Waters
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Waters Xevo TQ-XS Mass Spectrometry System

Overview and Maintenance Guide

715004990
Revision A

General information

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Trademarks

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Contacting Waters

Contact Waters with enhancement requests or technical questions regarding the use, transportation, removal, or disposal of any Waters product. You can reach us via the Internet, telephone, or conventional mail.

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System manufacturing information

Manufacturer:

Waters Corporation

34 Maple Street

Milford, MA 01757

USA

Manufacturing site:

Waters Technologies Ireland Ltd.

Wexford Business Park

Drinagh, Wexford, Ireland

Safety considerations

Some reagents and samples used with Waters instruments and devices can pose chemical, biological, or radiological hazards (or any combination thereof). You must know the potentially hazardous effects of all substances you work with. Always follow Good Laboratory Practice (GLP), and consult your organization's standard operating procedures as well as your local requirements for safety.

Considerations specific to the device

Power cord replacement hazard

Warning: To avoid electric shock, use the SVT-type power cord in the United States and HAR-type (or better) cord in Europe. The main power cord must be replaced only with one of adequate rating. For information regarding what cord to use in other countries, contact your local Waters distributor.

Solvent leakage hazard

The source exhaust system is designed to be robust and leak-tight. Waters recommends you perform a hazard analysis assuming a maximum leak into the laboratory atmosphere of 10% LC eluate.

Warning: To avoid exposure to toxic substances and biohazards from O-ring leaks in the source exhaust system, observe these precautions:

- Replace the source O-rings at intervals not exceeding one year.
- Prevent chemical degradation of the source O-rings, which can withstand exposure only to certain solvents, by determining whether any solvents you use are chemically compatible with the composition of the O-rings.

Bottle placement prohibition

Warning: To avoid injury from electrical shock or fire, and damage to the equipment, do not place vessels containing liquid atop the workstation or ancillary equipment or otherwise expose those units to dripping or splashing liquids.

Prohibited: Do not place vessels containing liquid—such as solvent bottles—atop the workstation or ancillary equipment or otherwise expose those units to dripping or splashing liquids.

Spilled solvents hazard

Prohibited: To avoid equipment damage caused by spilled solvent, do not place reservoir bottles directly atop an instrument or device or on its front ledge. Instead, place the bottles in the bottle tray, which serves as secondary containment in the event of spills.

Flammable solvents hazard

Warning: To prevent the ignition of flammable solvent vapors in the enclosed space of a mass spectrometer's ion source, ensure that these conditions are met:

- Nitrogen flows continuously through the source.
- A gas-fail device is installed, to interrupt the flow of LC solvent should the nitrogen supply fail.
- The nitrogen supply pressure does not fall below 400 kPa (4 bar, 58 psi) during an analysis requiring the use of flammable solvents.

When using flammable solvents, ensure that a stream of nitrogen continuously flushes the instrument's source, and the nitrogen supply pressure remains above 400 kPa (4 bar, 58 psi). You must also install a gas-fail device that interrupts the solvent flowing from the LC system in the event the supply of nitrogen fails.

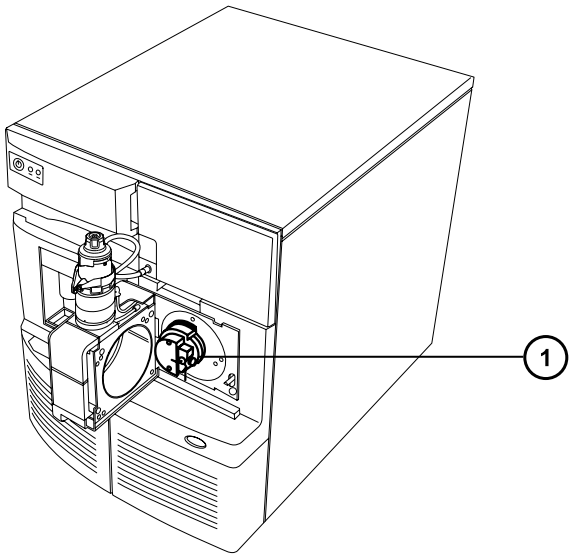
Glass breakage hazard

Warning: To avoid injuries from broken glass, falling objects, or exposure to toxic substances, never place containers on top of the instrument or on its front covers.

High temperature hazard

Warning: To avoid burn injuries, avoid touching the source ion block assembly when operating or servicing the instrument.

Mass spectrometer high temperature hazard



1 Source ion block assembly

Hazards associated with removing an instrument from service

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid puncture injuries, handle sample needles, syringes, fused silica lines, and borosilicate tips with extreme care.

Warning: To avoid eye injury from broken fused silica lines, use eye protection when performing this procedure.

When you remove the instrument from use to repair or dispose of it, you must decontaminate all of its vacuum areas. These are the areas in which you can expect to encounter the highest levels of contamination:

- Source interior
- Waste tubing
- Exhaust system
- Rotary pump oil (where applicable)

The need to decontaminate other vacuum areas of the instrument depends on the kinds of samples the instrument analyzed and their levels of concentration. Do not dispose of the instrument or return it to Waters for repair until the authority responsible for approving its removal from the premises specifies the extent of decontamination required and the level of residual

contamination permissible. That authority must also prescribe the method of decontamination to be used and the appropriate protection for personnel undertaking the decontamination process.

You must handle items such as syringes, fused silica lines, and borosilicate tips used to carry sample into the source area in accordance with laboratory procedures for contaminated vessels and sharps. To avoid contamination by carcinogens, toxic substances, or biohazards, you must wear chemical-resistant gloves when handling or disposing of used oil.

Electrical power safety notice

Do not position the instrument so that it is difficult to disconnect the power cord.

Safety hazard symbol notice

Documentation needs to be consulted in all cases where the  symbol is used to find out the nature of the potential hazard and any actions which have to be taken.

Equipment misuse notice

If equipment is used in a manner not specified by its manufacturer, protections against personal injury inherent in the equipment’s design can be rendered ineffective.

Safety advisories

Consult the "Safety advisories" appendix in this publication for a comprehensive list of warning advisories and notices.

Operating this device

When operating this device, follow standard quality-control (QC) procedures and the guidelines presented in this section.

Applicable symbols

Symbol	Definition
	Manufacturer

Symbol	Definition
	Date of manufacture
	Authorized representative of the European Community
	Confirms that a manufactured product complies with all applicable European Community directives
	Australia EMC compliant
	Confirms that a manufactured product complies with all applicable United States and Canadian safety requirements
	Consult instructions for use
	Alternating current
	Electrical and electronic equipment with this symbol may contain hazardous substances and should not be disposed of as general waste. For compliance with the Waste Electrical and Electronic Equipment Directive (WEEE) 2012/19/EU, contact Waters Corporation for the correct disposal and recycling instructions.
	Serial number
	Part number catalog number

Audience and purpose

This guide is for operators of varying levels of experience. It gives an overview of the device and explains how to prepare it for operation, change its modes of operation, and maintain it.

Intended use of the device

Waters designed the Xevo TQ-XS for use as a research tool to accurately, reproducibly, and robustly quantify target compounds present at the lowest possible levels in highly complex sample matrices. It is not for use in diagnostic procedures.

When fitted with Waters options (APCI, APGC, APPI, ASAP, ESCi, NanoFlow ESI, TRIZAIC, UniSpray, UPLC, ionKey), or optional third-party sources (DART, DESI, or LDTD), the Xevo TQ-XS does not comply with the European Union In Vitro Diagnostic Device Directive 98/79/EC.

Calibrating

To calibrate LC systems, adopt acceptable calibration methods using at least five standards to generate a standard curve. The concentration range for standards must include the entire range of QC samples, typical specimens, and atypical specimens.

When calibrating mass spectrometers, consult the calibration section of the operator's guide for the instrument you are calibrating. In cases where an overview and maintenance guide, not an operator's guide, accompanies the instrument, consult the instrument's online Help system for calibration instructions.

Quality control

Routinely run three QC samples that represent subnormal, normal, and above-normal levels of a compound. If sample trays are the same or very similar, vary the location of the QC samples in the trays. Ensure that QC sample results fall within an acceptable range, and evaluate precision from day to day and run to run. Data collected when QC samples are out of range might not be valid. Do not report these data until you are certain that the instrument performs satisfactorily.

EMC considerations

FCC radiation emissions notice

Changes or modifications not expressly approved by the party responsible for compliance, could void the user's authority to operate the equipment. This device complies with Part 15 of the FCC Rules. Operation is subject to the following two conditions: (1) this device may not cause harmful interference, and (2) this device must accept any interference received, including interference that may cause undesired operation.

