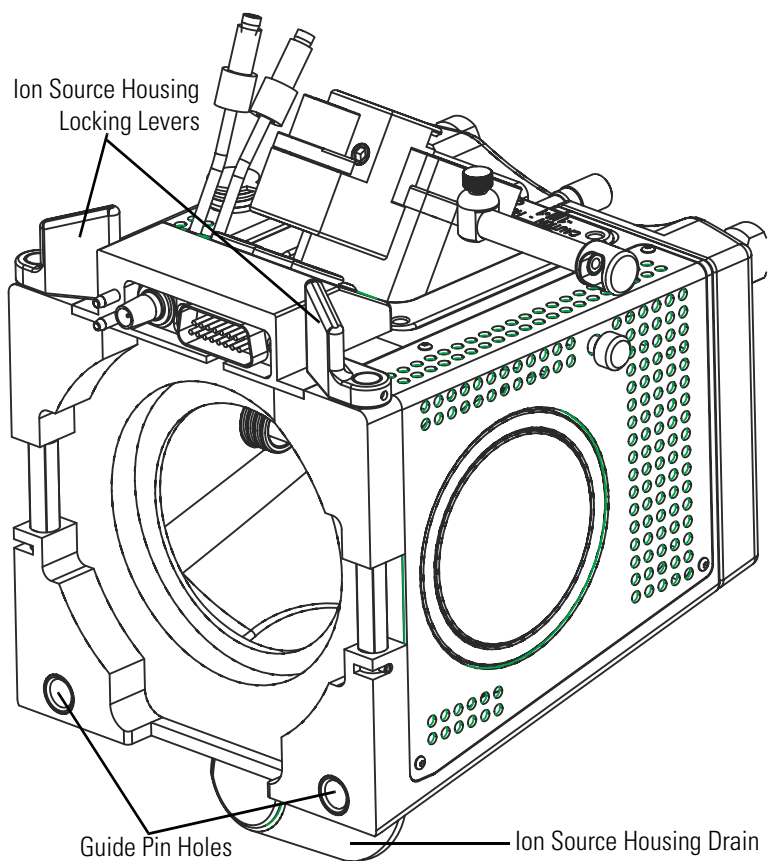
❖ **To reinstall the Ion Max API source housing**

1. Carefully align the two guide pin holes on the rear of the ion source housing with the ion source housing guide pins on the mass spectrometer. Carefully press the ion source housing onto the ion source mount. See [Figure 8-7](#) and [Figure 8-8](#).
2. Rotate the ion source housing locking levers 90 degrees to lock the ion source housing onto the ion source mount assembly.

**NOTICE** Prevent solvent waste from backing up into the ion source and mass spectrometer. Always make sure that liquid in the drain tube is able to drain to a waste container. ▲

3. Reinstall the ion source housing drain tube. See [“Connecting the Source Housing Drain to the Waste Container”](#) below for advice.

The Ion Max API source is now properly installed on the mass spectrometer.



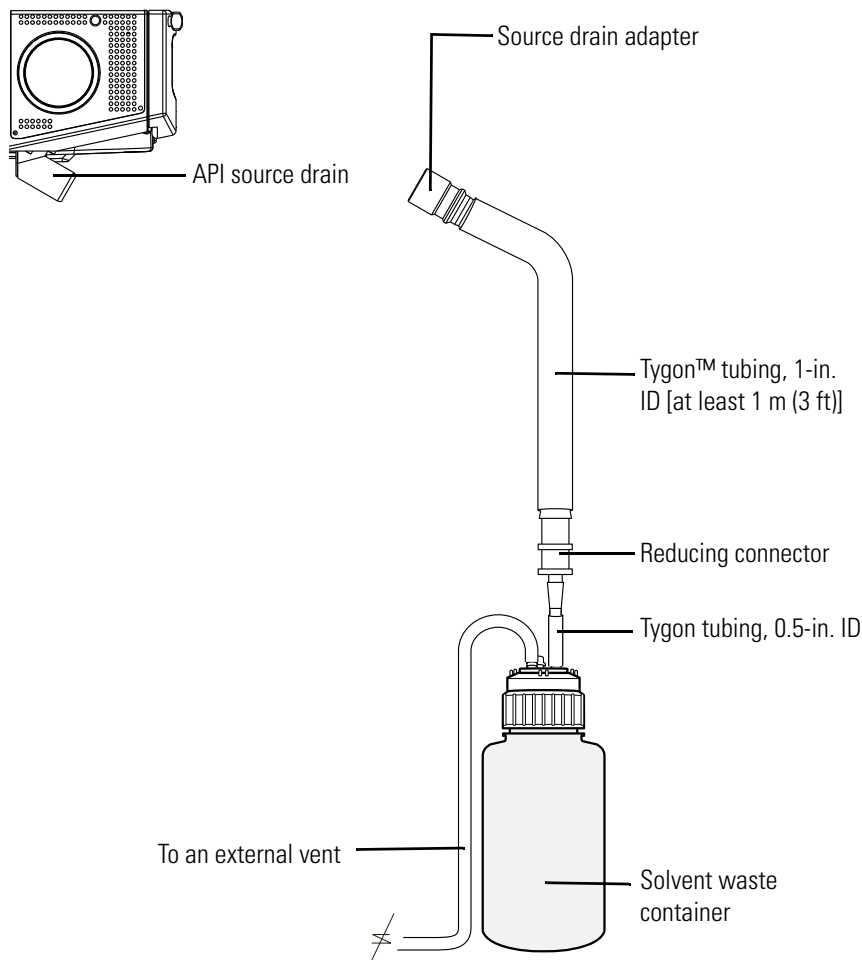
**Figure 8-7.** Rear view of the Ion Max API source housing



**Figure 8-8.** Ion source mount showing ion source housing guide pins

## Connecting the Source Housing Drain to the Waste Container

When you reinstall the Ion Max API source, reconnect the drain at the bottom of the source housing to the solvent waste container (see [Figure 8-9](#)).



**Figure 8-9.** View of the Ion Max API source and the drainage system

When you reconnect the drain tubing to the drain at the bottom of the Ion Max API source, make sure that you connect the Teflon™ source drain adapter to the source drain. It can withstand the high temperatures that are produced by the H-ESI probe or the APCI probe. In addition, make sure that the tubing assembly includes at least 1 m (3 ft) of 1 inch ID Tygon tubing.

**NOTICE** Make sure to comply with the following requirements:

- Do not connect Tygon™ tubing directly to the source drain. At high temperatures, Tygon releases volatile contaminants.
- Do not connect silicone tubing to the API source outlet drain. If silicone tubing is connected to the outlet drain, you might observe background ions at  $m/z$  536, 610, and 684. Use the silicone tubing that is provided with the filling/venting cap to connect the waste container to a fume exhaust system.



- Prevent solvent waste from backing up into the API source and mass spectrometer. Always make sure that the drain tubing is above the level of liquid in the waste container.
- To prevent the laboratory from being accidentally contaminated by solvent waste, protect the waste container against overturning.
- Your laboratory must have at least two fume exhaust systems:
  - The analyzer optics can become contaminated if the API source drain tube and the exhaust tubing from the forepump are connected to the same fume exhaust system. Route the exhaust tubing from the forepump to a dedicated fume exhaust system.
  - Do not vent the drain tube (or any vent tubing connected to the waste container) to the same fume exhaust system that you have connected the forepump to. Vent the waste container to a dedicated fume exhaust system. ▲

Table 8-5 lists the components of the solvent waste system. They are contained in the Exactive Series Installation Kit. During the initial installation of the mass spectrometer, a Thermo Fisher Scientific field service engineer installs the solvent waste system.

**Table 8-5.** Solvent waste system parts

Part description	Part number
DRAIN, ION MAX 2, LTQ	97055-20488
Source drain adapter, Teflon™	70111-20971
Reducing connector, single barbed fitting, 1-in. × 0.5-in.	00101-03-00001
Tube, 1-in. ID × 1.3/8-in. OD, Tygon™ 2001	00301-01-00020
Tubing, Tygon, 0.5-in. ID × 0.75-in. OD	00301-22920
Cap, filling/venting	00301-57022
Heavy-duty, 4 L Nalgene™ bottle	00301-57020

## API Source Housing Maintenance

The API source housing is designed to be serviced by Thermo Fisher Scientific field service engineers. User maintenance is limited to cleaning the ion source housing as necessary.

### ▲ CAUTION

**Hazardous Substance.** Methanol is highly flammable and noxious. Keep away from heat, sparks, and flame. Avoid accidental exposure. Use with adequate ventilation. When possible, dilute it with 50% water. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of methanol.

Follow all safety precautions in the sections regarding the installation and removal of the housing. For any additional service that might be required, contact your local Thermo Fisher Scientific field service engineer.

❖ **To clean the API source housing**

1. After the API source cools to room temperature, remove it from the mass spectrometer.
2. Put on appropriate eye-wear and gloves.
3. Under an appropriate fume hood, rinse the interior of the housing with UHPLC/MS-grade methanol.
4. Allow the housing to dry before you install it on the mass spectrometer.

## Removing, Cleaning, and Reinstalling the Ion Transfer Capillary

The bore of the ion transfer capillary can become blocked by buffer salts or high concentrations of sample. The ion transfer capillary can be removed for cleaning. You do not have to vent the system to remove the ion transfer capillary.

If the pressure in the source region (as measured by the Pirani gauge) drops considerably below 1 mbar (2.5 mbar in case of a Q Exactive HF-X MS), you should suspect a blocked ion transfer capillary. You can check the Pirani gauge pressure in the Tune software (Vacuum / Bakeout window > Fore vacuum).

### **WARNING**

**High Voltage.** High voltages capable of causing an electric shock are used in the instrument. Make sure that the electronics service switch is in the Service Mode position before you proceed.

### **CAUTION**

**Hot Parts.** During operation of the mass spectrometer, ion transfer capillary and sweep cone might reach temperatures up to 450 °C. This might cause severe burns upon touching or ignite combustible material. The external surface of the ion source housing can become hot enough to cause skin burns.

Do not touch the ion source housing when the mass spectrometer is in operation. Let the ion source cool down as described in this manual before you remove the ion source housing. Do not touch the ion source mount immediately after you have removed the ion source housing. Keep combustible materials away from the ion source mount. Do not let the instrument stay unattended when the housing is not mounted to the source.

**▲ CAUTION**

**Hazardous Substance.** Methanol is highly flammable and noxious. Keep away from heat, sparks, and flame. Avoid accidental exposure. Use with adequate ventilation. When possible, dilute it with 50% water. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of methanol.

**Maintenance of the Ion Transfer Capillary in Instruments with an S-Lens**

Table 8-6 lists the parts that are required when you perform maintenance of the ion transfer capillary. They are contained in the Installation Kit.

**Table 8-6.** Parts for maintenance of the ion transfer capillary

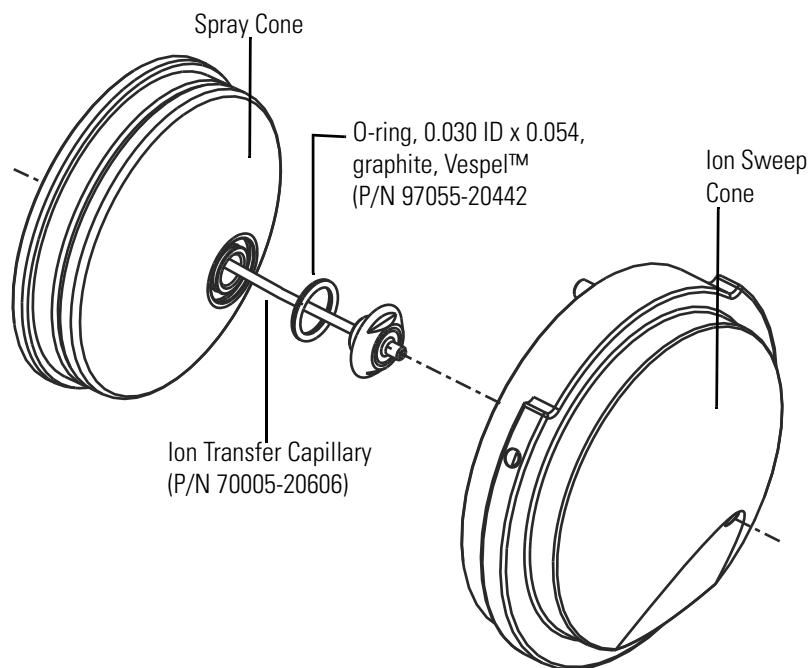
Part description	Part number
Ion transfer capillary	70005-20606
Tool, Capillary Removal, Quantum	70111-20258
O-ring, 0.030 ID x 0.054, graphite, Vespel™	97055-20442

**❖ To remove and clean the ion transfer capillary**

1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source.
2. Place the electronics service switch (located on the left side of the mass spectrometer) in the Service Mode position to remove power to all components of the mass spectrometer with the exception of the vacuum system. Wait for at least 60 minutes to let hot components cool down.
3. Remove the Ion Max API source housing from the front of the mass spectrometer as described in [“Removing the Ion Max API Source Housing”](#) on page 8-17.
4. Remove the ion sweep cone by grasping its outer ridges and pulling the cone straight off of the API cone seal.

**NOTICE** You might need to loosen the set screws on the ion sweep cone to remove it. ▲

5. Remove the ion transfer capillary by turning it counterclockwise with the custom removal tool until you can pull it free from the ion source interface. See [Figure 8-10](#).



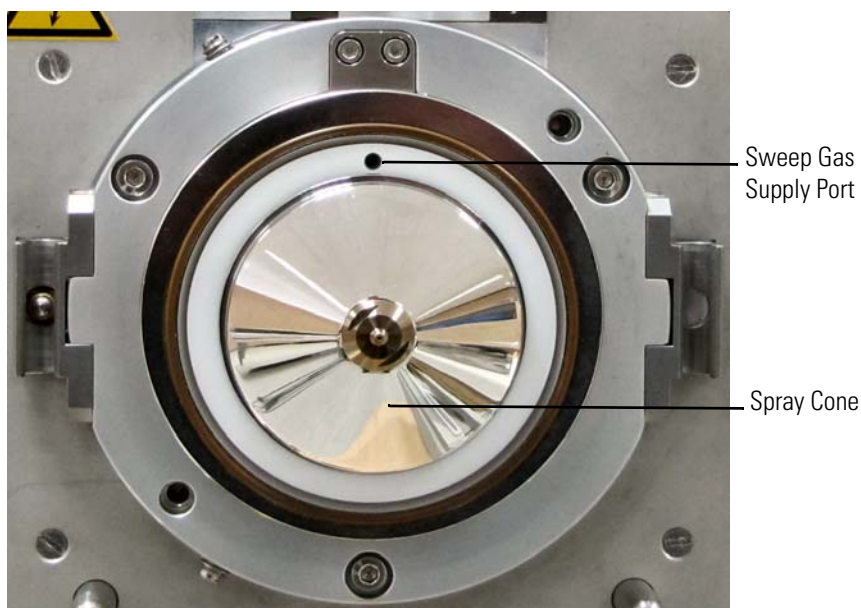
**Figure 8-10.** Spray cone, O-ring, ion transfer capillary, and ion sweep cone of the ion source interface with S-lens

6. Soak the ion transfer capillary in a dilute solution of nitric acid to remove contaminants.
7. Sonicate the ion transfer capillary in distilled water.
8. Clean the ion sweep cone by wiping the inside and outside with a lint-free tissue soaked in methanol.
9. Remove and inspect the O-ring that is seated in the spray cone under the entrance end of the ion transfer capillary. Clean it with methanol or replace it if necessary.
10. Reinsert the O-ring in the spray cone.

**NOTICE** Use caution when you reinstall the ion transfer capillary:

- Make sure that everything is properly aligned to prevent stripping the thread on the ion transfer capillary.
- Be careful not to bend the ion transfer capillary. Rotate the capillary while you insert it.
- To prevent mechanical damage to the transfer capillary, make sure that the capillary temperature is well below 200 °C. Let the spray cone cool down for at least 60 minutes to allow safe handling by laboratory personnel. See the warnings at the beginning of this topic. ▲

11. Insert the ion transfer capillary into the heater block. Rotate the capillary while you insert it. After it is inserted, turn the capillary clockwise until it is finger tight.



**Figure 8-11.** Ion source interface, showing the sweep gas supply port in the API cone seal



**Figure 8-12.** Ion sweep cone, showing the gas inlet

12. Align the gas inlet on the ion sweep cone with the sweep gas supply port on the ion source mount. Firmly press the ion sweep cone into ion source mount. See [Figure 8-11](#) and [Figure 8-12](#).

13. Reinstall the Ion Max API source housing on the mass spectrometer as described in “[Installing the Ion Max API Source Housing](#)” on page 8-18.
14. Place the electronics service switch in the Operating Mode position to supply power to all components of the mass spectrometer.

If you have unblocked the ion transfer capillary, then the Pirani gauge pressure should increase to a normal value (approximately 2 mbar). If you cannot clear the ion transfer capillary by this method, then replace it.

## Maintenance of the Ion Transfer Tube in Instruments with an Ion Funnel

Table 8-6 lists the parts that are required when you perform maintenance of the ion transfer tube. They are contained in the Installation Kit.

**Table 8-7.** Parts for maintenance of the ion transfer capillary

Part description	Part number
Tube, I.T, 1/4 turn, 2.5 dia, (0.6x1.6)	80500-20045
Tool, Transfer Tube Release	70005-20972
Seal, ITT 1/4 turn	70005-20922

### ▲ CAUTION

**Hot Surface.** To prevent mechanical damage to the ion transfer tube, make sure that the tube temperature is well below 200 °C before you touch it.

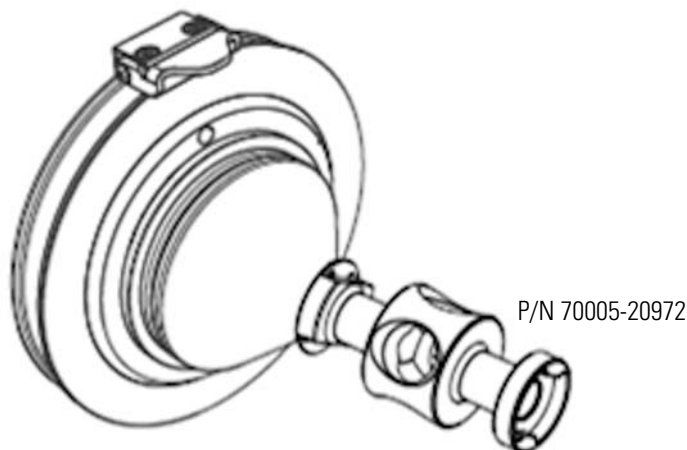
#### ❖ To remove and clean the ion transfer tube

1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source.
2. Place the electronics service switch (located on the left side of the mass spectrometer) in the Service Mode position to remove power to all components of the mass spectrometer with the exception of the vacuum system. Wait for at least 60 minutes to let hot components cool down.
3. Remove the Ion Max API source housing from the front of the mass spectrometer as described in “[Removing the Ion Max API Source Housing](#)” on page 8-17.
4. Remove the ion sweep cone by grasping its outer ridges and pulling the cone straight off of the API cone seal.

**NOTICE** You might need to loosen the set screws on the ion sweep cone to remove it. ▲

5. Rotate the ion transfer tube with the tool (see [Figure 8-13](#)) 1/4-turn counterclockwise. Then slowly pull the tube out of the API source interface.

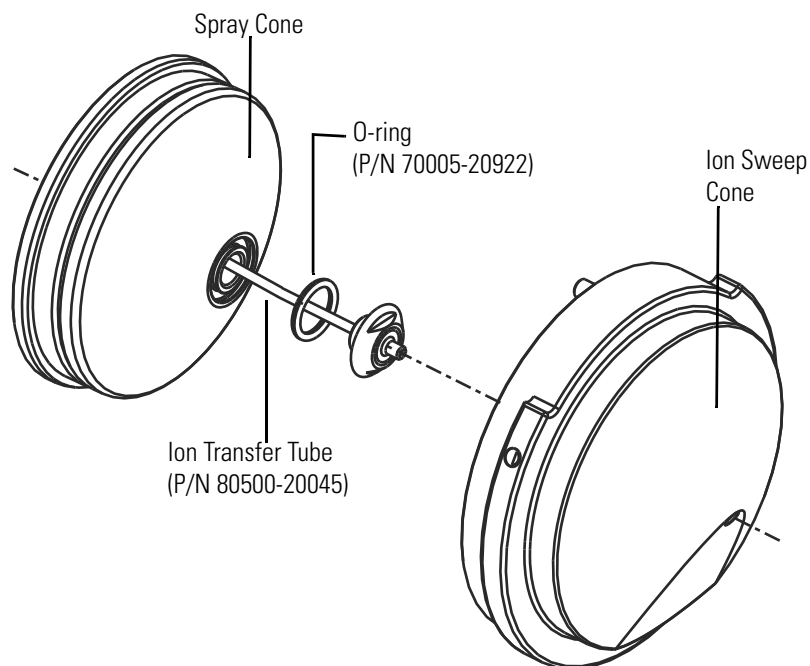
If necessary, insert a hex key through a side hole for leverage.



**Figure 8-13.** Ion transfer tube removal tool

6. Clean the ion transfer tube. If the ion transfer tube is extremely contaminated, then begin the cleaning with [step 6a](#) that uses Liquinox™. If the ion transfer tube is normally contaminated, then begin with [step 6e](#).
  - a. Sonicate the ion transfer tube overnight in water with 10% Liquinox.
  - b. Rinse the ion transfer tube with water forcing a strong stream of water through the orifice for 2 minutes.
  - c. Sonicate the ion transfer tube for 30 minutes in 100% water.
  - d. Clean the ion transfer tube as described in and following.
  - e. Sonicate the ion transfer tube for 30 minutes in a 50:50 solution of methanol/water containing 20% formic acid.
  - f. Rinse the ion transfer tube thoroughly with water.
  - g. Sonicate the ion transfer tube in deionized water for 15 minutes.
  - h. Rinse the ion transfer tube with methanol.
  - i. Sonicate the ion transfer tube in methanol for 15 minutes.
  - j. Blow the ion transfer tube with a stream of nitrogen gas until it is dry.
7. Clean the ion sweep cone by wiping the inside and outside with a lint-free tissue soaked in methanol.

8. Remove and inspect the O-ring that is seated in the spray cone under the entrance end of the ion transfer tube. Clean it with methanol or replace it if it is necessary.



**Figure 8-14.** Spray cone, O-ring, ion transfer tube, and ion sweep cone of the ion source interface with ion funnel (figure similar)

9. Reinsert the O-ring in the spray cone.
10. The bore of the ion transfer tube has a rectangular cross section. Insert the ion transfer tube with the tool while you keep the capillary slit horizontally. Then rotate the tube a 1/4 turn clockwise to lock the bayonet. This brings the slit and the flattened sides to the vertical orientation.
11. Align the gas inlet on the ion sweep cone with the sweep gas supply port on the ion source mount. Firmly press the ion sweep cone into ion source mount. See [Figure 8-11](#) and [Figure 8-12](#).
12. Reinstall the Ion Max API source housing on the mass spectrometer as described in [“Installing the Ion Max API Source Housing”](#) on [page 8-18](#).
13. Place the electronics service switch in the Operating Mode position to supply power to all components of the mass spectrometer.

If you have unblocked the ion transfer tube, then the Pirani gauge pressure should increase to a normal value (approximately 3.5 mbar). If you cannot clear the ion transfer tube by this method, then replace it.



## API Probe Maintenance

The HESI-II probe requires minimum maintenance. If the metal needle sample tube is blocked, replace it. Replacing the metal needle requires a partial disassembly of the probe.

Refer to the *Ion Max and Ion Max-S API Source Hardware Manual* and the *HESI-II Probe User Guide* for procedures for maintaining the API probes.

This section contains the following procedures:

- “Flushing the Sample Transfer Line and Sample Tube”, next section
- “Removing the HESI-II Probe” on page 8-30
- “Installing the HESI-II Probe” on page 8-34
- “Adjusting the Probe Position” on page 8-38
- “Replacing the Needle Insert” on page 8-40

### **▲ CAUTION**

**Hot Parts.** At typical operating temperatures between 350 and 450 °C, touching the vaporizer might cause severe burns. Let the HESI-II probe cool to room temperature (approximately 60 minutes) before you touch or remove it.

**NOTICE** For best results, do not operate the HESI-II probe at elevated temperatures without solvent flow. Letting the HESI-II probe to run dry at elevated temperatures can cause blockage of the replaceable metal needle. ▲

**NOTICE** Wear a new pair of lint- and powder-free gloves when you handle HESI-II probe components. See “[Personal Protective Equipment](#)” on [page 4-12](#) for a specification for the required gloves. ▲

## Flushing the Sample Transfer Line and Sample Tube

For best results, flush the sample transfer line, sample tube, and HESI-II probe for 15 minutes at the end of each working day (or more often if you suspect they are contaminated). Use a 50:50 methanol/distilled water solution from the LC system through the API source.

### ▲ CAUTION

**Hazardous Substance.** Methanol is highly flammable and noxious. Keep away from heat, sparks, and flame. Avoid accidental exposure. Use with adequate ventilation. When possible, dilute it with 50% water. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of methanol.

After 15 minutes, turn off the flow of liquid from the LC to the API source, but keep the API source on (including the sheath gas and auxiliary gas) for an additional 5 minutes. See [“Flushing Sample Transfer Line, Sample Tube, and API Probe”](#) on page 6-15.

## Removing the HESI-II Probe

### ▲ CAUTION

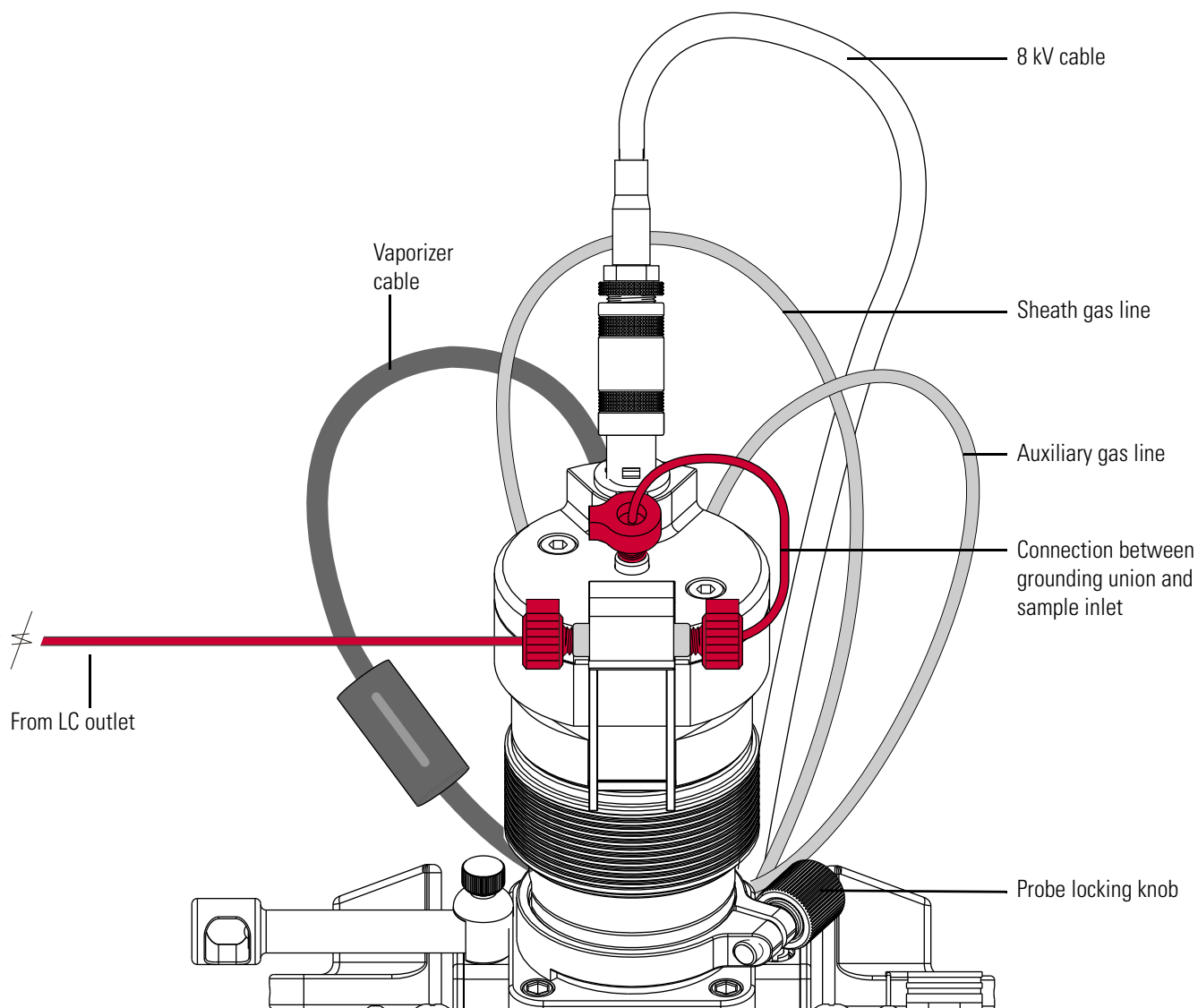
**Hot Parts.** At typical operating temperatures between 350 and 450 °C, touching the HESI-II probe might cause severe burns. Let the API probe cool to room temperature (approximately 60 minutes) before you remove it from the API source housing.

#### ❖ To remove the HESI-II probe from the API source housing

1. Place the Exactive Series mass spectrometer in Standby mode (see [“Setting the System in Standby Condition”](#) on page 6-7) and let the probe cool to room temperature.

Wait approximately 60 minutes for the probe to reach room temperature when it has been operating at high temperature. If the mass spectrometer is connected to an LC system, keep the solvent flow from the LC pump on while the probe is cooling to room temperature.

2. If the mass spectrometer is connected to an LC system, switch off the solvent flow from the LC pump, and then disconnect the tubing from the left side of the HESI-II probe grounding union ([Figure 8-15](#)).



**Figure 8-15.** Connections to the HESI-II probe (front view)

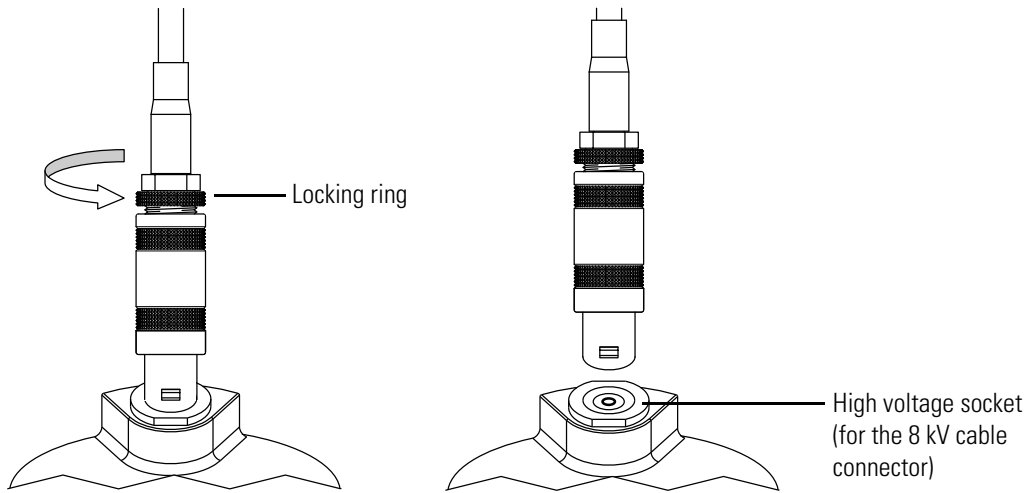
**⚠ WARNING**

**High Voltage.** Voltages up to 8 kV are used in the ion source. If you touch parts of the ion source while the mass spectrometer is in operation, you might receive an electric shock! The mass spectrometer must be in standby mode before you disconnect or connect the 8 kV cable.

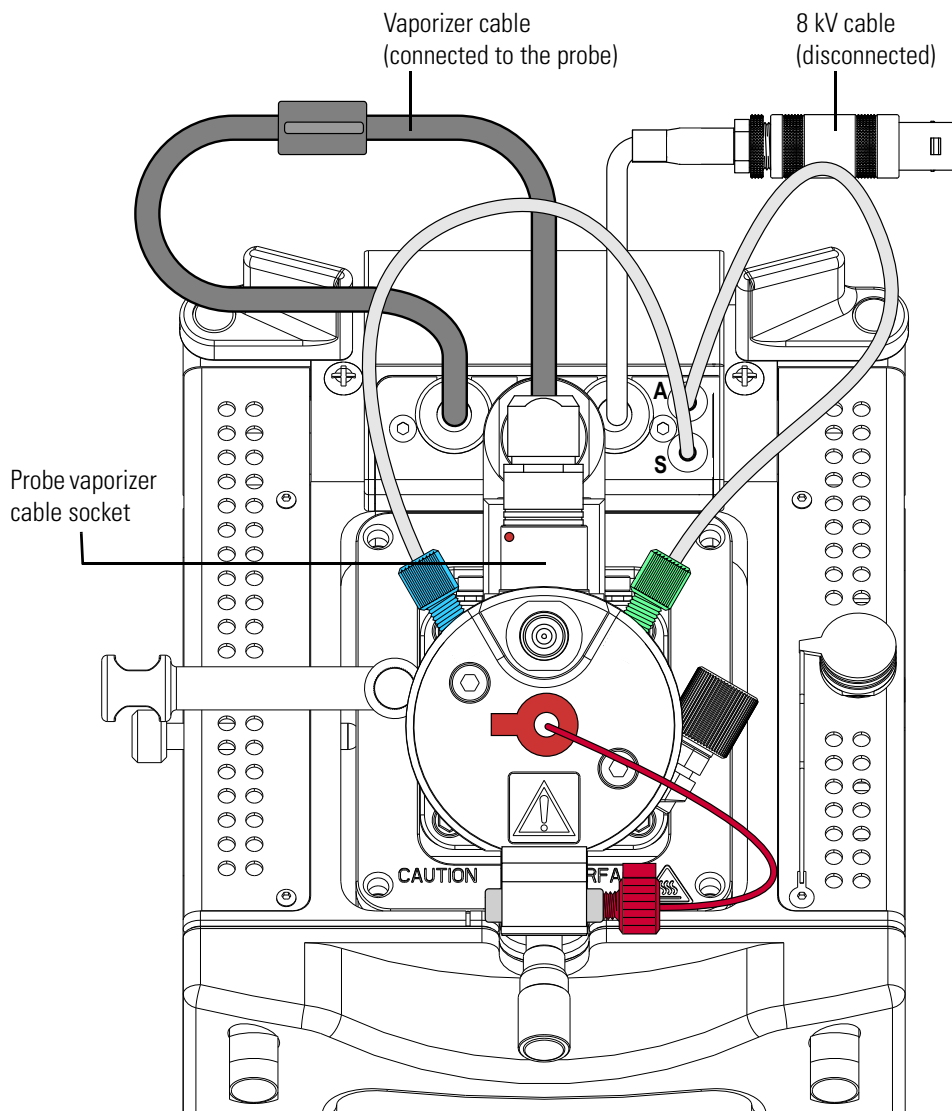
3. Disconnect the 8 kV cable from the probe high-voltage receptacle (Figure 8-16):
  - a. Unlock the cable by turning the locking ring counterclockwise.
  - b. Unplug the 8 kV cable from the probe high-voltage socket.

**Maintenance**

API Source Maintenance



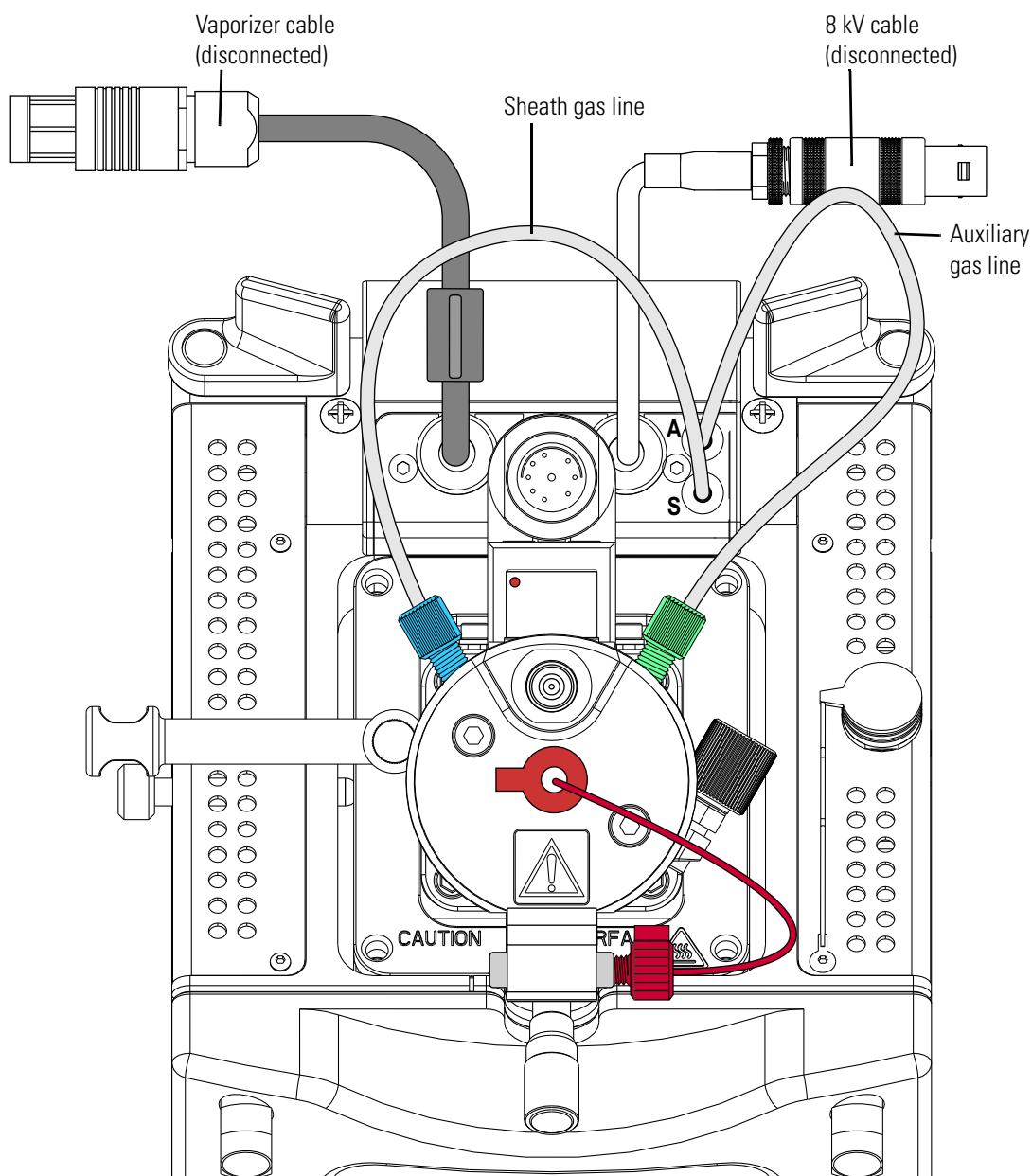
**Figure 8-16.** 8 kV cable connector (enlarged view)



**Figure 8-17.** API source housing and the HESI-II probe (top view)

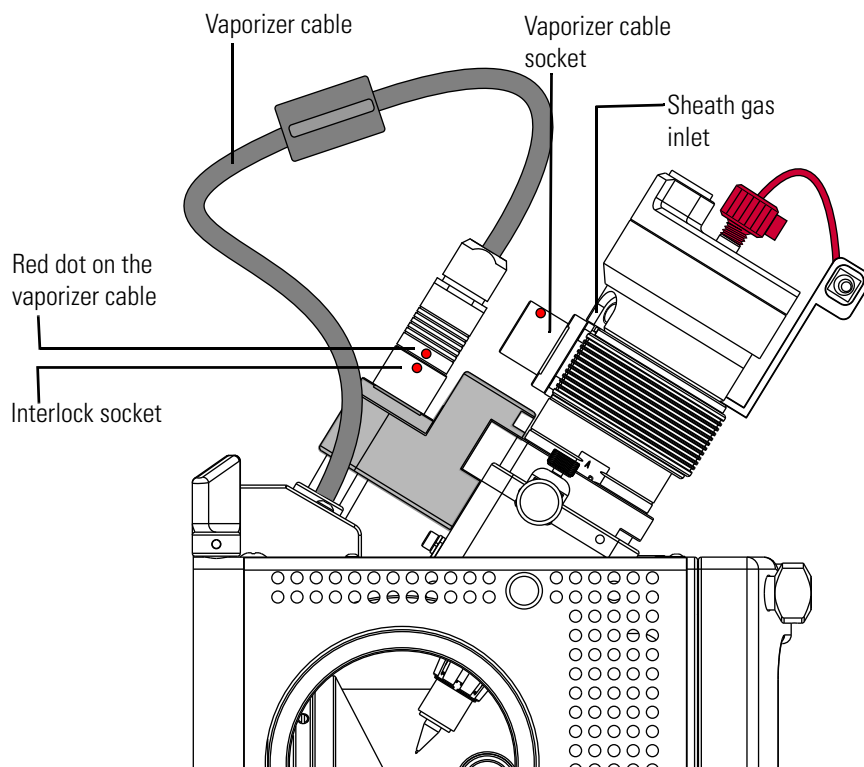
4. Disconnect the nitrogen gas lines (Figure 8-18):

- Disconnect the auxiliary gas fitting (green) from the auxiliary gas inlet (A) on the probe.
- Disconnect the sheath gas fitting (blue) from the sheath gas inlet (S) on the probe.