Canada spectrum management emissions notice

This class A digital product apparatus complies with Canadian ICES-001.

Cet appareil numérique de la classe A est conforme à la norme NMB-001.

ISM classification: ISM group 1 class A

This classification has been assigned in accordance with IEC CISPR 11 Industrial Scientific and Medical (ISM) instruments requirements.

Group 1 products apply to intentionally generated and/or used conductively coupled radio-frequency energy that is necessary for the internal functioning of the equipment.

Class A products are suitable for use in all establishments other than residential locations and those directly connected to a low voltage power supply network supplying a building for domestic purposes.

There may be potential difficulties in ensuring electromagnetic compatibility in other environments due to conducted as well as radiated disturbances.

EMC grounding requirements

Notice: To avoid difficulties in ensuring electromagnetic compatibility, if the instrument's pump control cable is attached to the vacuum hose, ensure that the cable is grounded to the mass spectrometer.

EC authorized representative

EC REP

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Table of contents

1 Waters Xevo TQ-XS Overview

The Xevo TQ-XS is a tandem quadrupole, atmospheric pressure ionization (API) mass spectrometer. It is designed for routine HPLC/MS/MS and UPLC/MS/MS analyses in quantitative and qualitative applications, and can operate at fast acquisition speeds compatible with UltraPerformance LC.

You can use theXevo TQ-XS with the following high-performance ZSpray dual-orthogonal API sources:

- Standard multi-mode electrospray ionization/atmospheric pressure chemical ionization/ combined electrospray ionization and atmospheric pressure chemical ionization (ESI/APCI/ ESCi)

  Requirement: Dedicated APCI operation requires an additional probe.
- Optional UniSpray source
- Optional dual-mode atmospheric pressure photoionization (APPI)/APCI
- Optional low-flow ESI
- Optional NanoFlow ESI
- Optional atmospheric solids analysis probe (ASAP)
- Optional atmospheric pressure gas chromatography (APGC)
- Optional TRIZAIC UPLC
- Optional ionKey source

You can also use the Xevo TQ-XS with the following optional third-party sources:

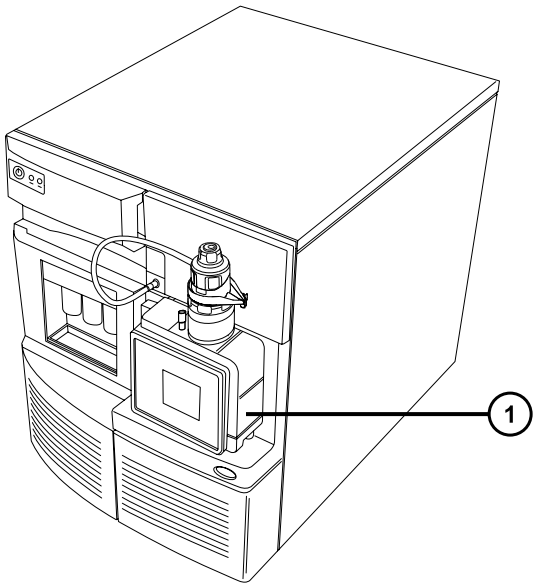
- Direct analysis in real time (DART)
- Desorption electrospary ionization (DESI)
- Laser diode thermal desorption (LDTD)

For additional details, refer to the appropriate manufacturer's documentation.

Available source options can vary, depending on the software you use to operate the Xevo TQ-XS. Refer to the MassLynx or UNIFI online Help for more information about supported sources.

For mass spectrometer specifications, see the *Waters Xevo TQ-XS Site Preparation Guide* (715005172).

Figure 1–1: Waters Xevo TQ-XS



1 Source enclosure

1.1 IntelliStart technology

IntelliStart technology monitors instrument performance and indicates when the instrument is ready for use.

The software automatically tunes and mass calibrates the instrument, displays performance readbacks, and enables simplified setup of the system for use in routine analytical and open-access applications.

The IntelliStart fluidics system[1] is built into the mass spectrometer. It delivers sample directly to the MS probe from the LC column or from three integral reservoirs. The integral reservoirs can also deliver sample through direct or combined infusion, enabling you to optimize instrument performance at analytical flow rates.

See IntelliStart fluidics system and the mass spectrometer's online Help for further details on IntelliStart technology.

[1] In Waters documents, the term "fluidics" refers to the IntelliStart Fluidics system, which is the instrument's onboard system that delivers sample and solvent to the probe of the mass spectrometer. It can also denote plumbing components and fluid pathways within and between system modules.

1.2 ACQUITY UPLC/MS Xevo TQ-XS systems

The Waters Xevo TQ-XS is compatible with the ACQUITY UPLC systems. If you are not using an ACQUITY UPLC system, refer to the documentation relevant to your LC system.

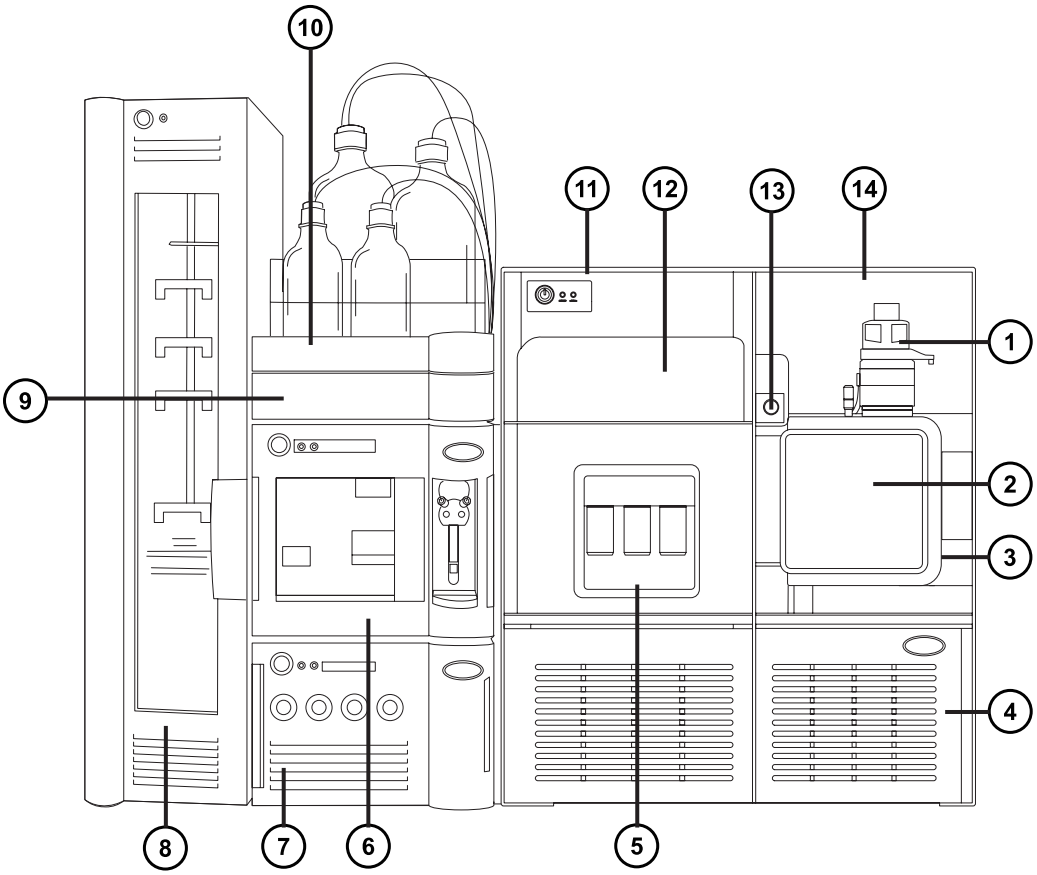
1.2.1 ACQUITY UPLC system

The ACQUITY UPLC system includes a binary or quaternary solvent manager, sample manager, column heater or column manager, optional sample organizer, one or more detectors, a specialized ACQUITY UPLC column, and software to control the system.

For additional information, see the *ACQUITY UPLC System Operator's Guide* or *Controlling Contamination in UltraPerformance LC/MS and HPLC/MS Systems* (part number 715001307). You can find these documents on www.waters.com; click **Services & Support** > **Support**.