**Figure 8-18.** Sheath and auxiliary gas lines connected to the probe (top view)

5. Connect the vaporizer cable to the interlock socket on the interlock block. To align the socket pins, align the red dot on the vaporizer cable connector with the red dot on the interlock socket (Figure 8-19).



**Figure 8-19.** API source housing (left side view)

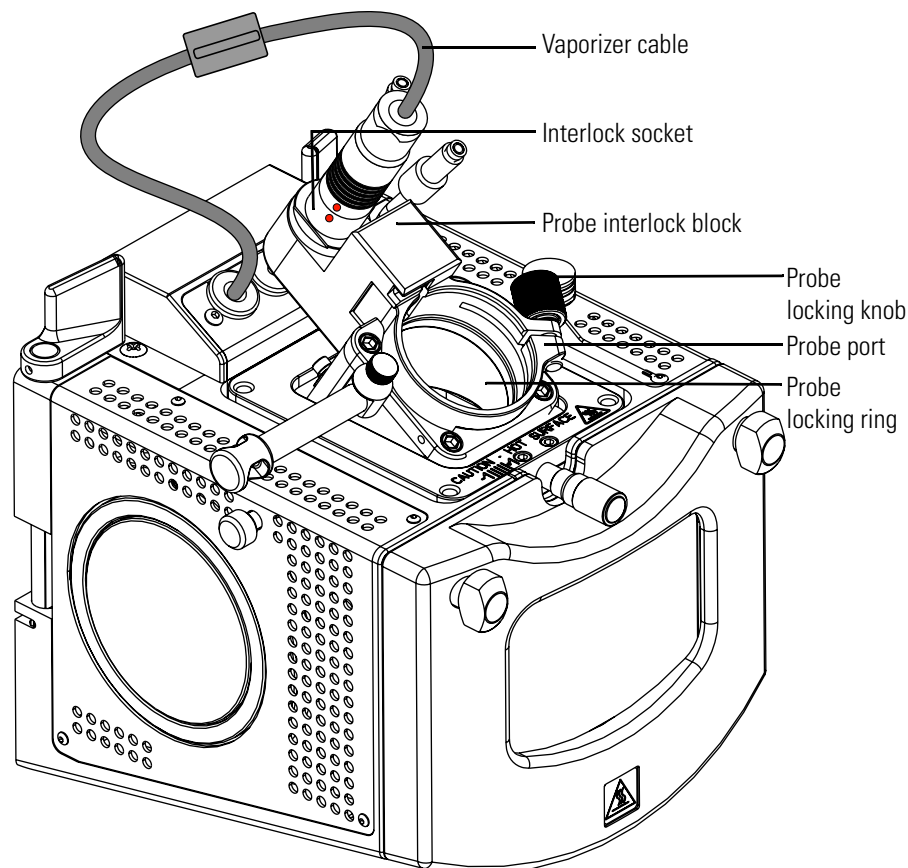
6. Unlock the probe locking ring by turning the probe locking knob (Figure 8-15 on page 8-31) counterclockwise.
7. Remove the probe from the port in the API source housing:
  - a. Slowly pull the probe out of the port until you feel the resistance caused by the probe guide pin meeting the interlock block.
  - b. Turn the probe counterclockwise until the guide pin is free of the interlock block.
  - c. When the guide pin is free of the interlock block, pull the probe out of the port.
8. Store the HESI-II probe in its original shipping container.

## Installing the HESI-II Probe

### ❖ To install the HESI-II probe

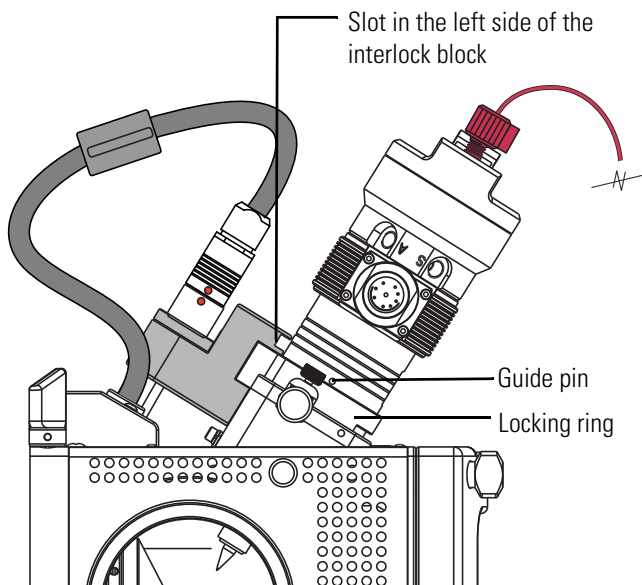
1. Make sure that the Exactive Series mass spectrometer is in Standby mode as described in “Setting the System in Standby Condition” on page 6-7.
2. If the mass spectrometer is set up for the APCI mode, remove the APCI probe and the corona needle (refer to the *Ion Max and Ion Max-S API Source Hardware Manual*).

3. Remove the HESI-II probe from its storage container. Inspect and clean it if necessary.
4. Turn the probe locking knob counterclockwise until the probe locking ring is opened to its widest position ([Figure 8-20](#)).

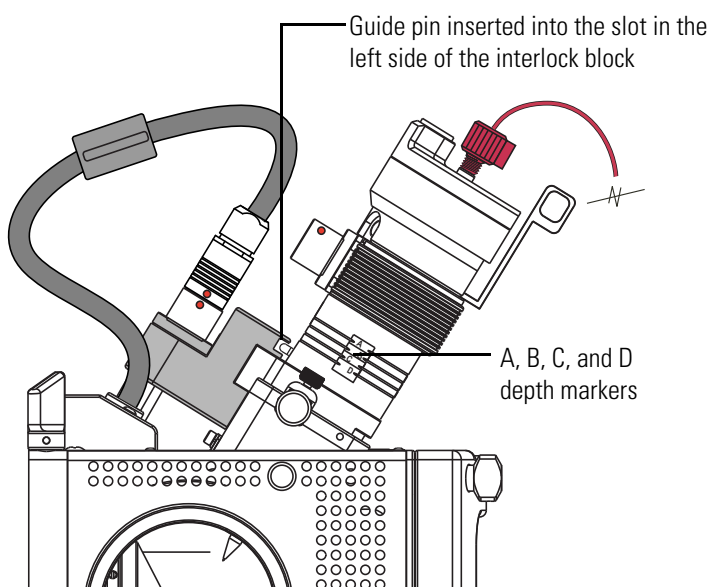


**Figure 8-20.** Ion Max API source housing without a probe

5. Seat the probe in the probe port:
  - a. Holding the probe with the nozzle facing down and the guide pin facing toward the left, slowly insert the probe into the port until the guide pin meets the locking ring on the API source housing ([Figure 8-21](#)).
  - b. Pull the probe slightly up until the guide pin is level with the slot on the left side of the interlock block. Then turn the probe clockwise until the guide pin meets resistance from the interlock block ([Figure 8-22](#)).
  - c. Push the probe down into the port to the appropriate depth indicated by the A, B, C, and D depth markers on the probe. In the ESI mode, insert the probe to a depth of B, C, or D. For high solvent flow rates, adjust the probe depth so that the nozzle is farther away from the ion interface (depth C or D). Conversely, for low solvent flow rates, adjust the probe depth so that the nozzle is closer to the ion interface (depth B or C).



**Figure 8-21.** Guide pin touching the locking ring



**Figure 8-22.** Guide pin inserted into the slot

6. Lock the probe in place by turning the probe locking knob (see [Figure 8-20](#) on [page 8-35](#)) clockwise until you feel resistance.
7. Connect the nitrogen gas lines to the HESI-II probe as follows:
  - Connect the sheath gas fitting (blue) to the sheath gas inlet (S).
  - Connect the auxiliary gas fitting (green) to the auxiliary gas inlet (A).
8. Unplug the vaporizer cable connector from the interlock socket and connect it to the vaporizer cable connector socket on the probe. To align the connector pins with the socket, align the red dot on the



connector with the red dot on the socket. [Figure 8-19](#) on [page 8-34](#) shows the red alignment dots on the connector and the socket.

**⚠ WARNING**

**High Voltage.** Voltages up to 8 kV are used in the ion source. If you touch parts of the ion source while the mass spectrometer is in operation, you might receive an electric shock! Always place the mass spectrometer in standby mode before you disconnect or connect the 8 kV cable.

9. Connect the 8 kV cable connector to the 8 kV cable connector socket on the probe. Tighten the locking ring (see [Figure 8-16](#) on [page 8-32](#)) on the 8 kV cable connector.
10. Make sure that the grounding union (stainless steel ZDV fitting) is seated in the grounding union holder on the probe.
11. Using two fingertight fittings, connect a short length of red PEEK tubing to the right side of the grounding union and to the probe sample inlet.
12. Using two fingertight fittings, connect a length of red PEEK tubing to the LC outlet and to the left side of the grounding union.

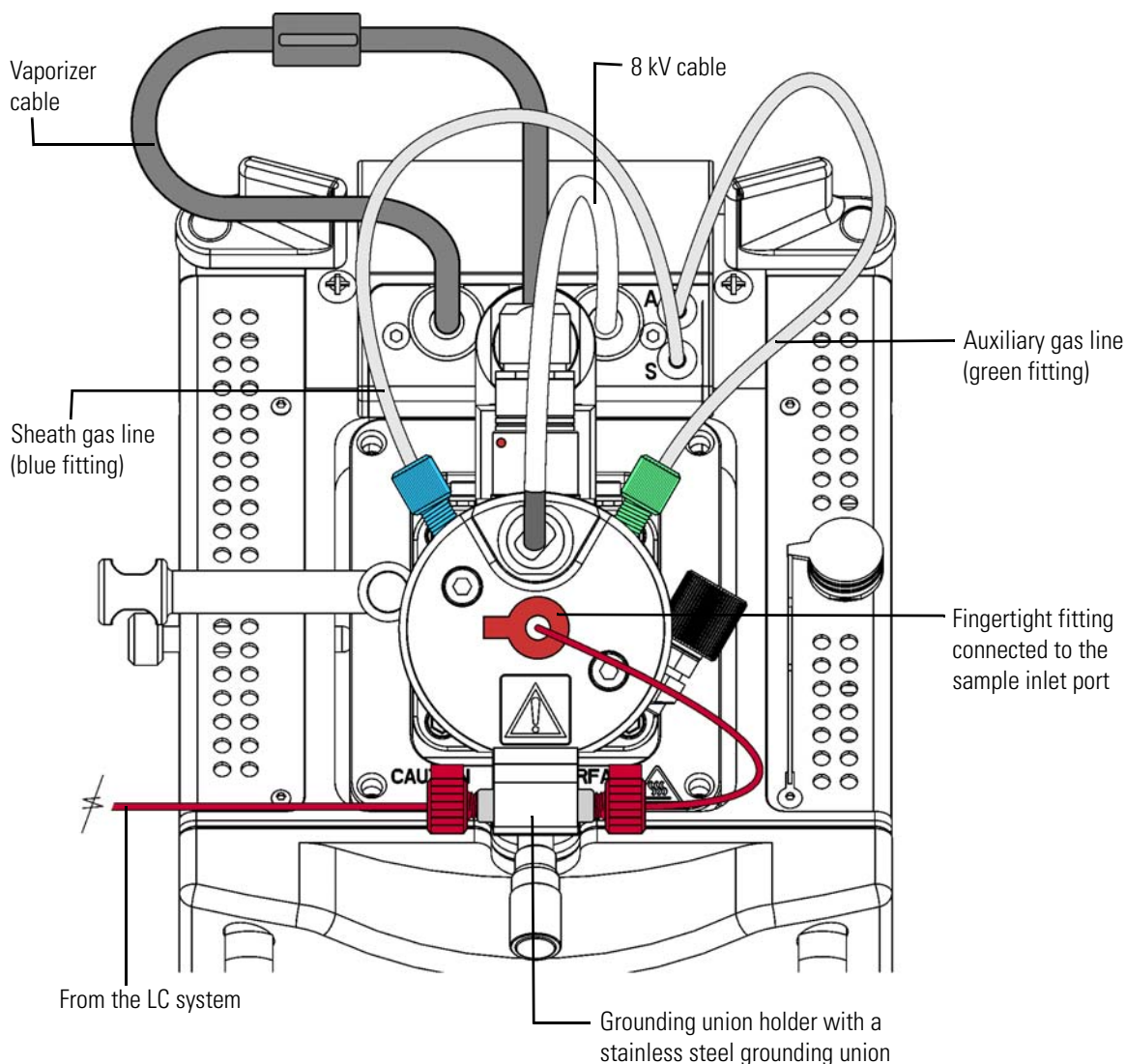
**⚠ WARNING**

**High Voltage.** If the sample tubing is directly connected to the probe inlet, the high voltage might be transmitted to you over the liquid. If you touch liquid that leaks from the probe sample inlet while the mass spectrometer is in operation, you might receive an electric shock. Always connect the sample with the grounding union.

[Figure 8-23](#) shows the HESI-II probe installed in the Ion Max API source.

## Maintenance

### API Source Maintenance



**Figure 8-23.** HESI-II probe installed in the Ion Max API source housing

## Adjusting the Probe Position

To maximize sensitivity, you can adjust the probe depth. You can also adjust the side-to-side and front-to-back probe position by a few millimeters. For best results, follow the guidelines in [Table 8-8](#) as a starting point. These guidelines are based on the liquid flow rate of your application.

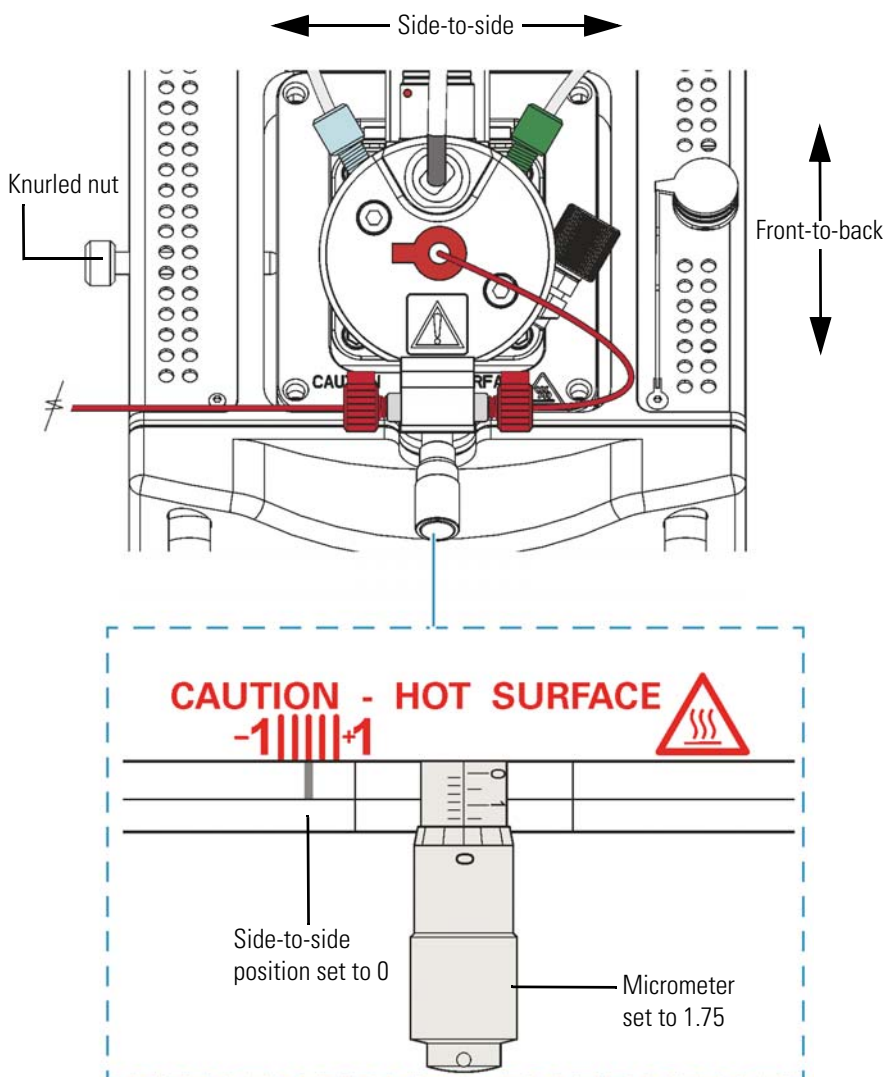
**Table 8-8.** Probe position guidelines

Liquid flow rate range ( $\mu\text{L}/\text{min}$ )	Front-to-back position (micrometer setting)	Probe depth (probe depth line)	Side-to-side position (+1 to -1 marks)
1 to 50	1.75 <sup>a</sup>	B	0
50 to 2000	1.75	C	0

<sup>a</sup> Fully turned to the right.

❖ **To adjust the probe position**

- Using the micrometer on the front of the Ion Max source housing, adjust the front-to-back probe position (see [Figure 8-24](#)).
- Using the knurled nut on the left side and the +1 to -1 markers on the top front of the Ion Max source housing, adjust the side-to-side probe position (see [Figure 8-24](#)).
- Using the A, B, C, and D markers on the probe as a guide, adjust the probe depth (see [Figure 8-22](#) on [page 8-36](#)).