1.2.2 Waters ACQUITY Xevo TQ-XS UPLC/MS system

Figure 1–2: Waters ACQUITY Xevo TQ-XS UPLC/MS System



1. Probe adaptor
2. Source enclosure
3. Source enclosure release
4. Xevo TQ-XS
5. Access door to the fluidics
6. Sample manager
7. Binary solvent manager or Quaternary solvent manager
8. Sample organizer (optional on the ACQUITY UPLC system)
9. Column heater
10. Solvent tray
11. Access door to the fluidics valve
12. Removable panel for ACQUITY arm
13. Probe high voltage connector
14. Source interface sliding door

1.2.3 ACQUITY UPLC M-Class system

The ACQUITY UPLC M-Class system is designed for nano-scale and micro-scale separations.

M-Class system components are optimized for use with sub-2µm particle liquid chromatography and use reduced fluid volumes. The supported flow rate for a gradient elution ranges from 200 nL/min to 100 µL/min at 15,000 psi.

For further information, see the *ACQUITY UPLC M-Class System Guide* or *Controlling Contamination in UltraPerformance LC/MS and HPLC/MS Systems* (part number 715001307). You can find these documents on www.waters.com; click **Services & Support** > **Support**.

1.2.4 Non-ACQUITY devices for use with the Xevo TQ-XS

The following non-ACQUITY LC devices are validated for use with the Xevo TQ-XS:

- Waters Alliance 2695 separations module
- Waters Alliance 2795 separations module

- Waters 2998 PDA detector
- Waters 2487 UV detector
- Waters 1525µ binary gradient pump + 2777 autosampler

1.2.5 Software and data system

You can use MassLynx software v4.2 to control the mass spectrometer. The software enables these major operations:

- Configuring the system
- Creating LC and MS/MS methods that define operating parameters for a run
- Using IntelliStart software to automatically tune and mass calibrate the mass spectrometer
- Running samples
- Acquiring data
- Monitoring the run
- Processing data
- Reviewing data
- Printing data

1.2.5.1 MassLynx software

MassLynx software acquires, analyzes, manages, and distributes mass spectrometry, ultraviolet (UV), evaporative light scattering (ELS), and analog data. OpenLynx and TargetLynx XS application managers are included with MassLynx software.

See the MassLynx software user documentation and online Help for information about using MassLynx software.

You configure settings, monitor performance, run diagnostic tests, and maintain the system and its modules via the MassLynx Instrument Control application.

The Instrument Control software, which functions independently of MassLynx software, does not recognize or control data systems.

See the online Help for the Instrument Console system for additional details.

1.3 Ionization techniques and source probes

Note: Available source options can vary depending on the software used to operate the Xevo TQ-XS. Refer to the instrument software's online Help for more information about supported sources.

1.3.1 Electrospray ionization

In electrospray ionization (ESI), a strong electrical charge is applied to the eluent as it emerges from a nebulizer. The droplets that compose the resultant aerosol undergo a reduction in size (solvent evaporation). As solvent continues to evaporate, the charge density increases until the droplet surfaces eject ions (ion evaporation). The ions can be singly or multiply charged.

To operate the source in ESI mode, you fit the source enclosure with an ESI probe adaptor and ESI probe assembly.

The standard ESI probe assembly accommodates flow rates of up to 2 mL/min, making it suitable for LC applications in the range of 100 µL/min to 2 mL/min. To reduce peak broadening for lower-flow-rate LC applications, such as 1-mm UPLC columns, use the optional, small-bore capillary, which can accommodate a maximum flow rate of 200 µL/min.

See also: ESI, ESCi, and APCI modes for further details.

1.3.2 ESCi

ESCi mode is supplied as standard equipment on the mass spectrometer. In ESCi, the standard ESI probe adaptor is used in conjunction with a corona pin, to allow alternating acquisition of ESI and APCI ionization data, which facilitates high throughput and wider compound coverage.

See ESI, ESCi, and APCI modes for further details.

1.3.3 APCI

An optional dedicated high-performance APCI interface is available. APCI produces singly charged protonated or deprotonated molecules for a broad range of nonvolatile analytes.

The APCI interface consists of the ESI/APCI/ESCi enclosure fitted with a corona pin and an APCI probe adaptor.

See ESI, ESCi, and APCI modes for further details.

1.3.4 Dual-mode APPI/APCI source

The optional, combined APPI/APCI source comprises an APCI probe adaptor and the APPI lamp drive assembly. The APPI lamp drive assembly comprises a UV lamp and a repeller electrode. In addition, a specially shaped, dual, APPI/APCI corona pin can be used. You can operate the source in APPI, APCI, or dual mode, which switches rapidly between APPI and APCI ionization modes.

See Combined APPI/APPI source for further details.

1.3.5 UniSpray

The UniSpray source enables the detection of a wide range of compounds in a single analysis. In contrast to Electrospray ionization, UniSpray uses a grounded capillary, and the resulting spray is directed at an impactor pin held at a voltage, creating smaller charged droplets, amenable to easy desolvation.

See UniSpray source for further details.

1.3.6 Low-flow ESI probe

The optional low-flow ESI probe is fitted with a narrow bore capillary suitable for use with flow rates from 5 µL/min to 100 µL/min. Its probe tip is optimized for this capillary.

The low-flow ESI probe replaces the standard ESI probe in the instrument's source housing.

See the *Low-flow ESI Probe Operator's Guide* for further details.

1.3.7 NanoFlow ESI source

NanoFlow is the name given to several techniques that use low flow rate ESI. The NanoFlow source allows ESI in the flow rate range of 5 to 1,000 nL/min. For a given sample concentration, the ion currents observed approximate those seen in normal flow rate electrospray. However, for similar experiments, NanoFlow's significant reduction in sample consumption accompanies significant increases in sensitivity.

The following options are available for the spraying capillary:

- Universal nebulizer sprayer (Nano LC).
  This option is for flow injection or for coupling to nano-UPLC. It uses a pump to regulate the flow rate downward to 100 nL/min. If a syringe pump is used, a gas-tight syringe is necessary to effect correct flow rates without leakage. A volume of 250 µL is recommended.
- Borosilicate glass capillaries (nanovials).
  Metal-coated, glass capillaries allow the lowest flow rates. They are usable for one sample, and then must be discarded.
- Capillary Electrophoresis (CE) or Capillary Electrochromatography (CEC) sprayer.
  This option uses a make-up liquid at the capillary tip that provides a stable electrospray. The make-up flow rate is less than 1 µL/min.
  See NanoFlow ESI source for further details.

1.3.8 Atmospheric solids analysis probe (ASAP)

The ASAP facilitates rapid analysis of volatile and semivolatile compounds in solids, liquids, and polymers. It is particularly suited to analyzing low-polarity compounds. The ASAP directly

replaces the ESI or APCI probe in the instrument's source housing and has no external gas or electrical connections.

See the *Atmospheric Solids Analysis Probe Operator's Guide Supplement* for further details.

1.3.9 APGC

The Waters APGC couples an Agilent GC with the Xevo TQ-XS. Doing so enables you to perform LC and GC analyses in the same system, without compromising performance. The APGC provides complementary information to the LC/MS instrument, enabling analysis of compounds of low molecular weight and low-to-intermediate polarity.

See the *Atmospheric Pressure GC Operator's Guide Supplement* for further details.

1.3.10 TRIZAIC UPLC source

The TRIZAIC UPLC source accepts a nanoTile device, which combines the functions of an analytical column, trapping column, and nanospray emitter. This technology simplifies the implementation of capillary-scale chromatography and analysis of limited-volume samples.

See the *TRIZAIC UPLC System Guide* for further details.

1.3.11 ionKey source

The ionKey source integrates UPLC separation into the source of the mass spectrometer. The source accepts an iKey Separation Device, which contains the fluidic connections, electronics, ESI interface, heater, e-cord, and chemistry. Inserting the iKey simultaneously engages the electronic and fluidic connections. This technology eliminates the need to manually connect electronic cables and tubing, and simplifies the user experience.

See the *ACQUITY UPLC M-Class System Guide* (part number 715003588) and the *ionKey/MS System Guide* (part number 715004028) for further details.

See also: ionKey source.