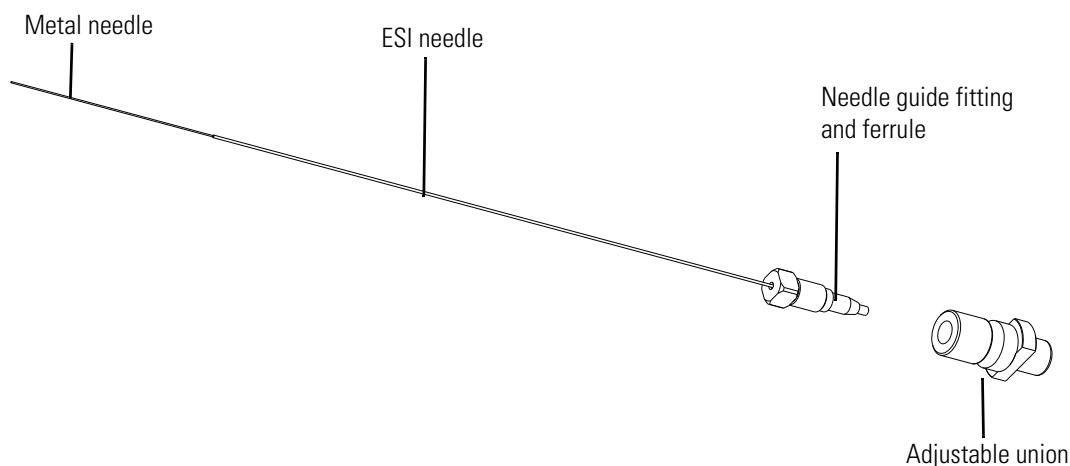
**Figure 8-24.** Top view of the Ion Max source housing with a HESI-II probe

**⚠ CAUTION**

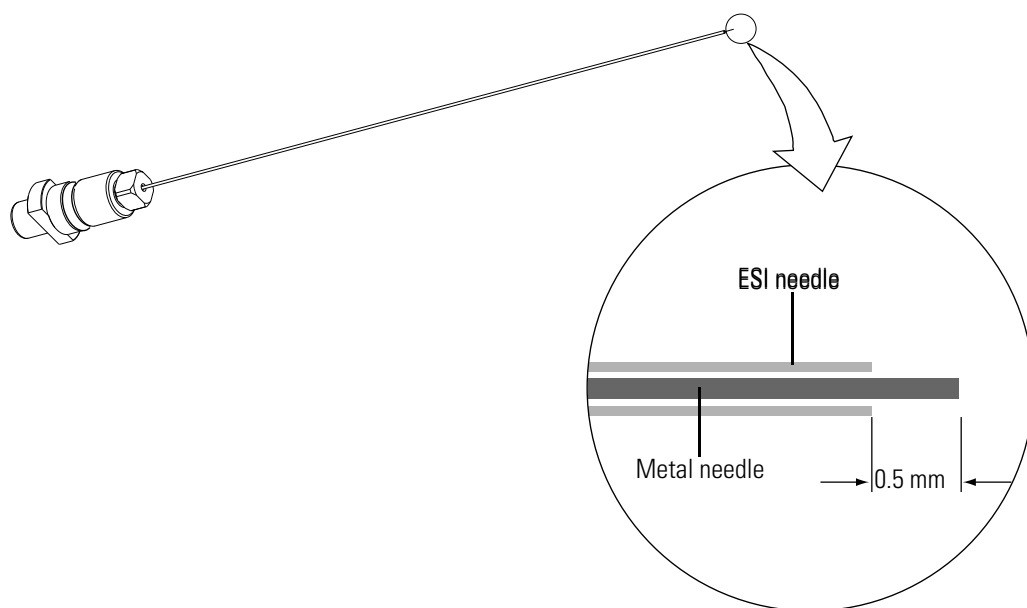
**Hot Parts.** When the system is in operation, the surface of the source housing can be hot enough to burn your skin. You may touch the micrometer and the knurled nut while the system is in operation, but do not touch other parts of the source housing.

## Replacing the Needle Insert

If the metal needle is blocked, you can replace the needle insert. The needle insert is assembled at the factory and consists of an adjustable union, a needle guide fitting, a ferrule, an O-ring, an ESI needle, and a metal needle (Figure 8-25). The ferrule is swaged onto the ESI needle. Factory adjusted, the metal needle protrudes 0.5 mm from the end of the ESI needle (Figure 8-26).



**Figure 8-25.** Needle insert components



**Figure 8-26.** Metal needle insert assembly with an enlarged view of the stainless steel needle tip

To support flow rates from 5 to 2000  $\mu\text{L}/\text{minute}$ , Thermo Fisher Scientific provides two metal needle inserts for the HESI-II probe. The difference between the two inserts is the size of the metal needle and supporting ferrule (Table 8-9).

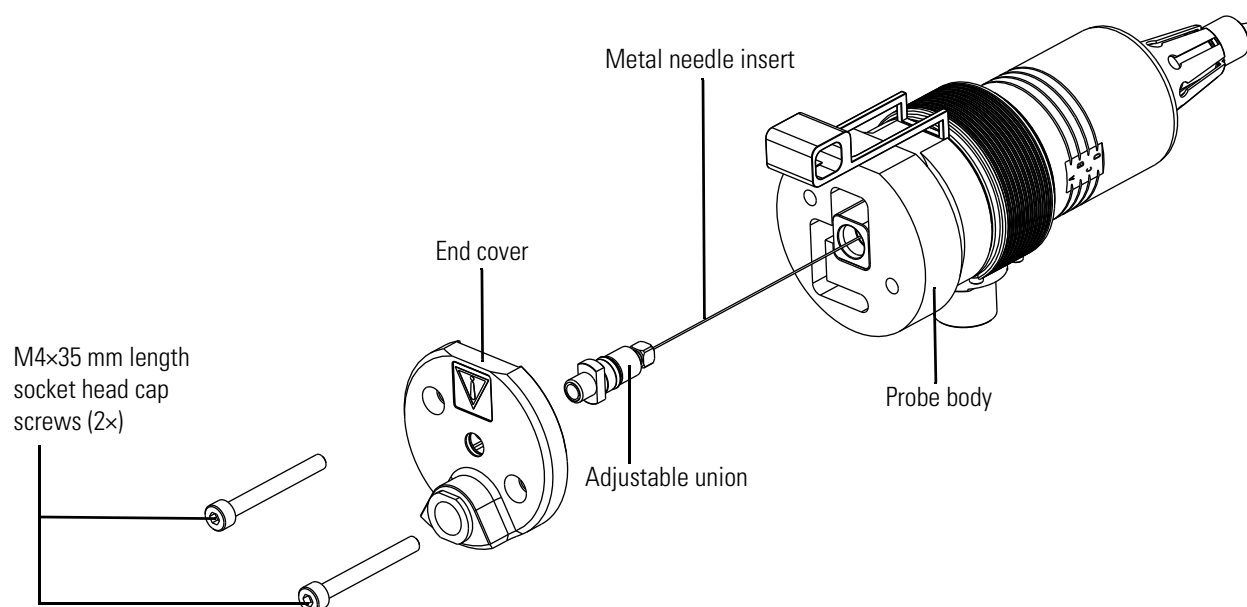
**Table 8-9.** Metal needle inserts

Description	Metal needle	Ferrule	Flow rate range	Part number
32-gauge needle insert, HESI-II probe	0.004 in. ID 0.009 in. OD	0.4 mm thru-hole	5 to 2000 $\mu\text{L}/\text{min}$	70005-60155
34-gauge needle insert, HESI-II probe	0.003 in. ID 0.007 in. OD	0.2 mm thru-hole	1 to 10 $\mu\text{L}/\text{min}$	70005-60180

To replace the metal needle insert, you must have a 3 mm (7/64 in.) hex wrench or ball driver.

❖ **To replace the metal needle insert**

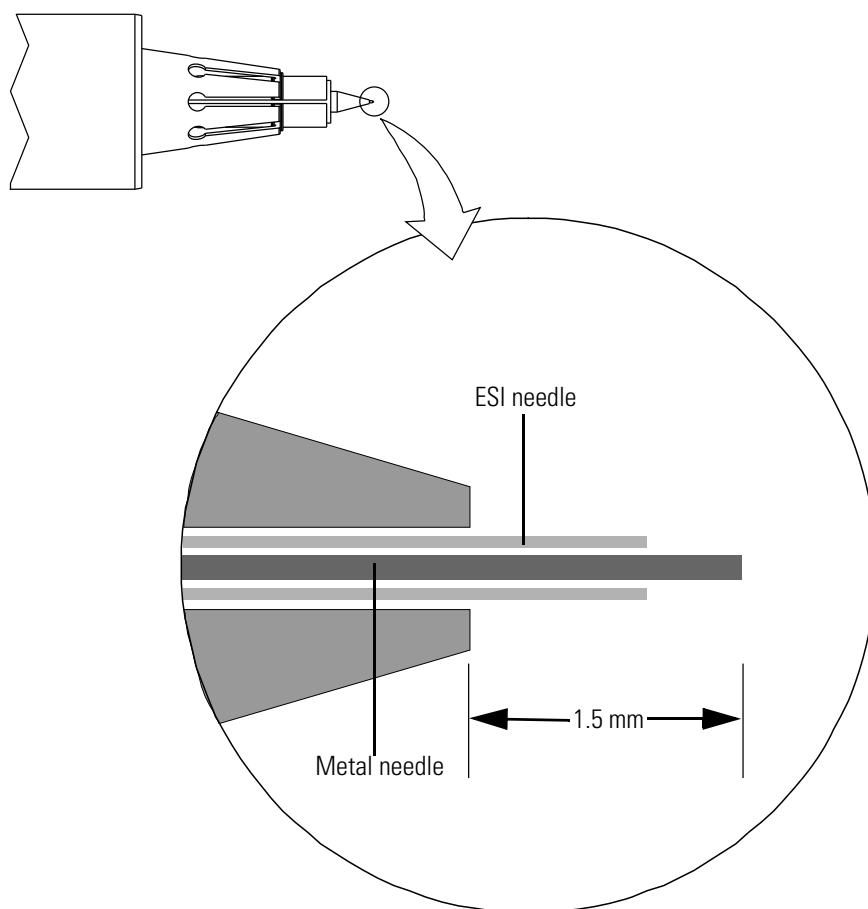
1. Remove the HESI-II probe from the Ion Max API source (see “Removing the HESI-II Probe” on page 8-30).
2. Unscrew the fingertight fitting from the sample inlet port (see Figure 8-23 on page 8-38).
3. Remove the metal needle insert from the probe as follows (Figure 8-27):
  - a. Using a 3 mm (7/64 in.) hex wrench or ball driver, remove the two M4×35 mm length, socket head cap screws.
  - b. Pull off the end cover of the probe.
  - c. Unscrew the metal needle insert, and then pull it out of the probe body.



**Figure 8-27.** HESI-II probe (exploded view)

4. Insert a new metal needle insert into the probe body.

5. Hand tighten the adjustable union fitting until the tip of the needle insert protrudes from the probe nozzle by 1.5 mm (Figure 8-28).



**Figure 8-28.** HESI-II probe nozzle (exploded view)

6. Put the end cover on the probe body.
7. Insert the two M4×35 mm length, socket head cap screws into the end cover, and then tighten them with a 3 mm (7/64 in.) hex wrench or ball driver.
8. Reinstall the HESI-II probe (see [“Installing the HESI-II Probe”](#) on page 8-34).

## Ion Source Interface Maintenance

The ion source interface assembly includes ion sweep cone, ion transfer capillary, exit lens, and S-lens or ion funnel. The ion transfer capillary has a finite lifetime. You need to replace it if its bore becomes corroded.

It is good practice to flush the ion sweep cone and the bore of the ion transfer capillary at the end of each working day with a 50:50 methanol:water solution. See [“Flushing Ion Sweep Cone and Ion Transfer Capillary”](#) on page 6-16.

For cleaning or replacement, you can remove the ion sweep cone and ion transfer capillary without venting the system. See [“Removing, Cleaning, and Reinstalling the Ion Transfer Capillary”](#) on page 8-22.

### Sequence of Steps

To maintain ion source interface assembly components other than the ion sweep cone and ion transfer capillary, proceed in the following order:

1. Shut down and vent the system
2. Remove the Ion Max API source housing
3. Remove the ion source interface assembly
4. Clean exit lens and S-lens or ion funnel
5. Reinstall the ion source interface assembly
6. Reinstall the Ion Max API source housing
7. Start up the system

The above steps are described in the following topics.

### Shutting Down and Venting the System

Shut down and vent the system as described in [“Shutting Down the System”](#) on page 6-8.

Continue with [“Removing the Ion Max API Source Housing.”](#)

### Removing the Ion Max API Source Housing

You need to remove the Ion Max API source housing to access the ion source interface assembly. Remove the Ion Max API source housing as described in [“Removing the Ion Max API Source Housing”](#) on page 8-17.

Continue with [“Removing the Ion Source Interface.”](#)

## Removing the Ion Source Interface

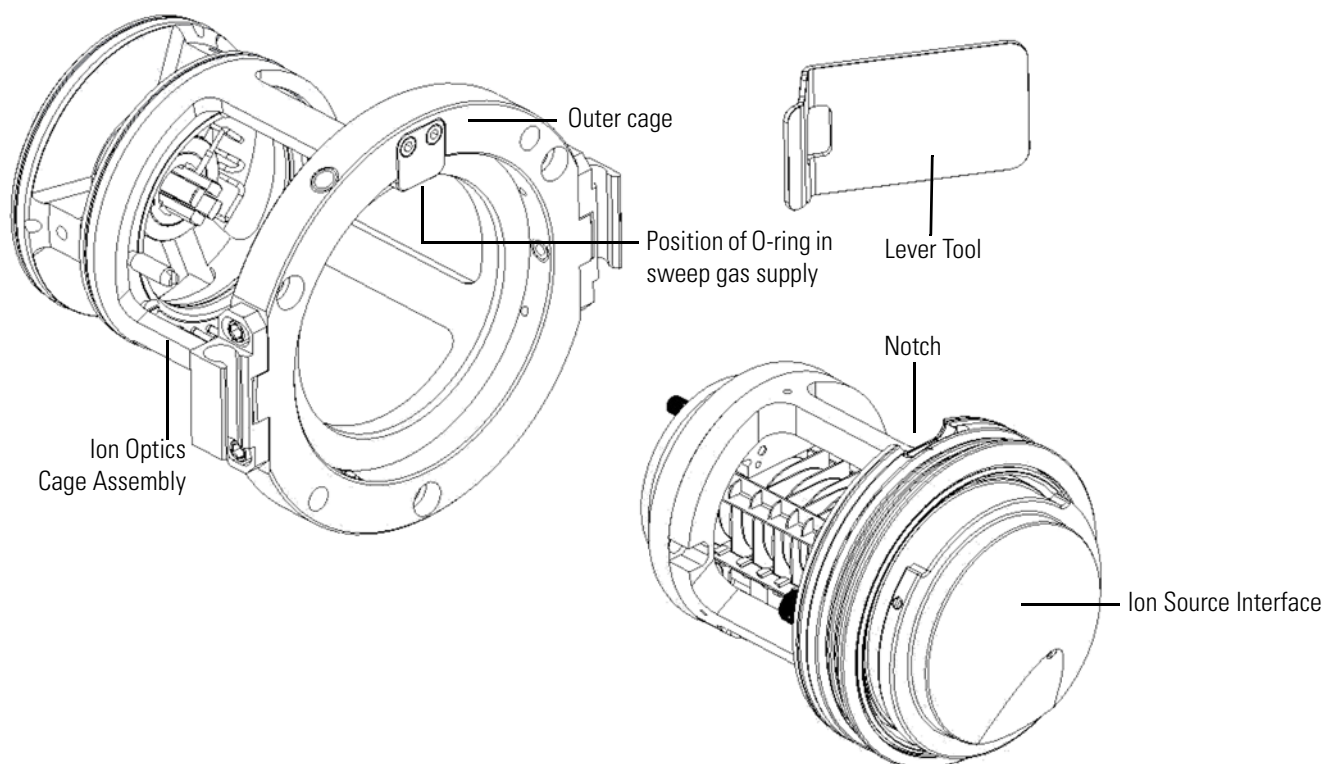
You need to remove the ion source interface to access the exit lens and the S-lens or the ion funnel.

### ⚠ CAUTION

**Hot Parts.** The ion source interface can become hot enough to cause severe burns when the mass spectrometer is in operation. Do not touch the ion source interface immediately after you have removed the ion source housing. Let the ion source interface cool to room temperature (approximately 2 hours) before you remove it from the mass spectrometer.

#### ❖ To remove the ion source interface

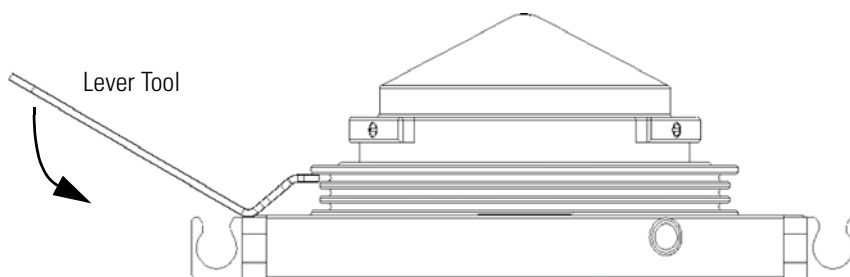
1. Put on clean, talc-free gloves. See [page 4-12](#) for a recommendation for the required gloves.
2. Grasp the ridges on either side of the ion source interface and firmly pull the assembly straight out.



**Figure 8-29.** Removing the ion source interface



Use the tool (P/N 1304960) to lever out the interface assembly. See [Figure 8-30](#).



**Figure 8-30.** Using the lever tool

3. Place the assembly on a clean, lint-free surface.

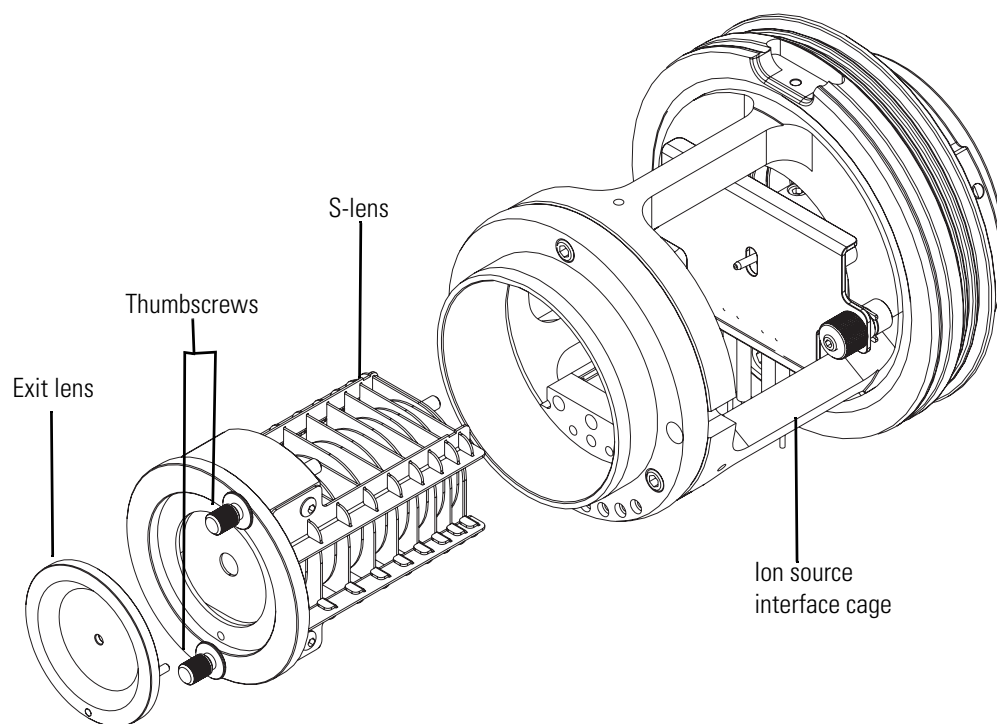
For instruments with an S-lens, continue with [“Removing, Cleaning, and Reinstalling the Exit Lens and the S-Lens.”](#) For instruments with an ion funnel, continue with [“Removing, Cleaning, and Reinstalling the Exit Lens and the Ion Funnel”](#) on page 8-48.

### Removing, Cleaning, and Reinstalling the Exit Lens and the S-Lens

Remove the S-lens and the exit lens from the ion source interface cage before you clean them.

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

1. Cover the area with lint-free paper to prepare a clean work surface.
2. Put on a new pair of lint- and powder-free gloves. See [page 4-12](#) for a recommendation for the required gloves.
3. Loosen and extend the two thumbscrews that secure the S-lens to the ion source interface cage and the exit lens to the S-lens ([Figure 8-31](#)).
4. Remove the exit lens from the S-lens and place it on a clean, lint-free surface.
5. Grasp the two thumbscrews and carefully pull the S-lens straight out of the ion source interface cage and place it on a clean, lint-free surface.