1.4 IntelliStart fluidics system

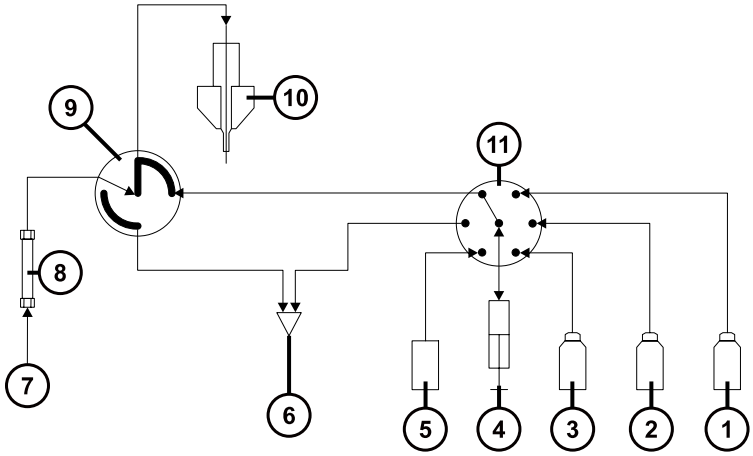
1.4.1 Overview

The IntelliStart fluidics system is a solvent delivery system built into the mass spectrometer. It delivers sample directly to the MS probe in one of these ways:

- From the LC column.
- From three integral reservoirs. (The reservoirs can also deliver sample, by direct or combined infusion, to enable optimization at analytical flow rates.)
- From a wash reservoir that contains solvent for automated flushing of the instrument's solvent delivery system.

For further information on the IntelliStart fluidics system, see IntelliStart Fluidics Plumbing and the diagram located on the inside of the fluidics access door (see Waters ACQUITY Xevo TQ-XS UPLC/MS system).

Figure 1–3: IntelliStart fluidics system:



1. Reservoir C
2. Reservoir B
3. Reservoir A
4. Pump
5. Wash bottle, located in solvent tray
6. To waste system
7. LC
8. Column
9. Diverter valve
10. Probe
11. 7-port selector valve

1.4.2 System components

The onboard system incorporates a 7-port selector valve, a multi-position diverter valve, a pump, and three sample reservoirs.

The sample reservoirs are mounted on the instrument's front panel. When you select a solvent from the instrument console, an LED illuminates the appropriate reservoir. You can simultaneously illuminate all three reservoirs or extinguish the LEDs for light-sensitive samples.

Recommendation: Use reservoir A for the calibrant solution, reservoir B for tuning compounds, and reservoir C for analyte/optimization solution.

1.4.3 System operation

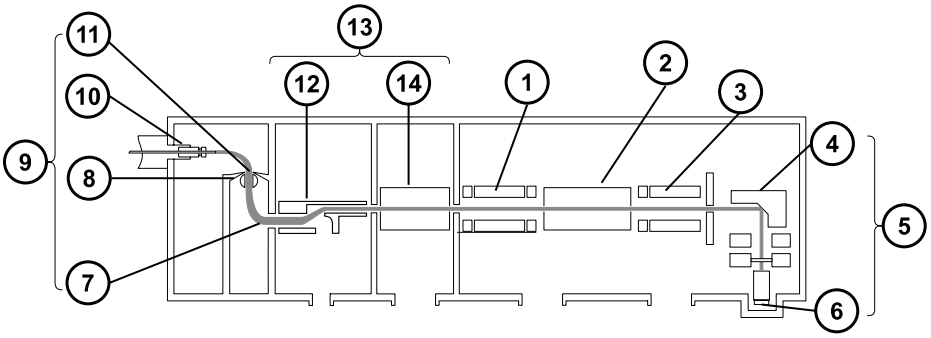
The software automatically controls solvent and sample delivery during auto-tuning, auto-calibration, and method development, via the instrument console.

See the mass spectrometer's online Help for additional details on IntelliStart software and operation of the instrument's solvent delivery system.

1.5 Ion optics

The mass spectrometer's ion optics operate as follows:

1. Samples from the LC or instrument's solvent delivery system are introduced at atmospheric pressure into the ionization source, where they are ionized.
2. The ions pass through the sample cone into the vacuum system.
3. The resulting ion beam passes through the source sampling orifice, undergoing a certain amount of expansion.
4. The ion beam then passes into the entrance of the StepWave transfer optics. The entrance is large enough to efficiently capture ions in the expanded beam. The StepWave transfer optics comprise two stages. The first stage (conjoined ion guide) focuses the ion beam and directs it to the second stage (T-Wave ion guide). The off-axis design ensures that any neutral materials entering the source sampling orifice are actively extracted from the system.
5. The ions then pass to the first quadrupole, where they can be filtered according to their mass-to-charge ratio (*m/z*).
6. The mass-separated ions pass into the T-Wave/ScanWave collision cell, where they undergo collision-induced dissociation (CID) or pass to the second quadrupole. Any fragment ions can then be mass-analyzed by the second quadrupole.
7. The transmitted ions are detected by the photomultiplier detection system.
8. The signal is amplified, digitized, and sent to the mass spectrometry software:



1. Quadrupole 1 (MS1)
2. T-Wave/ScanWave collision cell
3. Quadrupole 2 (MS2)
4. Conversion dynode
5. Detector assembly
6. Photomultiplier tube
7. Source sampling orifice
8. Isolation valve
9. Z-Spray ion source
10. Sample inlet
11. Sample cone
12. Conjoined ion guide
13. StepWave
14. T-Wave ion guide

1.6 MS operating modes

The following table shows the MS operating modes.

Table 1–1: MS operating modes:

Operating mode	MS1	Collision cell	MS2
MS	Pass all masses		Resolving (scanning)
SIR	Pass all masses		Resolving (static)
MS1	Resolving (scanning)	Pass all masses	

In MS mode, the instrument can acquire data at scan speeds as high as 20,000 Da/s. Use this mode for instrument tuning and calibration before MS/MS analysis. See the mass spectrometer's online Help for further information.

Use the selected ion recording (SIR) mode for quantitation when you cannot find a suitable fragment ion to perform a more specific multiple reaction monitoring (MRM) analysis (see MS/MS operating modes for further details) . In SIR and MRM modes, neither quadrupole is scanned, therefore no spectrum (intensity versus mass) is produced. The data obtained from SIR or MRM analyses derive from the chromatogram plot (specified mass intensity versus time).

1.7 MS/MS operating modes

The following table shows the MS/MS operating modes.

Table 1–2: MS/MS operating modes:

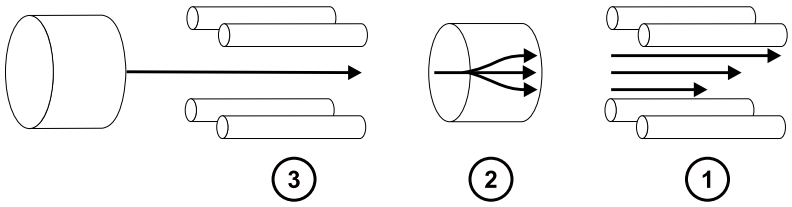
Operating mode	MS1	Collision cell	MS2
Product (daughter) ion spectrum	Static (at precursor mass)	Fragment precursor ions and pass all masses	Scanning
Precursor (parent) ion spectrum	Scanning		Static (at product mass)
MRM	Static (at precursor mass)		Static (at product mass)
Constant neutral loss spectrum	Scanning (synchronized with MS2)		Scanning (synchronized with MS1)
Constant neutral gain spectrum	Scanning (synchronized with MS2)		Scanning (synchronized with MS1)
ScanWave daughter scan	Static (at precursor mass)		Scanning (synchronized with collision cell)

RADAR is an additional mode with which you simultaneously collect data from the MRM and full scan MS modes. RADAR mode can also acquire all detectable ions in both positive and negative full scan MS.

1.7.1 Product (daughter) ion mode

Product ion mode is the most commonly used MS/MS operating mode. You can specify an ion of interest for fragmentation in the collision cell, thus yielding structural information.

Figure 1–4: Product ion mode:



1. MS1 - Static (at precursor mass)
2. Collision cell - Fragment precursor ions and pass all masses
3. MS2 - Scanning

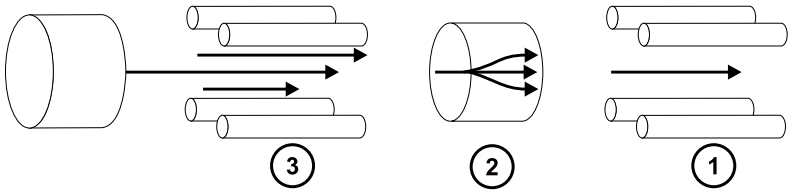
1.7.1.1 Typical applications

You typically use product ion mode for the following applications:

- Method development for MRM screening studies:
  - Identifying product ions for use in MRM transitions.
  - Optimizing CID tuning conditions to maximize the yield of a specific product ion to be used in MRM analysis.
- Structural elucidation (for example, peptide sequencing).