**Figure 8-31.** Exit lens and S-lens separated from the ion source interface cage

❖ **To clean S-lens and exit lens**

**NOTICE** Do not clean the exit lens or S-lens with abrasives, acidic or caustic substances, or detergents not stated in this chapter. ▲

**NOTICE** Do not disassemble the S-lens from its holder. Otherwise, you risk losing the correct alignment of the lens segments. ▲

1. Put on a new pair of lint- and powder-free gloves. See [page 4-12](#) for a recommendation for the required gloves.
2. Inspect the components under magnification for any lint, particulates, and sample buildup or coatings.
3. Sonicate the components for 10–15 minutes in a 50:50 solution of LC/MS grade methanol and water or a 1% solution of Liquinox™ in water. If a sonicator is not available, do the following:
  - a. To clean the exit lens, use a soft toothbrush with a 1% solution of Liquinox in water.
  - b. To clean the S-lens, use a chamois-tip swab with a 1% solution of Liquinox in water, and use the 6000 grit MICRO-MESH™

polishing swabs to clean the areas that are inaccessible to the chamois-tip swab.

**▲ CAUTION**

**Hazardous Substance.** Methanol is highly flammable and noxious. Keep away from heat, sparks, and flame. Avoid accidental exposure. Use with adequate ventilation. When possible, dilute it with 50% water. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of methanol.

4. For the exit lens, clean the bore by using the 6000 grit MICRO-MESH polishing swabs.
5. Rinse the components thoroughly with water.
6. Rinse the exit lens and S-lens with fresh methanol.
7. Air dry the exit lens and S-lens or blow them dry with oil-free nitrogen gas.
8. Make sure that all solvent has evaporated from the components before reassembly.
9. Inspect the components under magnification for any lint or particulates.

**NOTICE** Inspect the orifices to confirm that no lint or particulates are present in the bores of the orifices. Use tweezers or a similar tool to remove lint or particulates. ▲

❖ **To reinstall the S-lens and the exit lens**

1. Put on a new pair of lint- and powder-free gloves. See [page 4-12](#) for a recommendation for the required gloves.
2. Slide the S-lens into the ion source interface cage and align the thumbscrews with the screw holes ([Figure 8-31](#) on [page 8-46](#)).
3. Insert the exit lens into the S-lens, aligning the lead pin with the lead pin socket, and press until you hear a click.
4. Hand tighten the thumbscrews to secure the exit lens and the S-lens to the ion source interface cage.

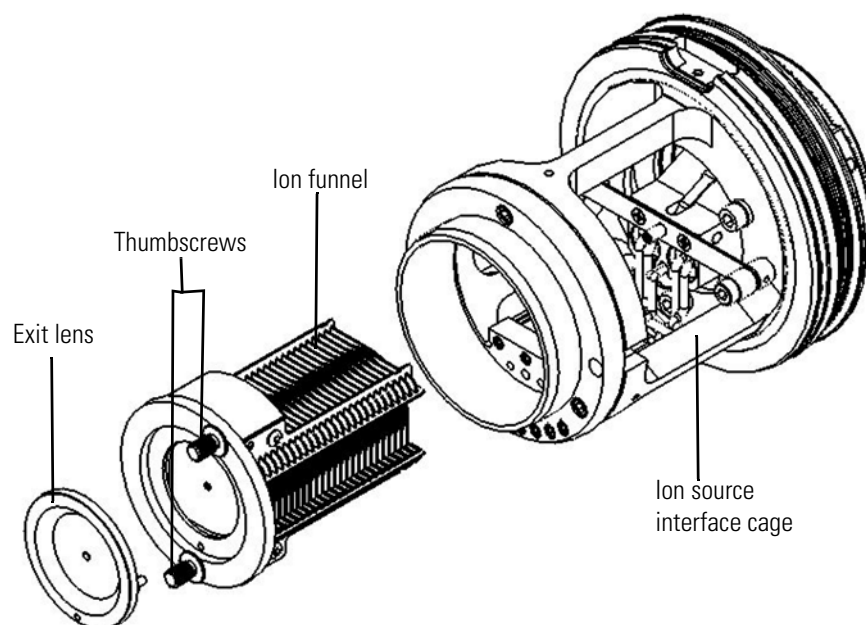
Continue with “[Reinstalling the Ion Source Interface Assembly](#)” on [page 8-50](#).

## Removing, Cleaning, and Reinstalling the Exit Lens and the Ion Funnel

Remove the ion funnel and the exit lens from the ion source interface cage before you clean them.

❖ **To remove exit lens and the ion funnel from the ion source interface cage**

1. Cover the area with lint-free paper to prepare a clean work surface.
2. Put on a new pair of lint- and powder-free gloves. See [page 4-12](#) for a recommendation for the required gloves.
3. Loosen and extend the two thumbscrews that secure the ion funnel to the ion source interface cage and the exit lens to the ion funnel.



**Figure 8-32.** Exit lens and ion funnel separated from the ion source interface cage

4. Remove the exit lens from the ion funnel and place it on a clean, lint-free surface.
5. Grasp the two thumbscrews and carefully pull the ion funnel straight out of the ion source interface cage and place it on a clean, lint-free surface.

❖ **To clean ion funnel and exit lens**

**NOTICE** Do not clean the exit lens or ion funnel with abrasives, acidic or caustic substances, or detergents not stated in this chapter. Always use LC/MS-grade methanol and LC/MS-grade water. ▲

**NOTICE** Do not disassemble the ion funnel from its PEEK holder. Otherwise, you risk losing the correct alignment of the ion funnel segments. ▲

1. Put on a new pair of lint- and powder-free gloves. See [page 4-12](#) for a recommendation for the required gloves.
2. Inspect the components under magnification for any lint, particulates, and sample buildup or coatings.
3. Sonicate the components for 10–15 minutes in a 50:50 solution of LC/MS grade methanol and water or a 1% solution of Liquinox™ in water.

**▲ CAUTION**

**Hazardous Substance.** Methanol is highly flammable and noxious. Keep away from heat, sparks, and flame. Avoid accidental exposure. Use with adequate ventilation. When possible, dilute it with 50% water. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of methanol.

4. Rinse the components thoroughly with water.
5. Rinse the exit lens and ion funnel with fresh methanol.
6. Air dry the exit lens and ion funnel or blow them dry with oil-free nitrogen gas.
7. Make sure that all solvent has evaporated from the components before reassembly.
8. Inspect the components under magnification for any lint or particulates.

**NOTICE** Inspect the orifices to confirm that no lint or particulates are present in the bores of the orifices. Use tweezers or a similar tool to remove lint or particulates. ▲

❖ **To reinstall the ion funnel and the exit lens**

1. Put on a new pair of lint- and powder-free gloves. See [page 4-12](#) for a recommendation for the required gloves.

2. Slide the ion funnel into the ion source interface cage and align the thumbscrews with the screw holes (Figure 8-31 on page 8-46).
3. Insert the exit lens into the ion funnel, aligning the lead pin with the lead pin socket, and press until you hear a click.
4. Hand tighten the thumbscrews to secure the exit lens and the ion funnel to the ion source interface cage.

Continue with “[Reinstalling the Ion Source Interface Assembly.](#)”

## Reinstalling the Ion Source Interface Assembly

### ❖ To reinstall the ion source interface assembly

1. Check the position of the little O-ring on the sweep gas supply before inserting the ion source interfaces. See Figure 8-29 on page 8-44. This O-ring sometimes comes out and breaks when you reinstall the ion source interface.
2. Orient the ion source interface assembly such that the sweep gas inlet notch on the ion source interface is aligned with the sweep gas supply block on the ion source mount.
3. Carefully slide the ion source interface assembly into the ion optics cage assembly.

Continue with “[Reinstalling the Ion Max API Source Housing.](#)”

## Reinstalling the Ion Max API Source Housing

Reinstall the Ion Max API source housing as described in “[Installing the Ion Max API Source Housing](#)” on page 8-18.

You may also need to reinstall an ion source probe and LC liquid lines, as appropriate.

Continue with “[Starting Up the System](#)” below.

## Starting Up the System

Start up the system as described in “[Starting Up the System after a Shutdown](#)” on page 6-10.

## Maintaining LCs or Autosamplers

For instructions on maintaining LCs or autosamplers, refer to the manual that came with the LC or autosampler.

## Consumables

For information on consumables such as fittings, nitrogen gas, or cleaning agents, refer to the *Exactive Series Pre-Installation Requirements Guide*, chapter *Consumables*.

For information on calibration- and test-chemicals or solvents, see [“Obtaining Calibration Solutions”](#) on [page 5-39](#).

The forepump oil is used for cooling, lubrication, and sealing of the forepump. See [page 9-4](#) for the specification of the forepump oil. See [“Maintenance of the Forepumps”](#) on [page 8-8](#) for information about forepump oil disposal. Also refer to the Material Safety Data Sheet (MSDS) for the forepump oil.

## Thermo Fisher Scientific Service

This section contains information concerning maintenance work that must be performed by Thermo Fisher Scientific personnel.

### CAUTION

**Hazardous Chemicals.** Hazardous material might contaminate certain parts of your system during analysis. To protect our employees, we ask you to adhere to special precautions when you return parts to the factory for exchange or repair.

If hazardous materials have contaminated instrument parts, Thermo Fisher Scientific can only accept these parts for repair if they have been properly decontaminated.

Materials that due to their structure and the applied concentration might be toxic or which are reported in publications to be toxic are regarded as hazardous. Materials that will generate synergetic hazardous effects in combination with other materials present are also considered hazardous.

Parts contaminated by radioisotopes must not be returned to Thermo Fisher Scientific—neither under warranty nor within the exchange part program. If you are unsure whether parts of the system are possibly contaminated by hazardous material, make sure that the Thermo Fisher Scientific field service engineer is informed before the engineer starts working on the system.

## Returning Parts

To protect our employees, we ask you for some special precautions when returning parts to the factory for exchange or repair.

Your signature on the Health and Safety Form confirms that the returned parts have been decontaminated and that they are free of hazardous materials. This form is available on [page A-5](#). Instead of copying or printing this page, request a copy from the Thermo Fisher Scientific field service engineer.



## Services to be Performed by Thermo Fisher Scientific Service Only

Table 8-10 lists services that must be performed by a Thermo Fisher Scientific field service engineer only. Depending on the actual workload of your Exactive Series mass spectrometer, you might increase the maintenance frequency.

**Table 8-10.** Thermo Fisher Scientific service procedures

MS Component	Procedure	Frequency
Forepump Agilent MS120	Pump overhaul	Every 30 000 operating hours
Source TMP	Change operating fluid reservoir	Every three years
	Change TMP bearing	Every four years
Analyzer TMP	Change standard bearing	Every 45 000 operating hours
	Exchange rotor assembly	Every 80 000 operating hours
API source	Clean outer cage	As needed

**Maintenance**

Thermo Fisher Scientific Service

## Chapter 9 Replaceable Parts

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

For information on how to order parts, see [“Contacting Us”](#) on [page 1-7](#).

### Contents

- [Ion Source Probes and Parts](#) on [page 9-2](#)
- [Ion Source Interface Parts](#) on [page 9-2](#)
- [Instrument Parts](#) on [page 9-4](#)

## Ion Source Probes and Parts

Refer also to the *Ion Max and Ion Max-S API Source Hardware Manual* and the *HESI-II Probe User Guide* for more lists of replaceable parts for the Ion Max API source and available API probes.

<b>ESI Probe Kit</b> .....	<b>OPTON-20011</b>
Safety Sleeve Kit .....	70005-62015
Stainless Steel Needle Kit, 32 gauge .....	OPTON-53003
Stainless Steel Needle Kit, 34 gauge .....	OPTON-30004
<b>APCI Probe Kit</b> .....	<b>OPTON-20012</b>
APCI Probe Nozzle Assembly .....	97055-60089
<b>HESI-II Probe Kit</b> .....	<b>OPTON-20037</b>
High-flow Needle Insert Assembly .....	OPTON-53010
Low-flow Needle Insert Assembly .....	OPTON-53011

## Ion Source Interface Parts

Exit lens. ....	70005-20419
O-ring, 2-033 Viton V884 (2 × 1/16) .....	00107-01-00006
O-ring, 2.625 ID x 3/32, AS-146, Viton™ .....	00107-11002
O-ring, 2-74 × 0.063, 2-039, Viton .....	00107-12550
O-ring, 0.030 ID x 0.054, graphite, Vespel™ .....	97055-20442
Lever tool (S-lens cage) .....	1304960

## Parts for Ion Source with S-Lens

Ion source interface assembly (S-lens) .....	70005-60255
S-lens. ....	70005-60182
Ion transfer capillary .....	70005-20606
Ion transfer capillary removal tool .....	70111-20258
Graphite Vespel seal ring .....	97055-20442

## Parts for Ion Source with Ion Funnel

Ion source interface assembly (ion funnel) .....	70005-60400
Ion funnel .....	70005-60005
Tube, I.T, 1/4 turn, 2.5 dia, (0.6x1.6) .....	80500-20045
Tool, transfer tube release .....	70005-20972
Seal, ITT 1/4 turn .....	70005-20922

## Source Accessory Parts

Ion Max Housing .....	70005-60176
Syringe 500 µL .....	1248730
Syringe Adaptor Kit .....	70005-62011

## Source Drain Parts

API source drain . . . . .	97055-20488
Source drain adaptor, Teflon™ . . . . .	70111-20971
Reducing connector, 1-in × 0.5-in. . . . .	00101-03-00001
Tygon™ tubing 1-in. ID . . . . .	00301-01-00020
Tygon tubing, 0.5-in. ID . . . . .	00301-22920
Solvent waste container . . . . .	00301-57020
Filling/venting cap . . . . .	00301-57022

## Instrument Parts

### Gas Supply Parts

Teflon hose 4 × 1 . . . . . 0690280

### Forevacuum Parts

Forevacuum pump SV65 BI FC . . . . . 1302380  
Sogevac oil LVO200, 2L . . . . . 1317640  
Exhaust filter Sogevac SV65 BI FC . . . . . 1306150  
Noise Reduction Cover, for SOGEVAC pump . . . . . 1296790  
Drip pan, with wheels . . . . . 1296680  
Exhaust hose, 13 × 3.5, PVC . . . . . 0690720  
Forevacuum hose with steel helix; ID=45 mm, 2 m . . . . . 1302410  
Hose nipple, DN 40, ISO-KF-45 . . . . . 1159230  
Centering ring; NW 40, Viton/stainless steel . . . . . 1168170  
KF Clamping chain; synthetic, DN 40 . . . . . 1258190  
KF Elbow; stainless steel, DN 40 . . . . . 1258200  
KF Adapter; stainless steel, DN 40, 125 mm long . . . . . 1258210  
Hose clamp, NW 40 . . . . . 1181320  
Elbow, DN 40, KF, aluminum . . . . . 1181310  
Tube clamp, 12-20 mm, W4 . . . . . 1005970  
T-piece, for exhaust hoses . . . . . 0512360  
Forevacuum hose with steel helix; ID=19 mm, 2 m . . . . . BRE0010135  
Noise Reduction Cover, for DUO 11 pump . . . . . BRE0008989  
Drip pan, without wheels . . . . . BRE0008985  
Forevacuum pump Agilent MS120 . . . . . BRE0010767  
Forevacuum pump Pfeiffer DUO11 . . . . . BRE0010768

### Ethernet Switch and Cables

Switch . . . . . 2108640  
Patch cord, RJ45 SFTP, 5 m . . . . . 2066750  
Patch cord, RJ45 SFTP, 1m . . . . . 2064990

### Plug Connectors (to connect other devices of the LC/MS system)

COMBICON\_MC1.5/8ST-3.81 . . . . . 2087270  
COMBICON\_MC1.5/6ST-3.81 . . . . . 2098690

### Power Cord

Power cord; 16A/230V, C19, 5M UL . . . . . 2112490

### Fan Filter

Fan Filter . . . . . 1234880

### Additional Hardware

Syringe pump Chemyx Fusion 100 . . . . . 1245740  
Switching Valve MXT 715-000 . . . . . 1239650  
Power strip . . . . . 2129880  
Holder assembly (Syringe Pump/Valves) . . . . . 1302140

# Appendix A Legal Documents

## Contents

- [FCC Compliance Statement](#) on page A-2
- [WEEE Compliance](#) on page A-3
- [Declaration of Conformity for Exactive Series MS](#) on page A-4
- [Health and Safety Form](#) on page A-5

# **FCC Compliance Statement**

THIS DEVICE COMPLIES WITH PART 18 OF THE FCC RULES.



## WEEE Compliance

This product is required to comply with the European Union's Waste Electrical & Electronic Equipment (WEEE) Directive 2012/19/EU. It is marked with the following symbol:



Thermo Fisher Scientific is registered with B2B Compliance ([B2Bcompliance.org.uk](http://B2Bcompliance.org.uk)) in the UK and with the European Recycling Platform ([ERP-recycling.org](http://ERP-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 Thermo Fisher Scientific Business-to-Business (B2B) Recycling Program, send an email request to [weee.recycle@thermofisher.com](mailto: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

**NOTICE** 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. ▲

## RoHS

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

# Declaration of Conformity for Exactive Series MS

-Original-

## EG-Konformitätserklärung EC Declaration of Conformity



**ThermoFisher**  
SCIENTIFIC

Thermo Fisher Scientific (Bremen) GmbH  
Hanna-Kunath-Str. 11  
28199 Bremen, Germany

**Wir erklären hiermit, dass die folgenden Produkte**

*We hereby declare that the following products*

**Bezeichnung:**

*Designation:*

**Massenspektrometer**

*Mass Spectrometer*

**Modell:**

*Model:*

**Thermo Scientific Exactive Serie**

*Thermo Scientific Exactive Series  
(Exactive Plus, Exactive Plus EMR, Q Exactive,  
Q Exactive Focus, Q Exactive HF, Q Exactive Plus,  
Q Exactive HF-X)*

**alle einschlägigen Anforderungen der folgenden Richtlinien erfüllt:**

*fulfills all the relevant requirements of the following directives:*

**Niederspannungsrichtlinie**

*Low Voltage Directive*

**Richtlinie über elektromagnetische  
Verträglichkeit**

*Electromagnetic Compatibility Directive*

**2014/35/EU**

*2014/35/EU*

**2014/30/EU**

*2014/30/EU*

**Die folgenden einschlägigen harmonisierten Normen wurden zugrunde gelegt:**

*The following relevant harmonized standards were used:*

**EN 61010-1:2010**

*EN 61010-1:2010*


**EN 61326-1:2013**

*EN 61326-1:2013*

**Für die Zusammenstellung der technischen Unterlagen ist bevollmächtigt:**

*Person authorized to compile the technical file:*

Jörg Behrens (Director Operations)  
Thermo Fisher Scientific (Bremen) GmbH

  
**Unterschrift**  
*Signature*

Bremen, 2017-04-13

**Datum**

*Date*

This Decontamination Declaration Form must be completed for all materials returned to Thermo Fisher Scientific, it should be sent to the destination by e-mail after printing and with an authorization signature. A hard copy should be attached to the outside of the package with shipping paperwork and a further copy should be placed inside the packaging. The receiving Thermo Fisher Scientific office can help with this form and supply a return number, shipping address and e-mail address. Use the text "not used" to indicate a field not being used. Where a Thermo Scientific part number is not known, add the supplier name (as for the examples below).

## 1. General Information

Customer	_____	Instrument type	_____
Address	_____	Instrument SN	_____
	_____	Order number	_____
Phone	_____	Return number	_____
E-Mail	_____		

Part Number	Quantity	Material Description	Error Description / Reason for Return	Return Part Serial #
e.g. Thermo Scientific PN				
e.g. Pfeiffer				
e.g. Leybold				
e.g. Edwards				

## 2. Condition of the material or instrument



Has the material or instrumentation been removed from the shipping packaging or in contact with










- pump fluids,
- service fluids,
- samples,
- standard solutions,
- other chemicals,
- or hazardous materials?

Tick the applicable check box.

- Yes → go to section 3  
 No → go to section 5

## 3. Contamination

To which compounds has the material/instrumentation been exposed? Biological  or radioactive  contaminated materials must not be shipped to Thermo Fisher Scientific. If any of the check boxes are ticked, go to section 4. If 'No ticks' is ticked, go to section 5.

	<input type="checkbox"/> toxic		<input type="checkbox"/> flammable		<input type="checkbox"/> serious health hazard
	<input type="checkbox"/> corrosive		<input type="checkbox"/> oxidizing		<input type="checkbox"/> hazardous to environment
	<input type="checkbox"/> explosive		<input type="checkbox"/> gas under pressure		<input type="checkbox"/> other harmful substances

Tick the applicable check box.

- At least one tick → go to section 4  
 No ticks → go to section 5

**4. Description of Process Substances and/or Compound**

Which substances have been in contact with the material or instrumentation? (trade name and/or chemical term of service fluids and substances; properties of substances or compounds according to material safety data sheet; e.g. toxic, flammable, corrosive, radioactive)

	Part Number	Serial Number	Trade Name	Chemical / Substance Name / Properties
a)				
b)				
c)				
d)				
e)				
f)				

**5. Legally binding declaration**

Has the material/instrument undergone a decontamination process?  Yes → go to section 6  No

Is the material/instrument safe to handle for Thermo Fisher Scientific and third party personnel?  Yes  No

Components, materials and/or instruments that have been contaminated to a harmful level by whatever substances and/or compounds as stated in sections 3. and 4. above will not be accepted without written evidence of proper decontamination.

I hereby declare that the instrument has undergone successfully all required decontamination procedures and is safe to handle for Thermo Fisher Scientific and/or third party service personnel or suppliers such as Pfeiffer Vacuum, Leybold Vacuum, Edwards Vacuum products, or others.

I confirm that all information, which is supplied on this form, is accurate, complete and sufficient to judge any contamination level. I acknowledge and agree that I will be liable for any personal injury or any other damage, which might result from a false, inaccurate or incomplete statement and that I will indemnify and defend Thermo Fisher Scientific and/or any other concerned third party for and against any liabilities, claims, losses, and/or damages of all kinds arising out of and/or caused by such false, inaccurate or incomplete statements.

Thermo Fisher Scientific reserves the right not to process refunds or returns where the declared or observed use or previous contamination of the product/material has by Thermo Fisher Scientific judgement impacted its integrity.

**6. Detailed description of the Decontamination Process used**

Part Number	Serial Number	Describe the decontamination process

Return Number	Name of authorized person (block letters)	Date	Signature	Company stamp

# Appendix B Component Suppliers' Documents

This chapter contains excerpts from component suppliers' documents with safety-relevant information that may concern users of Exactive Series mass spectrometers.

## Contents

- [Forepumps](#) on page B-2
- [Syringe Pump](#) on page B-7
- [Switching Valve](#) on page B-8

## Forepumps

Observe the following safety guidelines when you operate the forepumps.

### SOGEVAC Pump

Failure to observe the following precautions could result in serious personal injury!

Sogevac™ pumps are not designed:

- for pumping of dusty, aggressive, corrosive, flammable or explosive gases or gas mixtures,
- for pumping of oxygen or other highly reactive gases with a greater concentration than atmospheric concentration (>20%),
- for working in flammable, explosive or dusty environment.

For all these cases, special materials must be used. In case of doubt, contact Oerlikon Leybold Vacuum. See also the limits of use indicated in the CE declaration of conformity.

Pump must not be operated above 2000 m sea level.

#### **▲ WARNING**

**High Voltage.** When you touch parts at high electric voltages, there is the risk that you suffer severe injuries by an electric shock! Covers marked with this symbol must only be opened by trained electricians after having reliably deenergized (lockout/tagout) the equipment. Always operate the pump with a properly connected grounding conductor and make sure that the motor & FC connection box are closed.

#### **▲ WARNING**

**High Voltage.** Even if the pump is not operating, there is the risk of suffering severe injuries by an electric shock! Even after complete power disconnection, live voltage is present in the frequency converter. Wait a minimum of 10 minutes for a complete capacitor discharge.

#### **▲ WARNING**

**Explosion Hazard.** The standard pump is not suitable for installation in explosion hazard ATEX areas. Contact the pump manufacturer if you are planning such an application. Before you install the pump, you must reliably disconnect it from the electrical power supply and prevent the pump from running up inadvertently.

#### **▲ CAUTION**

**Tripping Hazard.** Lay electric feed lines so that there is no risk of tripping over these.

**⚠ CAUTION**

**Hot Parts.** In normal operation, the pump surface temperature can reach 85 °C. Touching parts of the forepump might cause burns. Switch off the pump and let it cool down before any intervention or take appropriate precautions. It is recommended to use an oil casing or pump touching protection at high ambient temperatures.

As a protection against touching, you can use the noise reduction cover. Always wear heat protective gloves when you work on a pump that is “still warm from operation.”

Handle the pump only while vented and after having let it cool down. Do not remove the oil-fill or oil-drain plugs while the pump is running. There exists the risk of suffering burns. Always wear protective gloves and protective goggles also for protection against the oil.

**⚠ CAUTION**

**Vacuum Hazard.** Risk of injury. Do not expose part of the body to the vacuum.

Do not operate the pump with an open and thus accessible inlet. Vacuum connections as well as oil filling and oil draining openings must not be opened during operation of the pump.

Depending on the process involved, dangerous substances and oil might escape from the pump. Take the necessary safety precautions! Disconnect the unit from the power supply before starting any work.

## Agilent Pump

Observe the following safety guidelines when you operate the Agilent forepump.

**⚠ WARNING**

Always disconnect the power supply to the pump before starting maintenance work. Place a special warning signs over the power supply breaker switch: **Machine Undergoing Maintenance - Do Not Power On.** When finished, remove the safety warning.

**⚠ WARNING**

**Electric Safety** Some components of the electric equipment are electrically charged during operation. Any contact may cause serious injuries to persons or objects.

**⚠ CAUTION**

**Hot Surfaces** The pump surfaces may exceed the temperature of 80 °C. Adopt the necessary safeguards to avoid burns due to chance contact. Before carrying out any maintenance on the pump, be sure the pump is cool.

**▲ CAUTION**

**Harmful Substances Emissions** The discharged air contains part of traces of oil mist (maximum residual 2 ppm/weight corresponding to 2.4 mg/m<sup>3</sup>). Check the compatibility with the environment. Make sure that a correct air change is allowed. Otherwise, convey the pump discharge outside. A failure or the seals wear can cause an oil leakage. Avoid the dispersion to the ground and the pollution of other materials. In case that any air containing dangerous substances must be pumped down (for example, biological or microbiological agents), make sure to adopt filtering systems before introducing air in the work environment.

**▲ CAUTION**

**Hazard Caused by Vacuum** Any contact with parts under vacuum can cause injuries. Avoid any contact with the pump inlet port during the pump operation. Introduce air in the inlet circuit before every operation cycle.

**▲ CAUTION**

**Hazard Caused by Pressure** The pump tank is pressurized. Do not open the oil filling and discharge plugs during operation.



**Fire Hazard** The use of the pump in situations unforeseen or not recommended by this manual, as well as lack of correct maintenance, may create high risks for overheating or fire. In case of a fire do not use water to extinguish but use a powder CO<sub>2</sub> extinguisher or other means compatible with the electrical equipment and lubricating oil.



The pump:

- is to be blocked by acting on the brakes on the wheels, on a horizontal plane.
- it must be accessible for correct and easy maintenance, by respecting the minimum distances from possible obstructions. It should be accessible to suitable lifting equipment.
- it must be protected from jets or sprays of water which could cause electrical shorts and / or to the electrocution of operators near to the machine.

The pump must not handle:

- liquids or solid substances
- dangerous, explosive or aggressive gases and vapors
- pure oxygen or air mixtures enriched with oxygen.

It is forbidden to install the pump in a potentially explosive environment.



## DUO Forepump

### WARNING

**Toxic Vapors** Risk of poisoning when igniting and heating synthetic operating fluids (e.g. F4/F5) above 300 °C. Observe the application instructions of the operating fluid manufacturer. Do not allow operating fluid to make contact with tobacco products; observe safety precautions when handling chemicals.

### WARNING

**Strong Magnetic Field in the Vicinity of the Drive System** Hazard to life for persons with cardiac pacemakers when the drive system is disassembled. Persons with cardiac pacemakers must not enter the area of the magnetic field. Disassembled magnetic couplings must be kept away from computers, data storage media and other electronic components.

### CAUTION

**Emission of Toxic Substances from the Exhaust** Risk of poisoning from emitted gases or vapors, which can be detrimental to health and/or can pollute the environment, depending on the particular application. Comply with the applicable regulations when working with toxic substances. Only officially approved filter systems may be used to separate out these substances.

### CAUTION

**Risk of Injury from Moving Parts** After power failure or motor shutdown due to overheating, the motor may restart automatically. Secure the motor so that it cannot be switched on while any work is being performed on the pump. If necessary, dismantle the pump from the installation for inspection.

### CAUTION

**Hot Surface** Risk of burns if hot parts are touched. Depending on the operating and ambient conditions, the surface temperature of the pump may rise above 70 °C. In this case, use suitable finger guards. The surface temperature of the pump may rise above 105 °C in case of malfunction. Carry out work on the pump only after it has cooled to a safe temperature

### CAUTION

**Pump Parts may be Contaminated from Pumped Media** Risk of poisoning due to contact with harmful substances. Decontaminate the pump before carrying out any maintenance work. In the event of contamination, take suitable safety precautions to prevent your health from being harmed by any dangerous substances.

**▲ CAUTION**

**Hot Operating Fluid** Risk of burns when draining due to contact with skin. Wear suitable protective clothing.

**▲ CAUTION**

**Operating Fluid may contain Toxic Substances from the Pumped Media** Danger of poisoning from the emission of harmful substances (radioactive, toxic, etc.) from the operating fluid. Wear suitable protective clothing and respirators. Dispose of operating fluid according to the local regulations.

## Syringe Pump

Observe the following safety guidelines when you operate the syringe pump.

**⚠ CAUTION**

**Pinch Hazard.** Do not place fingers between the pusher block and end block while the pump is running.

## Switching Valve

Observe the following safety guidelines when you operate the switching valve:



- Do not submerge the MX Series II Module in liquids.
- Confirm that there is adequate ground between your controlling instrument and the MX Series II Module. This is especially important with electrospray mass spectrometry.
- Plug the Universal Power Supply into the MX Series II Module first, and then plug the Universal Power Supply into an AC power source.
- When disconnecting, unplug at the AC power source first.

# Glossary

This section lists and defines terms used in this manual. It also includes acronyms, metric prefixes, symbols, and abbreviations.

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**
- A** ampere
- AC** alternating current
- ADC** analog-to-digital converter; a device that converts data from analog to digital form.
- adduct ion** An ion formed by the joining together of two species, usually an ion and a molecule, and often in the ion source, to form an ion containing all the constituent atoms of both species.
- AGC™** See [Automatic Gain Control™ \(AGC\)](#).
- APCI** See [atmospheric pressure chemical ionization \(APCI\)](#).
- APCI corona discharge current** The ion current carried by the charged particles in the APCI source. The voltage on the APCI corona discharge needle supplies the potential required to ionize the particles. The APCI corona discharge current is set; the APCI corona discharge voltage varies, as required, to maintain the set discharge current.
- See also [corona discharge](#) and [APCI corona discharge voltage](#).
- APCI corona discharge voltage** The high voltage that is applied to the corona discharge needle in the APCI source to produce the APCI corona discharge. The corona discharge voltage varies, as required, to maintain the set APCI spray current.
- See also [APCI spray current](#).
- APCI manifold** The manifold that houses the APCI sample tube and nozzle, and contains the plumbing for the sheath and auxiliary gas.
- APCI needle, corona discharge** A needle to which a sufficiently high voltage (typically  $\pm 3$  to  $\pm 5$  kV) is applied to produce a chemical ionization plasma by the corona discharge mechanism.
- See also [chemical ionization \(CI\)](#), [chemical ionization \(CI\) plasma](#), [atmospheric pressure chemical ionization \(APCI\)](#), and [corona discharge](#).
- APCI nozzle** The nozzle in the APCI probe that sprays the sample solution into a fine mist.
- See also [atmospheric pressure chemical ionization \(APCI\)](#).
- APCI sample tube** A fused silica tube that delivers sample solution to the [APCI nozzle](#). The APCI sample tube extends from the sample inlet to the APCI nozzle.
- See also [atmospheric pressure chemical ionization \(APCI\)](#), and [API stack](#).
- APCI source** Contains the APCI probe assembly, APCI manifold, and API stack.
- See also [atmospheric pressure chemical ionization \(APCI\)](#), [APCI manifold](#), and [API stack](#).
- APCI spray current** The ion current carried by the charged particles in the APCI source. The [APCI corona discharge voltage](#) varies, as required, to maintain the set spray current.
- APCI vaporizer** A heated tube that vaporizes the sample solution as the solution exits the sample tube and enters the atmospheric pressure region of the APCI source.
- See also [atmospheric pressure chemical ionization \(APCI\)](#).

**Glossary:** API—atmospheric pressure chemical ionization (APCI)

**API** See [atmospheric pressure ionization \(API\)](#).

**API atmospheric pressure region** The first of two chambers in the API source. Also referred to as the spray chamber.

**API capillary-skimmer region** The area between the capillary and the skimmer, which is surrounded by the tube lens. It is also the area of first-stage evacuation in the API source.

**API heated capillary** A tube assembly that assists in desolvating ions that are produced by the ESI or APCI probe.

See also [API heated capillary voltage](#).

**API heated capillary voltage** The DC voltage applied to the heated capillary. The voltage is positive for positive ions and negative for negative ions.

See also [API source](#) and [API heated capillary](#).

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

See also [API ion transfer capillary offset voltage](#) and [API ion transfer capillary temperature](#).

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

See also [API source](#) and [API ion transfer capillary](#).

**API ion transfer capillary temperature** The temperature of the ion transfer capillary, which should be adjusted for different flow rates.

See also [API source](#) and [API ion transfer capillary](#).

**API source** The sample interface between the LC and the mass spectrometer. It consists of the API probe (ESI or APCI) and API stack.

See also [atmospheric pressure ionization \(API\)](#), [ESI source](#), [APCI source](#), [ESI probe](#), and [API stack](#).

**API spray chamber** The first of two chambers in the API source. In this chamber the sample liquid exits the probe and is sprayed into a fine mist (ESI or NSI) or is vaporized (APCI) as it is transported to the entrance end of the ion transfer capillary.

**API spray shield** A stainless steel, cylindrical vessel that, in combination with the ESI or APCI flange, forms the atmospheric pressure region of the API source.

See also [atmospheric pressure ionization \(API\)](#).

**API stack** Consists of the components of the API source that are held under vacuum and includes the [API spray shield](#), [API ion transfer capillary](#), [API tube lens](#), [skimmer](#), the ion transfer capillary mount, and the tube lens and skimmer mount.

See also [atmospheric pressure ionization \(API\)](#) and [API source](#).

**API tube lens** A lens in the API source that separates ions from neutral particles as they leave the ion transfer capillary. A potential applied to the tube lens focuses the ions toward the opening of the skimmer and helps to dissociate adduct ions.

See also [API tube lens offset voltage](#), [API source](#), [API ion transfer capillary](#), and [adduct ion](#).

**API tube lens and skimmer mount** A mount that attaches to the heated capillary mount. The tube lens and skimmer attach to the tube lens and skimmer mount.

**API tube lens offset voltage** A DC voltage applied to the tube lens. The value is normally tuned for a specific compound.

See also [API tube lens](#), [adduct ion](#), and [source CID](#).

**AP-MALDI** See [atmospheric pressure matrix-assisted laser desorption/ionization \(AP-MALDI\)](#).

**APPI** See [Atmospheric Pressure Photoionization \(APPI\)](#).

**ASCII** American Standard Code for Information Interchange

**atmospheric pressure chemical ionization (APCI)** A soft ionization technique done in an ion source operating at atmospheric pressure. Electrons from a corona discharge initiate the process by ionizing the mobile phase vapor molecules. A reagent gas forms, which efficiently produces positive and negative ions of the analyte through a complex series of chemical reactions.

See also [electrospray ionization \(ESI\)](#).

**atmospheric pressure ionization (API)** Ionization performed at atmospheric pressure by using [atmospheric pressure chemical ionization \(APCI\)](#), [electrospray ionization \(ESI\)](#), or [nanospray ionization \(NSI\)](#).

**atmospheric pressure matrix-assisted laser desorption/ionization (AP-MALDI)** Matrix-assisted laser desorption/ionization in which the sample target is at atmospheric pressure.

See also [matrix-assisted laser desorption/ionization \(MALDI\)](#).

**Atmospheric Pressure Photoionization (APPI)** A soft ionization technique in which an ion is generated from a molecule when it interacts with a photon from a light source.

**atomic mass unit** Atomic Mass Unit (u) defined by taking the mass of one atom of carbon-12 as being 12u; unit of mass for expressing masses of atoms or molecules.

**Automatic Gain Control™ (AGC)** Sets the ion injection time to maintain the optimum quantity of ions for each scan. With AGC on, the scan function consists of a prescan and an analytical scan.

See also [ion injection time](#).

**autosampler** The device used to inject samples automatically into the inlet of a chromatograph.

**auxiliary gas** The outer-coaxial gas (nitrogen) that assists the sheath (inner-coaxial) gas in dispersing and/or evaporating sample solution as the sample solution exits the APCI, ESI, or H-ESI nozzle.

**auxiliary gas flow rate** The relative rate of flow of [auxiliary gas](#) (nitrogen) into the API source reported in arbitrary units.

**auxiliary gas inlet** An inlet in the API probe where auxiliary gas is introduced into the probe.

See also [auxiliary gas](#) and [atmospheric pressure ionization \(API\)](#).

**auxiliary gas plumbing** The gas plumbing that delivers outer coaxial nitrogen gas to the ESI or APCI nozzle.

**auxiliary gas valve** A valve that controls the flow of auxiliary gas into the API source.

## B

**b** bit

**B** byte (8 b)

**baud rate** data transmission speed in events per second

**BTU** British thermal unit, a unit of energy

## C

**°C** degrees Celsius

**CE** central electrode (of the Orbitrap analyzer);

European conformity. Mandatory European marking for certain product groups to indicate conformity with essential health and safety requirements set out in European Directives.

**cfm** cubic feet per minute

**chemical ionization (CI)** The formation of new ionized species when gaseous molecules interact with ions. The process can involve transfer of an electron, proton, or other charged species between the reactants.

**chemical ionization (CI) plasma** The collection of ions, electrons, and neutral species formed in the ion source during chemical ionization.

See also [chemical ionization \(CI\)](#).

**CI** See [chemical ionization \(CI\)](#).

**CID** See [collision-induced dissociation \(CID\)](#).

**cm** centimeter

**cm<sup>3</sup>** cubic centimeter

**collision gas** A neutral gas used to undergo collisions with ions.

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

**consecutive reaction monitoring (CRM) scan type** A scan type with three or more stages of mass analysis and in which a particular multi-step reaction path is monitored.

**corona discharge** In the APCI source, an electrical discharge in the region around the corona discharge needle that ionizes gas molecules to form a chemical ionization (CI) plasma, which contains CI reagent ions.

See also [chemical ionization \(CI\) plasma](#) and [atmospheric pressure chemical ionization \(APCI\)](#).

**CPU** central processing unit (of a computer)

**CRM** See [consecutive reaction monitoring \(CRM\) scan type](#).

**C-Trap** curved linear trap

**<Ctrl>** control key on the terminal keyboard

## D

***d*** depth

**Da** dalton

**DAC** digital-to-analog converter

**damping gas** Helium gas introduced into the ion trap mass analyzer that slows the motion of ions entering the mass analyzer so that the ions can be trapped by the RF voltage fields in the mass analyzer.