1.7.2 Precursor (parent) ion mode

Figure 1–5: Precursor ion mode:



1. MS1 - Scanning
2. Collision cell - Fragment precursor ions and pass all masses
3. MS2 - Static (at product mass)

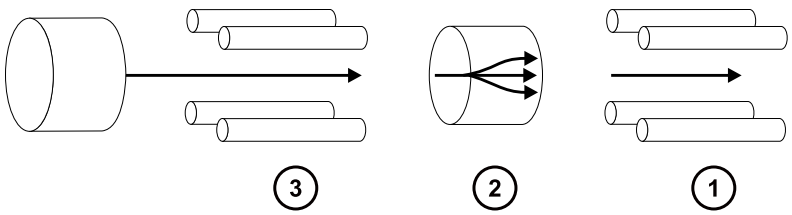
1.7.2.1 Typical application

You typically use the precursor ion mode for structural elucidation—that is, to complement or confirm product scan data—by scanning for all the precursors of a common product ion.

1.7.3 MRM mode

MRM mode is the highly selective MS/MS equivalent of SIR. Because both MS1 and MS2 are static, greater dwell time on the ions of interest is possible, so the sensitivity achieved is better, compared with scanning-mode MS/MS. This mode is the most commonly used acquisition mode for quantitative analysis, allowing the compound of interest to be isolated from the chemical background noise.

Figure 1–6: MRM mode:



1. MS1 - Static (at precursor mass)
2. Collision cell - Fragment precursor ions and pass all masses
3. MS2 - Static (at product mass)

1.7.3.1 Typical application

You typically use MRM mode to quantify known analytes in complex samples:

- drug metabolite and pharmacokinetic studies
- environmental studies; for example, pesticide and herbicide analysis
- forensic or toxicology studies; for example, screening for target drugs in sports testing

MRM mode does not produce a spectrum, because only one transition is monitored at a time. As in SIR mode, a chromatogram is produced.

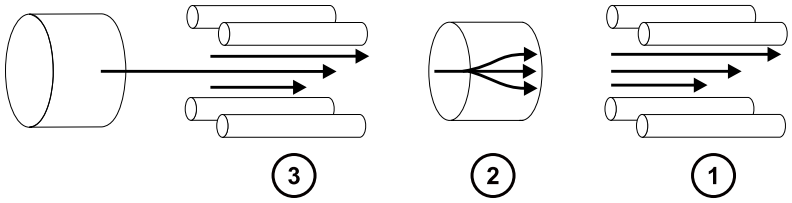
1.7.4 Constant neutral loss mode

Constant neutral loss mode detects the loss of a specific neutral fragment or functional group from an unspecified precursor or precursors.

The scans of MS1 and MS2 are synchronized. When MS1 transmits a specific precursor ion, MS2 determines whether that precursor loses a fragment of a certain mass. If it does, the loss registers at the detector.

In constant neutral loss mode, the spectrum shows the masses of all precursors that lost a fragment of a certain mass.

Figure 1–7: Constant neutral loss mode:



1. MS1 - Scanning (synchronized with MS2)
2. Collision cell - Fragment precursor ions and pass all masses
3. MS2 - Scanning (synchronized with MS1)

1.7.4.1 Typical application

You typically use constant neutral loss mode to screen mixtures for a specific class of compound that is characterized by a common fragmentation pathway, indicating the presence of compounds containing a common functional group.

1.7.5 Constant neutral gain mode

Similar to constant neutral loss mode, constant neutral gain mode detects the gain of a specific neutral fragment or functional group from an unspecified precursor or precursors. The mode is infrequently used because the mass selected by MS2 is seldom higher than that of MS1.

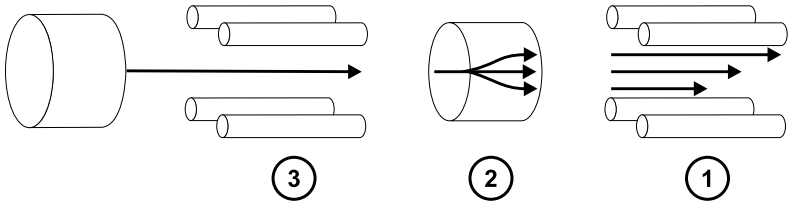
See also: Constant neutral loss mode.

1.7.6 ScanWave daughter scan mode

This operating mode is very similar to the conventional product ion mode in that you can specify an ion of interest for fragmentation in the collision cell, yielding structural information. In this ScanWave mode, the cell accumulates fragment ions and then releases them, according to their

mass, in synchrony with the second quadrupole mass analyzer. This mode results in a significant increase in the signal intensity of full scan spectra.

Figure 1–8: ScanWave daughter scan mode:



1 MS1 - Scanning

2 Collision cell - ScanWave enabled, fragments precursor ions, accumulates fragment ions and passes all masses

3 MS2 - Scanning (synchronized with collision cell)

1.7.6.1 Typical applications

You typically use product ion mode for the following applications:

- Method development for MRM screening studies:
  - Identifying product ions for use in MRM transitions.
  - Optimizing CID tuning conditions to maximize the yield of a specific product ion to be used in MRM analysis.
- Structural elucidation (for example, peptide sequencing).

1.8 Leak sensors

Leak sensors in the instrument's drip trays continuously monitor for liquid leaks. A leak sensor stops system flow when its optical sensor detects about 1.5 mL of accumulated leaked liquid in its surrounding reservoir. At the same time, the software displays an error message alerting you that a leak has developed. Consult the *Waters ACQUITY UPLC Leak Sensor Maintenance Instructions* (part number 71500082506) for complete details.

1.9 Vacuum system

An external roughing (rotary vane) pump and three internal turbomolecular pumps create the source vacuum. The turbomolecular pumps evacuate the analyzer and ion transfer region.

Vacuum leaks and electrical or vacuum pump failures cause vacuum loss. To protect the instrument in the event of vacuum loss, the vacuum interlock switches off the Operate voltages.

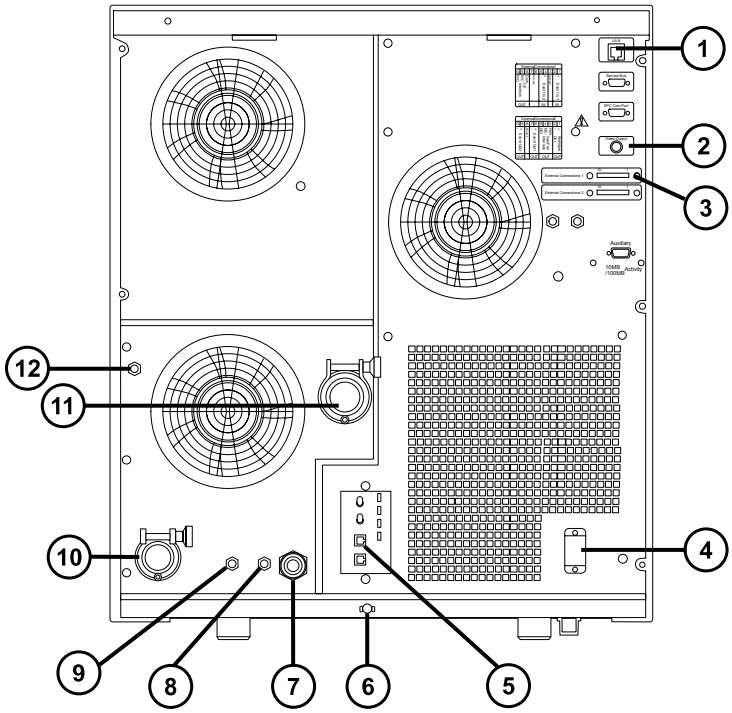
The system monitors the turbomolecular pump speeds and continuously measures vacuum pressure with built-in Pirani and Penning gauges. The gauges also serve as switches, stopping operation when vacuum loss is detected.

A vacuum isolation valve isolates the source sample cone from the mass analyzer, allowing you to perform routine maintenance without venting the system.

1.10 Rear panel

The following figure shows the rear panel locations of the connectors used to operate the mass spectrometer with external devices. For further details, see External connections.

Figure 1–9: Mass spectrometer rear panel:



1. Shielded Ethernet
2. Video connection (for use with the optional NanoFlow ESI or ionKey source)
3. Event inputs and outputs
4. Power connection
5. Roughing pump connections
6. Roughing pump grounding connection

7 Source vent

8 Nitrogen inlet

9 Pilot valve port

10 Turbo vacuum

11 Source vacuum

12 Collision cell gas inlet

2 Preparing the mass spectrometer for operation

This chapter describes how to start and shut down the mass spectrometer.

2.1 Preparing to start the mass spectrometer

This instrument is compatible with the ACQUITY UPLC system; if you are not using an ACQUITY UPLC system, refer to the documentation relevant to the system you are using (see Non-ACQUITY devices for use with the Xevo TQ-XS).

Notice: To avoid causing severe damage to the instrument, use only compatible solvents.

See also: For more details, refer to the following sources:

- Appendix Materials of Construction and Compatible Solvents of this guide, for mass spectrometer solvent information.
- Appendix C of the *ACQUITY UPLC System Operator's Guide* for solvent compatibility with ACQUITY devices.

To prepare the mass spectrometer:

1. On the rear panel, ensure that the nitrogen supply is connected to the instrument's nitrogen inlet connection (see the figure Connecting the nitrogen gas supply).

   Requirements:

   - The nitrogen must be dry and oil-free, with a purity of at least 95% or, for APGC use, at least 99.999%. Regulate the supply at 600 to 690 kPa (6.0 to 6.9 bar, 90 to 100 psi).
   - A gas-fail device must be installed, to interrupt the flow of LC solvent should the nitrogen supply fail.

2. Ensure that the wash solvent bottle is placed in the solvent tray on top of the instrument and that the end of the tubing from the fluidics valve is fully submerged in the solvent.

   Note: For additional information on the fluidics connections, see the diagram on the inside of the fluidics valve access door, and Plumbing schematic.

3. Ensure that the collision gas supply is connected to the instrument's collision cell gas inlet.

Requirement: The collision gas is argon; it must be dry and of high purity (99.997%). Regulate the supply at 50 kPa (0.5 bar, 7 psi).

2.2 Starting the mass spectrometer

Starting the mass spectrometer comprises powering-on the workstation, logging in, powering-on the mass spectrometer and all other instruments, and then starting the software.

Requirements:

- Ensure that you have prepared the mass spectrometer. See Preparing to start the mass spectrometer.
- Power-on and log in to the workstation, to ensure that it assigns the IP addresses of the system instruments.

See also: The mass spectrometer's online Help for details on the software.

To start the mass spectrometer:

1. Power-on the workstation, and log in.
2. Press the power switch on the top, left-hand side of the ACQUITY instruments and then the mass spectrometer.

   Result: Each system instrument runs a series of startup tests.
3. Wait three minutes for the embedded PC to initialize, as indicated by an audible alert.

   Tip: The power and operate LEDs change as follows:

   - During initialization, the binary solvent manager LED and sample manager LED flash green.
   - After the instruments are successfully powered-on, all power LEDs show steady green. The binary solvent manager flow LED, the sample manager run LED, and the mass spectrometer Operate LED remain off.
4. Start the MassLynx software, and monitor the Instrument Console software for messages and LED indications.
5. Pump down (evacuate) the mass spectrometer by following these steps:

   a. In the lower, left-hand corner of the MassLynx main window, click **IntelliStart**.

      Result: The mass spectrometer console appears. The mass spectrometer is in Standby mode.

   b. To start the roughing pumps, click **Control** > **Pump**.

      Tip: The Operate LED remains off.

   c. Wait a minimum of three hours for the instrument to be fully pumped-down (evacuated).

Tips:

- In the Instrument Console, the System Ready indicator shows green when the instrument is fully pumped-down (evacuated).
- Expect the Analyzer Penning gauge readback to show less than 1e-5 mbar vacuum.

Warning: To prevent the ignition of flammable solvent vapors in the enclosed space of a mass spectrometer's ion source, ensure that these conditions are met:

- Nitrogen flows continuously through the source.
- A gas-fail device is installed, to interrupt the flow of LC solvent should the nitrogen supply fail.
- The nitrogen supply pressure does not fall below 400 kPa (4 bar, 58 psi) during an analysis requiring the use of flammable solvents.

6. Start the nitrogen gas flowing through the source by clicking **API**  .

7. Click **Operate**  .

   Result: When the mass spectrometer is in good operating condition, IntelliStart software displays `Ready` in the Instrument Console.

2.3 Verifying the instrument's state of readiness

When the instrument is in good operating condition, the power and Operate LEDs show steady green. You can view any error messages in IntelliStart software (MassLynx).

2.4 Monitoring the mass spectrometer LEDs

LED on the mass spectrometer indicate its operational status.

2.4.1 Power LED

The power LED, located on the top, left-hand side of the mass spectrometer's front panel, indicates when the mass spectrometer is powered-on or powered-off.

2.4.2 Operate LED

The Operate LED, located on the right-hand side of the power LED, indicates the operating condition.

See the mass spectrometer's online Help topic "Monitoring the mass spectrometer LEDs" for details on the Operate LED indications.

2.5 Tuning and calibration information

You must tune and, if necessary, calibrate the instrument prior to use. You can perform these tasks using IntelliStart (MassLynx) software . For further instruction, see the mass spectrometer's online Help.

2.6 Running the mass spectrometer at high flow rates

The ACQUITY UPLC system runs at high flow rates. To optimize desolvation and sensitivity, run the ACQUITY Xevo TQ-XS system at appropriate gas flows and desolvation temperatures. When you specify a flow rate, IntelliStart software automatically specifies the settings shown in the following table.

Table 2–1: Flow rate versus temperature and gas flow:

Flow rate (mL/min)	Source temperature (°C)	Desolvation temperature (°C)	Desolvation gas flow (L/h)
0.000 to 0.020	150	200	800
0.021 to 0.100	150	300	800
0.101 to 0.500	150	500	1000
>0.500	150	600	1000

If you are using an APCI interface, IntelliStart software automatically sets the parameters according to the following table.

Table 2–2: Flow rate versus APCI probe temperature and gas flow:

Flow rate (mL/min)	APCI probe temperature (°C)	Desolvation gas flow (L/h)
0.000 to 0.020	400	800
0.021 to 0.500	500	1000
>0.500	600	1000

2.7 Preparing the IntelliStart Fluidics system

For additional information, see Connecting liquid waste lines.

Prohibited: To avoid equipment damage caused by spilled solvent, do not place reservoir bottles directly atop an instrument or device or on its front ledge. Instead, place the bottles in the bottle tray, which serves as secondary containment in the event of spills.

2.7.1 Installing the reservoir bottles

Use standard reservoir bottles (30-mL) for instrument setup and calibration. Use the Low-volume Adaptor Kit (included) to infuse smaller volumes. The low-volume vials have a volume of 1.5 mL.

Required materials

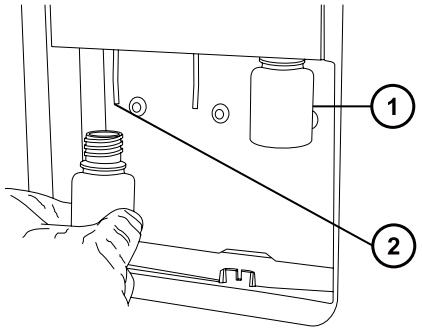
Chemical-resistant, powder-free gloves

To install the reservoir bottles:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

1. Remove the reservoir bottle caps.
2. Screw the reservoir bottles onto the mass spectrometer, as shown below.

   Figure 2–1:



   1 Reservoir bottle

   2 Solvent delivery tube

3. For each reservoir bottle, ensure that the ends of the solvent delivery tubes are positioned so that they are close to, but do not touch, the bottom of the bottle (see Adjusting the solvent delivery tube positions).

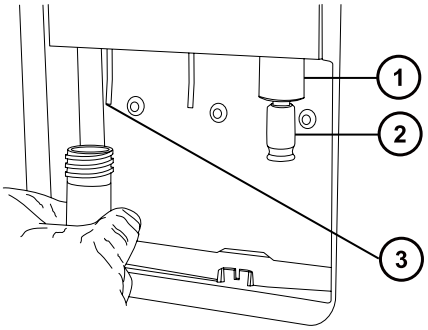
2.7.2 Installing the low-volume vials

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

To install low-volume vials:

1. If a standard reservoir bottle is fitted, remove it.
2. Screw the low-volume adaptors into the manifold and finger-tighten them.