**data-dependent scan** A scan mode that uses specified criteria to select one or more ions of interest on which to perform subsequent scans, such as MS/MS or ZoomScan.

**DC** direct current

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

**DS** data system

**DSP** digital signal processor

## E

**ECD** See [electron capture dissociation \(ECD\)](#).

**EI** electron ionization

**electron capture dissociation (ECD)** A method of fragmenting gas-phase ions for tandem mass spectrometric analysis. ECD involves the direct introduction of low energy electrons to trapped gas-phase ions.

See also [electron transfer dissociation \(ETD\)](#) and [infrared multiphoton dissociation \(IRMPD\)](#).

**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.

**electron transfer dissociation (ETD)** A method of fragmenting peptides and proteins. In electron transfer dissociation (ETD), singly charged reagent anions transfer an electron to multiply protonated peptides in the ion trap mass analyzer. This leads to a rich ladder of sequence ions derived from cleavage at the amide groups along the peptide backbone. Amino acid side chains and important modifications such as phosphorylation are left intact.

See also [fluoranthene](#).

**electrospray ionization (ESI)** A type of atmospheric pressure ionization that is currently the softest ionization technique available to transform ions in solution into ions in the gas phase.

**EMBL** European Molecular Biology Laboratory

**<Enter>** Enter key on the terminal keyboard

**ESD** ElectroStatic Discharge. Discharge of stored static electricity that can damage electronic equipment and impair electrical circuitry, resulting in complete or intermittent failures.

**ESI** See [electrospray ionization \(ESI\)](#).

**ESI flange** A flange that holds the [ESI probe](#) in position next to the entrance of the heated capillary, which is part of the API stack. The ESI flange also seals the atmospheric pressure region of the API source and, when it is in the engaged position against the spray shield, compresses the high-voltage safety-interlock switch.



**ESI probe** A probe that produces charged aerosol droplets that contain sample ions. The ESI probe is typically operated at liquid flows of 1  $\mu\text{L}/\text{min}$  to 1  $\text{mL}/\text{min}$  without splitting. The ESI probe includes the ESI manifold, sample tube, nozzle, and needle.

**ESI source** Contains the ESI probe and the API stack.

See also [electrospray ionization \(ESI\)](#), [ESI probe](#), and [API stack](#).

**ESI spray current** The flow of charged particles in the ESI source. The voltage on the ESI spray needle supplies the potential required to ionize the particles.

**ESI spray voltage** The high voltage that is applied to the spray needle in the ESI source to produce the ESI spray current. In ESI, the voltage is applied to the spray liquid as it emerges from the nozzle.

See also [ESI spray current](#).

**ETD** See [electron transfer dissociation \(ETD\)](#).

**eV** Electron Volt. The energy gained by an electron that accelerates through a potential difference of one volt.

**Extensible Markup Language** See [XML \(Extensible Markup Language\)](#).

**external lock mass** A lock that is analyzed in a separate MS experiment from your sample. If you need to run a large number of samples, or if accurate mass samples will be intermingled with standard samples, you might want to use external lock masses. These allow more rapid data acquisition by eliminating the need to scan lock masses during each scan.

See also [internal lock mass](#).

## F

**f** femto ( $10^{-15}$ )

**°F** degrees Fahrenheit

**.fasta file** extension of a SEQUEST™ search database file

**ft** foot; feet

**Fast Fourier Transform (FFT)** An algorithm that performs a Fourier transformation on data. A Fourier transform is the set of mathematical formulas by which a time function is converted into a frequency-domain function and the converse.

**FFT** See [Fast Fourier Transform \(FFT\)](#).

**fluoranthene** A reagent anion that is used in an [electron transfer dissociation \(ETD\)](#) experiment.

**firmware** Software routines stored in read-only memory. Startup routines and low-level input/output instructions are stored in firmware.

**forepump** The pump that evacuates the foreline. A rotary-vane pump is a type of forepump.

**Fourier transform (FT)** The mathematical operation that converts the image current signal detected in an ICR trap or Orbitrap mass spectrometer to a set of  $m/z$  values. The Fourier components correspond to ion mass and the Fourier coefficients correspond to ion abundance.

**Fourier Transform - Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS)** A technique that determines the mass-to-charge ratio of an ion by measuring its cyclotron frequency in a strong magnetic field.

**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.

**fragmentation** The dissociation of a molecule or ion to form fragments, either ionic or neutral. When a molecule or ion interacts with a particle (electron, ion, or neutral species) the molecule or ion absorbs energy and can subsequently fall apart into a series of charged or neutral fragments. The mass spectrum of the fragment ions is unique for the molecule or ion.

**FT** Fourier Transformation

**FT-ICR MS** See [Fourier Transform - Ion Cyclotron Resonance Mass Spectrometry \(FT-ICR MS\)](#).

**FTMS** Fourier Transformation Mass Spectrometry

**full-scan type** Provides a full mass spectrum of each analyte or parent ion. With the full-scan type, the mass analyzer is scanned from the first mass to the last mass without interruption. Also known as single-stage full-scan type.

**FWHM** Full Width at Half Maximum

## G

**g** gram

**G** Gauss; giga ( $10^9$ )

**GC** gas chromatograph; gas chromatography

**GC/MS** gas chromatography / mass spectrometer

**GUI** graphical user interface

## H

**h** hour

**h** height

**handshake** A signal that acknowledges that communication can take place.

**HCD** See [higher energy collision-induced dissociation \(HCD\)](#).

**header information** Data stored in each data file that summarizes the information contained in the file.

**heated-electrospray ionization (H-ESI)** Converts ions in solution into ions in the gas phase by using [electrospray ionization \(ESI\)](#) in combination with heated [auxiliary gas](#).

### **higher energy collision-induced dissociation (HCD)**

Collision-induced dissociation that occurs in the HCD cell of the [Orbitrap mass analyzer](#). The HCD cell consists of a straight multipole mounted inside a collision gas-filled tube. A voltage offset between C-Trap and HCD cell accelerates parent ions into the collision gas inside the HCD cell, which causes the ions to fragment into product ions. The product ions are then returned to the Orbitrap analyzer for mass analysis. HCD produces triple quadrupole-like product ion mass spectra.

### **high performance liquid chromatography (HPLC)**

Liquid chromatography in which the liquid is driven through the column at high pressure. Also known as high pressure liquid chromatography.

**HPLC** See [high performance liquid chromatography \(HPLC\)](#).

**HV** high voltage

**Hz** hertz (cycles per second)

## I

**ICR** ion cyclotron resonance

**ID** inside diameter

**IEC** International Electrotechnical Commission

**IEEE** Institute of Electrical and Electronics Engineers

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

**in.** inch

**infrared multiphoton dissociation (IRMPD)** In infrared multiphoton dissociation (IRMPD), multiply charged ions consecutively absorb photons emitted by an infrared laser until the vibrational excitation is sufficient for their fragmentation. The fragments continue to pick up energy from the laser pulse and fall apart further to ions of lower mass.

See also [electron capture dissociation \(ECD\)](#).

**instrument method** A set of experiment parameters that define Xcalibur operating settings for the autosampler, liquid chromatograph (LC), mass spectrometer, divert valve, syringe pump, and so on. Instrument methods are saved as file type .meth.

**internal lock mass** A lock that is analyzed during the same MS experiment as your sample and is contained in the sample solution or infused into the LC flow during the experiment. Internal lock masses provide the most accurate corrections to the data.

See also [external lock mass](#).

**I/O** input/output

**ion gauge** Measures the pressure in the mass analyzer region (high-vacuum region) of the vacuum manifold.

**ion injection time** The amount of time that ions are allowed to accumulate in the ion trap mass analyzer when AGC is off. With AGC on, the ion injection time is set automatically (up to the set maximum ion injection time) based on the AGC target value.

See also: [Automatic Gain Control™ \(AGC\)](#).

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

**ion source** A device that converts samples to gas-phase ions.

**ion sweep cone** A removable cone-shaped metal cover that fits on top of the [API ion transfer capillary](#) and acts as a physical barrier to protect the entrance of the capillary.

**ion sweep gas** Extra nitrogen gas that flows along the axis of the API ion transfer capillary (between the ion sweep cone and the capillary block) towards the API spray. The sweep gas flow is thus countercurrent to the flow of the ions.

See also [ion sweep gas pressure](#).

**ion sweep gas pressure** The rate of flow of the sweep gas (nitrogen) into the API source. A measurement of the relative flow rate (in arbitrary units) to provide the required flow of nitrogen gas out from the Ion Sweep cone towards the API spray.

See also [ion sweep gas](#).

**IRMPD** See [infrared multiphoton dissociation \(IRMPD\)](#).

**IS** interstage

## K

**k** kilo ( $10^3$ , 1000)

**K** kilo ( $2^{10}$ , 1024)

**KEGG** Kyoto Encyclopedia of Genes and Genomes

**kg** kilogram

## L

**l** length

**L** liter

**LAN** local area network

**lb** pound

**LC** See [liquid chromatography \(LC\)](#).

**LC/MS** See [liquid chromatography / mass spectrometry \(LC/MS\)](#).

**LED** light-emitting diode

**LHe** liquid helium

**liquid chromatography (LC)** A form of elution chromatography in which a sample partitions between a stationary phase of large surface area and a liquid mobile phase that percolates over the stationary phase.

**liquid chromatography / mass spectrometry (LC/MS)** An analytical technique in which a high-performance liquid chromatograph (LC) and a mass spectrometer (MS) are combined.

**LN2** liquid nitrogen

**lock mass** A known reference mass in the sample that is used to correct the mass spectral data in an accurate mass experiment and used to perform a real-time secondary mass calibration that corrects the masses of other peaks in a scan. Lock masses with well-defined, symmetrical peaks work best. You can choose to use [internal lock mass](#) or [external lock mass](#).

**log file** A text file, with a .log file extension, that is used to store lists of information.

## M

**μ** micro ( $10^{-6}$ )

**m** meter; milli ( $10^{-3}$ )

**M** mega ( $10^6$ )

**M<sup>+</sup>** molecular ion

**MALDI** See [matrix-assisted laser desorption/ionization \(MALDI\)](#).

**matrix-assisted laser desorption/ionization**

**(MALDI)** A method of ionizing proteins where a direct laser beam is used to facilitate vaporization and ionization while a matrix protects the biomolecule from being destroyed by the laser.

See also [atmospheric pressure matrix-assisted laser desorption/ionization \(AP-MALDI\)](#).

**MB** Megabyte (1048576 bytes)

**MH<sup>+</sup>** protonated molecular ion

**microscan** One mass analysis (ion injection and storage or scan-out of ions) followed by ion detection. Microscans are summed, to produce one scan, to improve the signal-to-noise ratio of the mass spectral data. The number of microscans per scan is an important factor in determining the overall scan time.

**min** minute

**mL** milliliter

**mm** millimeter

**MRFA** A peptide with the amino acid sequence methionine–arginine–phenylalanine–alanine.

**MS** mass spectrometer; mass spectrometry

**MS scan modes** Scan modes in which only one stage of mass analysis is performed. The scan types used with the MS scan modes are [full-scan type](#) and [selected ion monitoring \(SIM\) scan type](#).

**MSDS** Material Safety Data Sheet

**MS/MS** Mass spectrometry/mass spectrometry, or tandem mass spectrometry is an analytical technique that involves two stages of mass analysis. In the first stage, ions formed in the ion source are analyzed by an initial analyzer. In the second stage, the mass-selected ions are fragmented and the resultant ionic fragments are mass analyzed.

**MS<sup>n</sup> scan mode** The scan power equal to 1 to 10, where the scan power is the power *n* in the expression MS<sup>n</sup>. MS<sup>n</sup> is the most general expression for the scan mode, which can include the following:

- The scan mode corresponding to the one stage of mass analysis in a single-stage full-scan experiment or a selected ion monitoring (SIM) experiment

- The scan mode corresponding to the two stages of mass analysis in a two-stage full-scan experiment or a selected reaction monitoring (SRM) experiment
- The scan mode corresponding to the three to ten stages of mass analysis (*n* = 3 to *n* = 10) in a multi-stage full-scan experiment or a consecutive reaction monitoring (CRM) experiment

See also [MS scan modes](#) and [MS/MS](#).

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

***m/z*** Mass-to-charge ratio. An abbreviation used to denote the quantity formed by dividing the mass of an ion (in u) by the number of charges carried by the ion. For example, for the ion C<sub>7</sub>H<sub>7</sub><sup>2+</sup>, *m/z*=45.5.

## N

**n** nano (10<sup>-9</sup>)

**nanospray ionization (NSI)** A type of electrospray ionization (ESI) that accommodates very low flow rates of sample and solvent on the order of 1 to 20 nL/min (for static nanospray) or 100 to 1000 nL/min (for dynamic nanospray).

**NCBI** National Center for Biotechnology Information (USA)

**NIST** National Institute of Standards and Technology (USA)

**NMR** Normal Mass Range

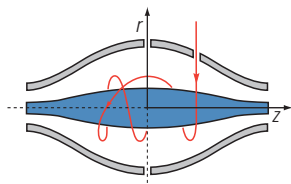
**NSI** See [nanospray ionization \(NSI\)](#).

## O

**octapole** An octagonal array of cylindrical rods that acts as an ion transmission device. An RF voltage and DC offset voltage applied to the rods create an electrostatic field that transmits the ions along the axis of the octapole rods.

**OD** outside diameter

**Orbitrap mass analyzer** The Orbitrap™ mass analyzer consists of a spindle-shaped central electrode surrounded by a pair of bell-shaped outer electrodes. Ions inside the mass analyzer orbit in stable trajectories around the central electrode with harmonic oscillations along it.



Two detection electrodes record an image current of the ions as they undergo harmonic oscillations. A Fourier transformation extracts different harmonic frequencies from the image current. An ion's mass-to-charge ratio  $m/z$  is related to the frequency  $f$  of its harmonic oscillations and to the instrumental constant  $k$  by:

$$m/z = k/f^2$$

**OT** Orbitrap

See [Orbitrap mass analyzer](#).

**OVC** outer vacuum case

$\Omega$  ohm

**P**

**p** pico ( $10^{-12}$ )

**Pa** pascal

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

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

See also [parent ion](#).

**PCB** printed circuit board

**PDA detector** The Photodiode Array detector is a linear array of discrete photodiodes on an integrated circuit chip. It is placed at the image plane of a spectrometer to allow a range of wavelengths to be detected simultaneously.

**PE** protective earth

**PID** proportional / integral / differential

**P/N** part number

**p-p** peak-to-peak voltage

**ppm** parts per million

**PQD** pulsed-Q dissociation

**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 (PR) can be a molecular ion or an electrically charged fragment of a molecular ion. Also known as parent ion.

**precursor mass** Mass of the corresponding precursor (or parent) ion or molecule.

**psig** pounds per square inch, gauge

**PTM** posttranslational modification

**pulsed Q dissociation (PQD)** Collision-induced dissociation that involves precursor ion activation at high Q, a time delay to allow the precursor to fragment, and then a rapid pulse to low Q where all fragment ions are trapped. The fragment ions can then be scanned out of the ion trap mass analyzer and detected. PQD eliminates the “1-3 Rule” low-mass cutoff for MS/MS data.

**Q**

**quadrupole** A symmetrical, parallel array of four hyperbolic rods that acts as a mass analyzer or an ion transmission device. As a mass analyzer, one pair of opposing rods has an oscillating radio frequency (RF) voltage superimposed on a positive direct current (DC) voltage. The other pair has a negative DC voltage and an RF voltage that is 180 degrees out of phase with the first pair of rods. This creates an electrical field (the quadrupole field) that efficiently transmits ions of selected mass-to-charge ratios along the axis of the quadrupole rods.

## R

**RAM** random access memory

**raw data** Uncorrected liquid chromatograph and mass spectrometer data obtained during an acquisition. Xcalibur and Xcalibur-based software store this data in a file that has a .raw file extension.

**resolution** The ability to distinguish between two points on the wavelength or mass axis.

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

**RF** radio frequency

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

**RF voltage** An AC voltage of constant frequency and variable amplitude that is applied to the ring electrode or endcaps of the mass analyzer or to the rods of a multipole. Because the frequency of this AC voltage is in the radio frequency (RF) range, it is referred to as RF voltage.

**RMS** root mean square

**RoHS** Restriction of Hazardous Substances. EU directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment.

**ROM** read-only memory

**rotary-vane pump** A mechanical vacuum pump that establishes the vacuum necessary for the proper operation of the turbomolecular pump. (Also called a roughing pump or forepump.)

**RS-232** An accepted industry standard for serial communication connections. This Recommended Standard (RS) defines the specific lines and signal characteristics used by serial communications controllers to standardize the transmission of serial data between devices.

**RT** An abbreviated form of the phrase [retention time \(RT\)](#). This shortened form is used to save space when the retention time (in minutes) is displayed in a header, for example, RT: 0.00-3.75.

## S

**s** second

**sample loop** A loop of calibrated volume that is used to perform flow injection analysis.

**scan mode and scan type combinations** A function that coordinates the three processes in the MS detector: ionization, mass analysis, and ion detection. You can combine the various scan modes and scan types to perform a wide variety of experiments.

**selected ion monitoring (SIM) scan type** A scan type in which the mass spectrometer acquires and records ion current at only one or a few selected mass-to-charge ratios.

See also [selected reaction monitoring \(SRM\) scan type](#).

**selected reaction monitoring (SRM) scan type** A scan type with two stages of mass analysis and in which 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.

**SEM** secondary electron multiplier

**Serial Peripheral Interface (SPI)** hardware and firmware communications protocol

**serial port** An input/output location (channel) for serial data transmission.

**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.

**sheath gas flow rate** The rate of flow of sheath gas into the API source. A measurement of the relative flow rate (in arbitrary units) that needs to be provided at the sheath gas inlet to provide the required flow of [sheath gas](#) to the ESI or APCI nozzle.



**sheath gas inlet** An inlet in the API probe where [sheath gas](#) is introduced into the probe.

**sheath gas plumbing** The gas plumbing that delivers [sheath gas](#) to the ESI or APCI nozzle.

**sheath gas pressure** The rate of flow of sheath gas (nitrogen) into the API source. A measurement of the relative flow rate (in arbitrary units) that needs to be provided at the sheath gas inlet to provide the required flow of inner coaxial nitrogen gas to the ESI or APCI nozzle. A software-controlled proportional valve regulates the flow rate.

See also [sheath gas](#).

**sheath gas valve** A valve that controls the flow of [sheath gas](#) into the API source. The sheath gas valve is controlled by the data system.

**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.

**SIM** See [selected ion monitoring \(SIM\) scan type](#).

**skimmer** A vacuum baffle between the higher-pressure capillary-skimmer region and the lower-pressure region. The aperture of the skimmer is offset with respect to the bore of the ion transfer capillary.

**source CID** A technique for fragmenting ions in an [atmospheric pressure ionization \(API\)](#) source. Collisions occur between the ion and the background gas, which increase the internal energy of the ion and stimulate its dissociation.

**SPI** See [Serial Peripheral Interface \(SPI\)](#).

**SRM** See [selected reaction monitoring \(SRM\) scan type](#).

**sweep gas** Nitrogen gas that flows out from behind the sweep cone in the API source. Sweep gas aids in solvent declustering and adduct reduction.

See also [sweep gas flow rate](#).

**sweep gas flow rate** The rate of flow of sweep gas into the API source. A measurement of the relative flow rate (in arbitrary units) to provide the required flow of nitrogen gas to the sweep cone of the API source.

See also [sweep gas](#).

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

## T

**T** Tesla

**target compound** A compound that you want to identify or quantitate or that a specific protocol (for example, an EPA method) requires you look for. Target compounds are also called analytes, or target analytes.

**TIC** See [total ion current \(TIC\)](#).

**TMP** See [turbomolecular pump](#).

**Torr** A unit of pressure, equal to 1 mm of mercury and 133.32 Pa.

**total ion current (TIC)** The sum of the ion current intensities across the scan range in a mass spectrum.

**tube lens offset** The voltage offset from ground that is applied to the tube lens to focus ions toward the opening of the skimmer.

See also [source CID](#).

**Tune Method** A defined set of mass spectrometer tune parameters for the ion source and mass analyzer. Tune methods are defined by using the instrument software's tune window and saved as tune file.

A tune method stores tune parameters only. (Calibration parameters are stored separately, not with the tune method.)

**tune parameters** Instrument parameters whose values vary with the type of experiment.

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

**TWA** time weighted average

## U

**u** atomic mass unit

**UHV** ultra high vacuum

**ultra-high performance liquid chromatography (U-HPLC)** See [high performance liquid chromatography \(HPLC\)](#).

**Ultramark 1621** A mixture of perfluoroalkoxycyclotriphosphazenes used for ion trap calibration and tuning. It provides ESI singly charged peaks at  $m/z$  1022.0, 1122.0, 1222.0, 1322.0, 1422.0, 1522.0, 1622.0, 1722.0, 1822.0, and 1921.9.

**UMR** Universal Mass Range

## V

**V** volt

**V AC** volts alternating current

**V DC** volts direct current

**vacuum manifold** A thick-walled, aluminum chamber with machined flanges on the front and sides and various electrical feedthroughs and gas inlets that encloses the API stack, ion optics, mass analyzer, and ion detection system.

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

**vent valve** A valve that allows the vacuum manifold to be vented to air or other gases. A solenoid-operated valve.

## W

**w** width

**W** watt

**WEEE** European Union Waste Electrical and Electronic Equipment Directive. Provides guidelines for disposal of electronic waste.

## X

**XML (Extensible Markup Language)** A general-purpose markup language that is used to facilitate the sharing of data across different information systems, particularly via the Internet.



# Index

## Numerics

- 1 V max port 3-13
- 10 V max port 3-13
- 8 kV power supply 3-49
- 90° flatapole 3-24, 3-26, 3-28

## A

- Active Pirani gauge (APG) 3-16
- adjustment, of API probe position 3-18
- air
  - circulation 5-5
  - duct 5-12
  - leaks 6-5, 7-6
- alert 3-45, 6-11
- analog signals 3-51
- analyzer chamber 3-40
- analyzer gauge 3-40
- analyzer TMP
  - cooling 3-45, 3-51
  - forevacuum 3-44
  - function 3-40
  - housing 3-45
  - inlets 3-44
  - maintenance 8-11
- APCI
  - corona discharge voltage 3-19
  - heater control 3-49
  - mode 3-49
  - vaporizer cable 3-19
  - vaporizer temperature 6-17
- API accessory kit 5-45
- API source
  - cleaning frequency 8-16
  - drainage 8-20
  - gas supply 3-46
  - replaceable parts 9-2
  - solvent drainage 3-18
- APPI lamp 3-49
- Automatic Gain Control (AGC) 3-26, 3-29, 3-31
- autosampler 6-9–6-10
- auxiliary forepump 3-15
  - power supply 3-14, 5-9
  - vacuum hose 3-42
- auxiliary gas 3-46–3-47
- axial oscillations 3-34

## B

- background ions 8-20
- bakeout 3-45, 8-12
- bath gas 3-3, 3-6, 3-31, 3-46
- bent flatapole 3-24–3-26, 3-28
- buck/boost transformer 5-9

## C

- caffeine methanol solution 5-41
- calibration parameters 6-6
- calibration solutions
  - cesium iodide 5-46
  - negative mode 5-45
  - ordering 5-39
  - positive mode 5-45
- capillary
  - removal tool 8-23
  - replaceable parts 9-2
  - voltage 3-24
- capillary temperature 7-9
- central electrode
  - schematics 3-32
  - voltages 3-33, 3-52
- central electrode pulser board 3-52
- cesium iodide
  - calibration solution 5-46
  - ordering 5-46
- checking leaks, in gas lines 8-7
- chemicals, ordering 5-41
- circuit breakers 3-12
- cleaning
  - fan filters 8-15
  - frequency 8-16
  - instrument surface 8-6
  - ion sweep cone 6-16
  - ion transfer capillary 6-16, 8-23, 8-26
- clothing 4-12
- collector
  - function 3-31
  - location 3-24, 3-26, 3-28
- collision gas, for HCD 3-31
- Compact Cold Gauge 3-16
- consumables 8-51
- contact closure 3-13, 3-37, 5-24
- control elements 3-17
- C-Trap
  - connection to HCD cell 3-35
  - function 3-31–3-32, 3-35

- gas supply 3-47
  - schematics 3-24, 3-26, 3-28
- C-Trap RF main board 3-31, 3-51
- C-Trap RF voltage 3-31

## D

- data acquisition (DAQ) board 3-48–3-49
- data system
  - communication 3-14, 6-14
  - log file 7-4
  - startup 6-10
  - wall outlets 5-9
- Declaration of Conformity A-4
- decommissioning, the instrument 4-7
- deflector electrode voltages 3-52
- dimensions, of instrument 5-3–5-4
- distilled water 8-6
- drip pan 3-41–3-42
- D-sub ports
  - APCI-ESI 3-19, 4-4
  - APPI-MALDI 3-19, 4-4
  - forepump control 3-14
  - forepump switch cord 3-14
- dynamic range 3-3–3-4, 3-7–3-9

## E

- electrodynamic squeezing, of ions 3-33
- electronic components 5-12
- electronics service switch
  - function 3-11
  - location 3-12
- emergency shutdown 4-9, 5-5
- emission sound pressure level 5-14
- Enhanced Resolution Option 3-7
- entrance lens 3-24, 3-26, 3-28–3-29
- entrance voltage 3-31, 3-51
- error diagnosis 7-7–7-9
- ESI
  - mode 3-49
  - spray voltage 3-19
- Ethernet
  - port 3-14
  - replaceable parts 9-4
  - switch 3-49
- exhaust
  - hose 3-41–3-42
  - system 3-41, 8-21
- exit lens 3-24, 3-26, 3-28
- exit voltage 3-31, 3-51
- extracting voltage 3-32
- extraction, of ion packets 3-32

## F

- fan filters
  - access 5-5
  - checking frequency 8-14
  - location 8-14
  - replacement 8-14, 9-4
- fans
  - failure 3-45, 3-51
  - inserts 3-43
  - power supply DAQ board 3-52
- Fast Fourier Transformation (FFT) 3-48
- FCC Compliance A-2
- fingerprints, removing 8-6
- flatpole exit lens 3-25
- flow rates
  - gases 3-49
    - HCD collision gas 3-47
- focusing potentials 3-52
- forepump
  - exhaust filter 8-9
  - exhaust plumbing 5-13
  - function 3-40–3-41
  - lifting 8-10
  - location 3-41, 5-13
  - maintenance 8-8–8-9
  - MSDS for oil 8-9, 8-51
  - oil 4-7, 8-9
  - oil level 6-4
  - on/off board 3-53
  - operating voltage 3-41
  - power cord 3-41
  - power supply 6-4
  - purging oil 6-19
  - replaceable parts 9-4
  - switching 3-53
  - vibration 5-13
  - warning labels 8-6, 8-9
- forevacuum port 3-11
- front side, LEDs 3-10
- FT adapter board 3-50, 3-53

## G

- gas
  - pressure 3-46, 6-12
  - pressure regulator 3-46
- gas ballast 6-4
- gas supply
  - C-Trap 3-47
  - leak check 8-7
  - nitrogen 3-15
  - replaceable parts 9-4
  - schematics 3-46
- gloves 4-12, 8-4
- goggles 4-12

ground bolt, for peripherals 3-14–3-15, 5-9  
grounding cable 5-10

## H

halogen bulbs 3-45  
handles, at the instrument 5-5–5-6  
harmonic oscillations 3-33  
hazardous chemicals 5-40  
HCD  
    collision gas valve 3-51  
    flow rate, of collision gas 3-47  
    fragment spectra 3-35  
HCD cell  
    description 3-35  
    location 3-24, 3-26, 3-28, 3-46  
Health and Safety Form 8-52, A-5  
heated capillary  
    heaters 3-49  
    location 3-24, 3-26  
    temperature 3-16, 7-5  
heater block 3-20  
heaters 3-20, 3-45  
heating cartridges 3-20, 3-45  
HESI source window 7-9  
high voltage (8 kV) socket 3-19  
high voltage electronics 3-51, 6-11  
high voltage power supply board 3-31, 3-52  
high-vacuum chamber 7-5  
holder, for syringe pump and switching valves 3-36  
humidity 5-12–5-13

## I

I/O board 3-53  
IKR 251 3-16, 6-11  
IKR 270 3-16, 3-40, 6-11  
image current 3-33–3-34, 3-48  
infusion line 5-23  
injection flatapole 3-5, 3-25–3-26  
input connection 3-12  
in-source CID, offset voltage 3-24  
Installation Kit 3-13, 5-11, 5-35, 8-21, 8-23, 8-26  
installation requirements 5-42  
instrument  
    dimensions 5-3–5-4  
    forevacuum measurement 3-16  
    high-vacuum measurement 3-16  
    lifting 5-8  
    moving 5-6, 5-8  
    operating voltage 3-15  
    performance 5-13  
    power cord 5-9, 9-4  
    rear side 3-14

    software 3-45  
    warning labels 8-6  
    weight 5-5–5-6  
instrument status window 6-12, 7-8–7-9, 8-12  
interflatapole lens 3-25, 3-27  
interlocks 3-19, 8-33–8-36  
internal computer 3-48  
internal standard 3-3–3-4, 3-7–3-9  
ion dephasing 3-35  
Ion Funnel 3-27  
ion optic supply DC board 3-49  
ion optic supply RF board 3-50  
ion optics cage assembly 8-44  
ion oscillation 3-32  
ion packets 3-32  
    shape 3-34  
ion pre-filtering mode 3-27  
ion source  
    housing 3-18  
    housing guide pins 3-19  
    interface 3-20–3-21, 8-44  
    mount 3-19  
    type 3-49  
ion sweep cone  
    cleaning 6-16  
    function 3-21  
    removal 8-24, 8-28  
ion trajectory 3-32  
ion transfer capillary  
    blockage 8-22  
    cleaning 6-16  
    function 3-20  
    offset voltage 3-19  
ions  
    detection 3-34  
    electrodynamic squeezing 3-33  
    image current 3-34  
    packet shape 3-34–3-35

## L

lab coat 4-12  
laboratory  
    exhaust system 3-41, 8-21  
    gas supplies 3-15  
    room temperature 5-12  
LC  
    flow control 3-37  
    leaks 3-18  
leak check, in gas lines 8-7  
LEDs  
    system status 3-10  
    vacuum 3-10  
lens system 3-31  
lever tool 8-44–8-45, 9-2

lifting, the instrument 5-8  
lock masses 3-3–3-4, 3-7–3-9  
log file 7-4  
loop injector 3-37, 5-24

## M

main power circuit breaker switch  
  function 3-15, 3-43  
  location 3-11–3-12, 4-9, 7-4  
  status 3-10  
  usage 3-11, 6-7–6-8, 6-10  
main RF supply 3-51  
mains failure 7-4, 8-12  
mains supply connector 3-14, 5-9  
maintenance  
  procedures 8-5  
  vacuum system 8-8  
mass accuracy 3-3–3-4, 3-7–3-9, 6-6–6-7, 6-15  
mass calibration 5-12  
Material Safety Data Sheet (MSDS) 5-40  
messages window 7-7–7-8  
micro controller 3-50  
mobile phones 4-6  
modifiers 5-42  
moving  
  forepump 8-10  
  instrument 5-6  
MRFA  
  ordering 5-41  
  stock solution 5-43

## N

*n*-butylamine  
  ordering 5-41  
  stock solution 5-44  
negative ion mode, calibration solution 5-39, 5-45  
nitric acid 8-24  
nitrogen  
  connection to source 5-11  
  consumption 6-4–6-5, 6-7, 6-9  
  gas flow 3-47  
  inlet 3-14, 3-46, 5-9, 5-11  
  inlet port 3-46  
  pressure 3-47  
  purity 5-11  
  supply 3-15, 6-4  
noise emission 5-14  
noise reduction cover 3-41–3-42

## O

oil level, of forepump 6-4

oil vapor 5-2, 5-13, 6-2  
operating fluid reservoir, of TMP 8-11  
operating vacuum 3-10  
Orbitrap analyzer  
  central electrode 3-52  
  deflector electrode 3-52  
  differential pumping 3-32  
  electrodes 3-34  
  ion extraction 3-32  
  ion trajectories 3-34  
  lenses 3-32  
  measuring principle 3-33  
  principle 3-32  
  schematics 3-24, 3-26, 3-28  
  temperature 3-52  
  voltages 3-34  
ordering  
  calibration solutions 5-39  
  chemicals 5-41  
  replaceable parts 9-1  
output connection 3-12  
overheat, avoiding 5-5, 8-14  
oxygen, in the ion source 6-4, 6-13

## P

pallet jack 5-6  
part numbers 9-1  
Peltier element 3-52  
performance, of instrument 5-13  
peripherals  
  connecting 9-4  
  grounding 3-15  
  power supply 3-15  
personal protective equipment (PPE) 4-12  
Pirani gauge 3-40, 6-10  
placing, the instrument 5-12  
plug connectors 9-4  
polarity switching 3-3–3-4, 3-7–3-9  
polarity, of central Orbitrap electrode 3-52  
positive ion mode, calibration solution 5-39, 5-45  
power  
  failure 3-44, 7-4  
  fuses 3-41, 5-9  
power column 3-11, 3-14  
power cords 3-42  
  forepump 3-41  
  instrument 5-9, 8-2, 9-4  
power fail detector 7-4  
Power LED 6-14  
power panel 3-11  
power supply 1 board 3-50  
power supply DAQ board 3-52  
power supply, for forepump 3-14, 5-9  
preamplifier 3-48

Preinstallation Kit 1-5, 5-1  
 pressure relief valves 3-46  
 pressure, of nitrogen 6-4  
 printed circuit boards 3-48  
 probe sensor 3-20  
 PT-100 3-52  
 pumping inlets 3-43–3-44  
 pumping, the system 8-12  
 pumps, manuals 8-8  
 purging, forepump oil 6-19

## Q

quad exit lens 3-29  
 quadrupole  
   board 3-50  
   function 3-29  
   location 3-26, 3-28  
   offset voltage 3-31  
 quality, of vacuum 3-51

## R

rating plate 4-5  
 Ready Out port 3-12  
 reagents 5-42  
 rebooting, of instrument 7-4  
 receptacles 3-41, 5-9  
 removing  
   gases 8-12  
   stains 8-6  
 replaceable parts  
   API source 9-2  
   capillary 9-2  
   Ethernet 9-4  
   fan filter 8-14, 9-4  
   forepump 9-4  
   gas supply 9-4  
   source drain 9-3  
 reset button 3-13, 4-9  
 reset switch 3-53  
 resetting, the instrument 6-14  
 resolution 3-3–3-4, 3-7–3-9, 6-6  
 RF C-Trap main board 3-52  
 RF output control 3-50  
 RF voltage supply 3-51  
 room temperature 5-12  
 rotor assembly 8-11  
 RS232 serial interface 3-13, 3-37

## S

safety glasses 4-12

safety labels 4-3  
 safety relay 3-18, 3-49  
 sensitivity, of instrument 3-3–3-4, 3-7–3-9  
 serial number 4-5  
 Serial Source Interface 3-49–3-50  
 setting up, conditions for operation 6-12  
 sheath gas 3-46–3-47  
 short circuits 5-12  
 shutdown 6-8, 6-10  
 shutting off, power 3-12  
 S-lens  
   function 3-21  
   location 3-24, 3-26  
 S-Lens RF generator board 3-50, 3-53  
 sodium dodecyl sulfate  
   ordering 5-41  
   stock solution 5-45  
 sodium taurocholate  
   ordering 5-41  
   stock solution 5-45  
 software 3-48, 6-10  
 solvent waste  
   container 6-19, 8-20  
   removal 8-21  
 solvents  
   for operating the instrument 5-42  
   recommendations 5-42  
 solvents, drainage 3-18  
 source board 3-10, 3-46, 3-49  
 source chamber 3-40  
 source drain, replaceable parts 9-3  
 source TMP  
   cooling 3-45  
   forevacuum 3-41–3-43  
   function 3-40, 3-43  
   inlets 3-43–3-44  
   maintenance 8-11  
 spectrum 3-35  
 SPI bus 3-49–3-52  
 split lens 3-26, 3-28–3-29, 3-50  
 spray cone 6-18, 8-24, 8-28  
 stains, removing 8-6  
 standby condition 6-7  
 Start In input 5-37  
 Start Out port 3-12  
 starting up, instrument 6-10  
 static electricity 5-12  
 Status LED 6-14  
 stock solutions  
   caffeine 5-43  
   MRFA 5-43, 5-45  
   *n*-butylamine 5-44  
   sodium dodecyl sulfate 5-44  
   sodium taurocholate 5-44  
   Ultramark 1621 5-43

support points, of instrument 5-8  
sweep cone, location 3-19  
sweep gas  
  flow 6-7  
  flow setting 6-7  
  inlet 6-18, 8-25  
  supply port 6-18  
sweep gas, flow setting 6-5  
switching on, the vacuum system 3-16  
switching valve 3-13, 3-37, 3-49, 9-4  
syringe  
  connecting to LC union 5-23  
  connecting to LC union Tee 5-25  
syringe pump  
  control 3-49, 3-53  
  interface 3-13  
  part number 9-4  
  port 3-12, 5-34  
  usage 5-19, 5-22  
system  
  bakeout 3-10, 3-45, 8-12  
  rebooting 7-4  
  reset button 3-12  
  resetting 6-14  
  shutdown 6-8  
  standby 6-7  
  starting up 6-10  
  status LEDs 3-10, 3-49  
  venting 7-4  
System LED 6-14

## T

temperature  
  checks 3-45  
  fluctuations 5-12  
  monitor 5-12  
  probe 3-20, 3-52  
temperatures  
  heated capillary 7-5  
  ion source 3-49  
thermal overload 3-12  
third-party manuals 1-6  
tilt angle, of instrument 5-8  
TK lens 3-28  
TPR 280 3-16, 3-40  
transfer multipole 3-24, 3-26, 3-28–3-29  
transport pallet 5-5–5-6  
trigger cable 3-13  
tune parameters 6-6  
turbomolecular pumps  
  bearing 8-11  
  communication 3-51

  maintenance 8-11  
  status 3-43  
Tygon tubing 8-20

## U

UHV chamber 3-44  
Ultramark 1621  
  ordering 5-41  
  stock solution 5-43  
uninterruptible power supply 7-4  
USB interface 3-48–3-50  
USB port 3-13  
user maintenance 8-1, 8-5

## V

vacuum  
  analyzer chamber 3-44  
  compartments 3-40  
  control 3-16  
  deterioration 3-45  
  establishing 6-10  
  failure 6-11  
  gauges 3-16, 3-51  
  manifold 3-40  
  quality 3-51  
  source chamber 3-43  
Vacuum / Bakeout window 6-12, 8-22  
vacuum control board 3-45  
vacuum hose 3-43  
Vacuum LED 3-10, 6-11  
vacuum system  
  controls 3-44  
  maintenance 8-11  
  moisture 3-45  
  schematics 3-40  
Valve 1 port 3-13, 5-34  
Valve 2 port 3-13, 5-34  
valve, for HCD collision gas 3-51  
vent prevent ball 3-20  
vent tubing 5-13  
vent valve  
  function 3-44  
  location 3-40, 3-46–3-47  
  switching 3-51  
ventilation slots 3-11, 5-5, 8-14  
venting, waste drain tubing 5-13  
vertical clearance, of instrument 5-5  
vibration 5-13  
view ports, at the ion source housing 3-18  
voltage sags 5-9

**W**

warning labels

forepump 8-9

instrument 4-3

location 8-6

waste

drain tubing 5-13

solvent 3-18

WEEE Compliance A-3

weight, of instrument 5-5

wheels, of the instrument 5-8

workbench, for instrument 5-5

**X**

Xcalibur 3-48

**Z**

Z-lens 3-3, 3-6, 3-24, 3-26, 3-28, 3-44