   Figure 2–2:

   1 Low-volume adaptor

   2 Low-volume vial

   3 Solvent delivery tube

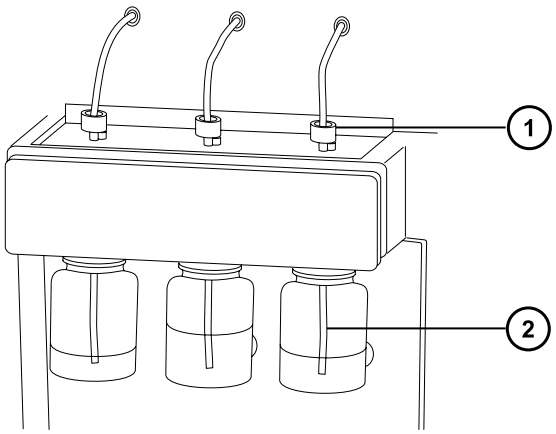
   Warning: To avoid laceration injuries caused by the shattering of fragile, low-volume glass vials, take care when screwing them in, and never use force.
3. Screw the low-volume vials into the adaptors.
4. For each low-volume vial, ensure that the ends of the solvent delivery tubes are positioned so that they are close to, but do not touch, the bottom of the vial (see Adjusting the solvent delivery tube positions).

2.7.3 Adjusting the solvent delivery tube positions

For correct operation of the IntelliStart Fluidics system, you must adjust each solvent delivery tube so that its end is close to, but does not touch, the bottom of the reservoir bottle or low volume vial.

To adjust the position of a solvent delivery tube:

1. Open the access door to the fluidics pump (see Waters ACQUITY Xevo TQ-XS UPLC/MS system).
2. Loosen the finger-tight fitting for the solvent delivery tube you are adjusting.



1. Finger-tight fitting
2. Solvent delivery tube

3. Move the solvent delivery tube so that its end is close to, but does not touch, the bottom of the reservoir bottle or low volume vial.
4. Tighten the finger-tight fitting.
5. Close the access door.

2.8 Purging the fluidics

Whenever you replace a solution bottle, purge the fluidics with the solution that you are going to use next. See the mass spectrometer's online Help for details.

Requirement: Ensure that the end of the tubing is fully submerged in the solvent in the wash reservoir.

Tip: Depending on the solutions used, the system can require more than one purge cycle to minimize carryover.

2.9 Rebooting the mass spectrometer

Pressing the reset button shuts down the electronics momentarily and causes the mass spectrometer to reboot.

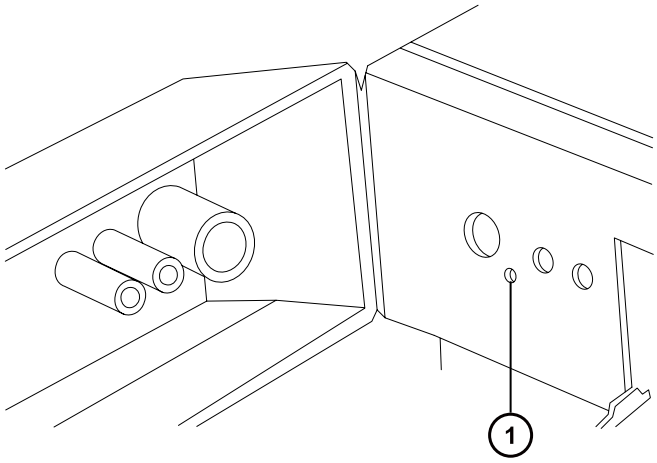
Reboot the mass spectrometer when either of these conditions applies:

- The software fails to establish communication or loses communication with the mass spectrometer.
- You perform a software upgrade.

To reboot the mass spectrometer:

1. Ensure that the mass spectrometer software is closed.
2. Open the mass spectrometer's front, left-hand door.
3. Insert a short length (7.5 cm) of PEEK tubing, or similar object, into the reset button aperture to operate the reset button.

   Figure 2–3:



   (1) Reset button aperture

4. Remove the PEEK tubing from the reset button aperture.
5. Close the mass spectrometer's door.
6. Wait until the reboot sequence completes before starting the mass spectrometer software.

   Tip: An audible alert sounds when the reboot sequence completes.

2.10 Leaving the mass spectrometer ready for operation

Leave the mass spectrometer in **Operate mode**, except in the following cases:

- when performing routine maintenance
- when changing the source
- when leaving the mass spectrometer unused for a long period

In these instances, put the mass spectrometer in **Standby mode** (see the online Help for details).

Notice: For ionKey operation, to protect the iKey when you leave the mass spectrometer in **Operate mode** with no flow, set the capillary voltage to zero.

2.11 Emergency shutdown of the mass spectrometer

Warning: To avoid electric shock, observe the following procedure to isolate the instrument from the main power supply. The instrument's power switch does not isolate it from the main power supply.

Notice: To avoid losing data, use the following procedure only in an emergency. To reboot the mass spectrometer, follow the procedure in Rebooting the mass spectrometer.

To shut down the mass spectrometer in an emergency:

1. Press the power button on the front of the mass spectrometer.
2. Disconnect the power cable from the rear panel.

3 Changing the mode of operation

3.1 Changing the Mode of Operation

This chapter describes how to prepare the mass spectrometer for the following modes of operation:

- ESI (electrospray ionization)
- ESCi (combined electrospray and atmospheric pressure chemical ionization)
- APCI (atmospheric pressure chemical ionization)
- Combined atmospheric pressure photoionization (APPI/APCI)
- Low flow ESI
- UniSpray
- NanoFlow ESI
- ionKey source

For details about other Waters and third-party source options, refer to the documentation supplied with the source.

3.2 ESI, ESCi, and APCI modes

ESI, ESCi, and APCI modes are all configured using a standard source enclosure.

3.2.1 ESI mode

To operate in ESI mode, you must fit the ESI probe adaptor to the source enclosure, and install a probe assembly.

The ESI probe adaptor fitted with a standard ESI probe assembly accommodates eluent flow rates as fast as 2 mL/min.

For further details, see ESI.

3.2.2 ESCi mode

To operate in ESCi mode, you must fit an ESI probe adaptor and corona pin to the source enclosure.

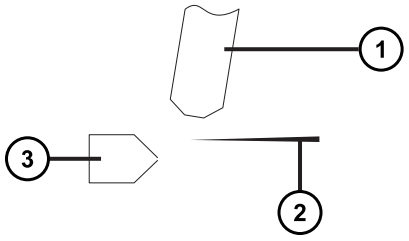
The system, with the ESI probe adaptor installed and corona discharge pin fitted, can alternate between ESI and APCI ionization modes, facilitating data acquisition in ESI and APCI modes in parallel.

3.2.3 APCI mode

APCI mode, an option for the mass spectrometer, produces singly charged protonated or deprotonated molecules for a broad range of nonvolatile analytes.

The APCI interface consists of the ESI/APCI/ESCi enclosure fitted with a corona pin and an APCI probe adaptor. Mobile phase from the LC column enters the probe, where it is pneumatically converted to an aerosol, rapidly heated, and vaporized or gasified at the probe tip.

Figure 3–1: APCI mode:



APCI probe

2 Corona pin

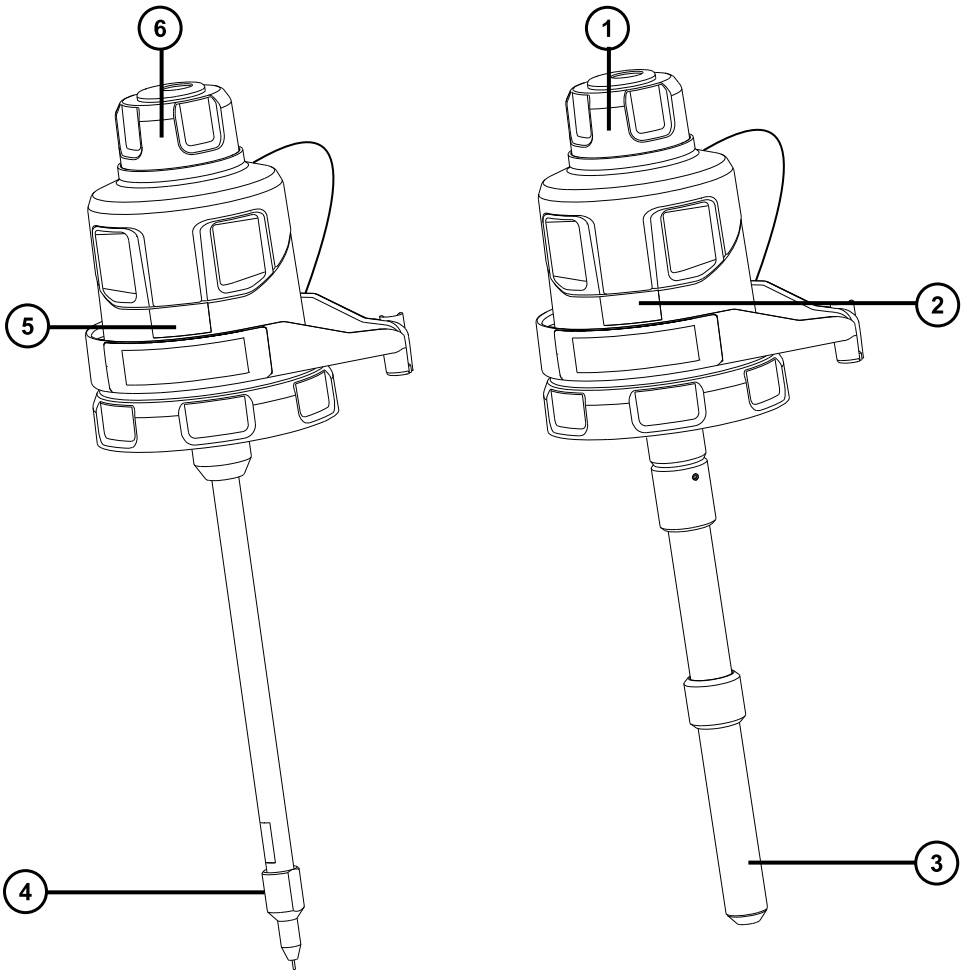
3 Sample cone

Hot gas from the APCI probe passes between the sample cone and the corona pin, which is typically operated with a discharge current of 5 µA. Mobile phase molecules rapidly react with ions generated by the corona discharge to produce stable reagent ions. Analyte molecules introduced into the mobile phase react with the reagent ions at atmospheric pressure and typically become protonated (in the positive ion mode) or deprotonated (in the negative ion mode). The sample and reagent ions then pass through the sample cone and into the mass spectrometer.

3.2.4 Configuring for ESI/ESCi/APCI modes

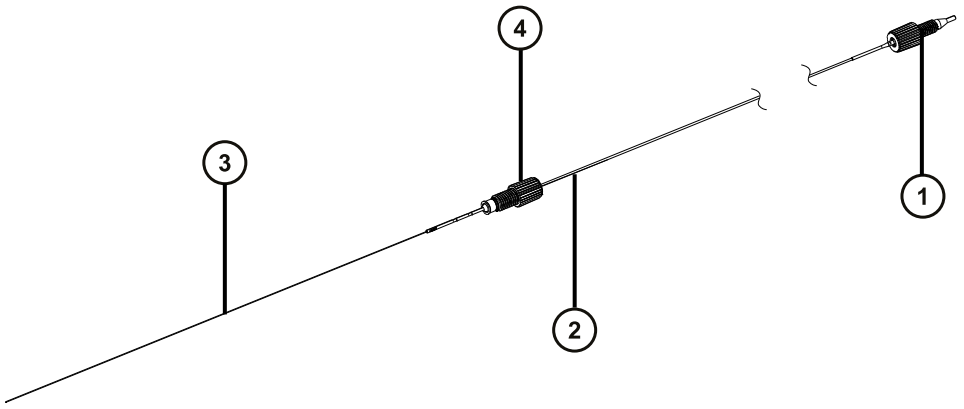
To operate in ESI, ESCi or APCI mode, you must fit the correct probe adaptor and install a probe assembly.

Figure 3–2: Probe adaptor types



1. APCI probe adaptor
2. APCI label
3. APCI probe heater
4. ESI probe tip
5. ESI label
6. ESI probe adaptor

Figure 3–3: Probe assembly



1. Probe inlet PEEK fitting
2. Identification label for part number
3. Capillary
4. Probe adaptor PEEK fitting

For ESCi and APCI modes, you must also install a corona pin.

Table 3–1: Configuration for ESI/ESCi/APCI modes

Mode	Probe adaptor	Install corona pin
ESI	ESI	No
ESCi	ESI	Yes
APCI	APCI	Yes

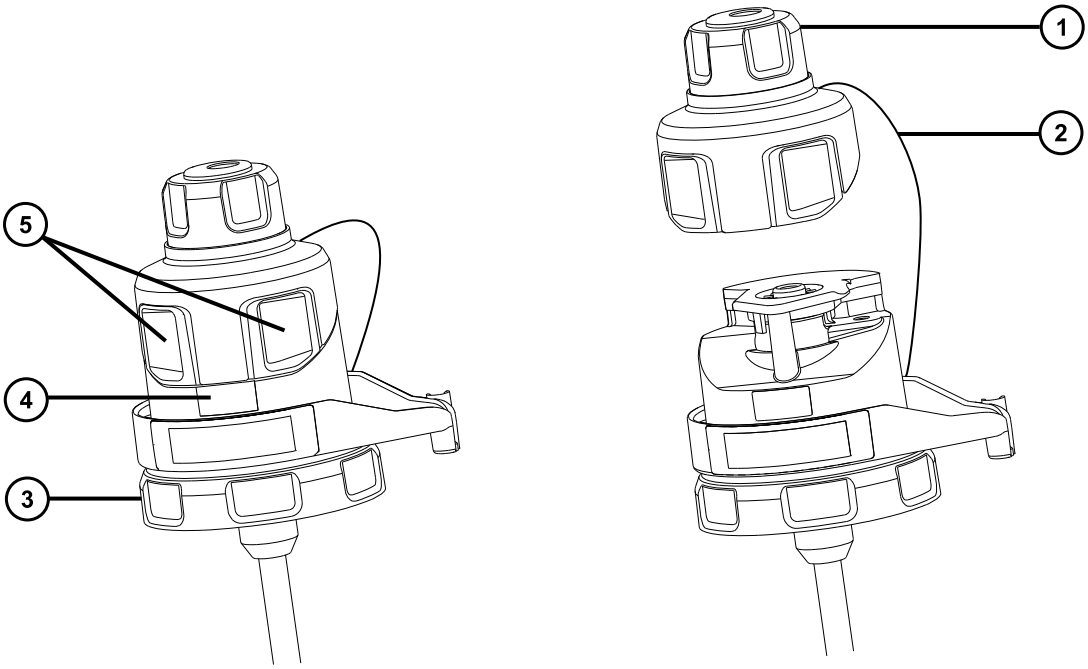
For more information on using each mode, see the Xevo TQ-XS system online Help.

The following sections explain how to complete the following tasks:

- Installing the probe adaptor
- Installing the probe assembly
- Removing the probe adaptor
- Installing and removing the corona pin

3.2.5 Installing the probe adaptor

Figure 3–4: Probe adaptor parts



1. Probe adaptor cap removed from probe adaptor
2. Probe adaptor cap tether
3. Locking ring
4. Probe adaptor identification label
5. Probe adaptor cap release buttons

Required materials

- Chemical-resistant, powder-free gloves

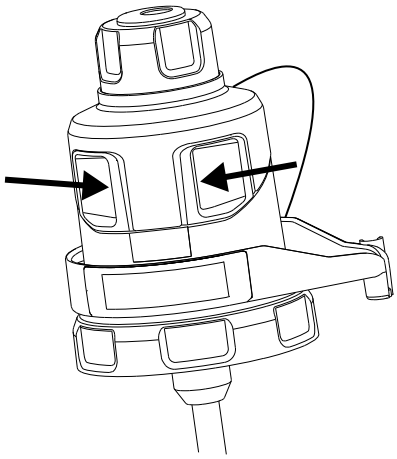
To install the probe adaptor:

Warning: To avoid personal contamination with biohazards or compounds that are toxic, wear clean, chemical-resistant, powder-free gloves when performing this procedure.

Warning: To avoid puncture wounds, handle sharp parts and materials with care.

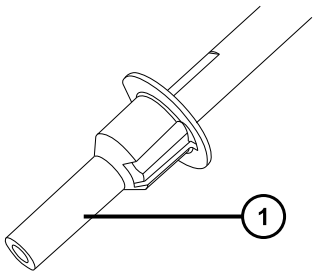
1. To prepare for installing a probe assembly, press together the probe-adaptor-cap release buttons, in the direction shown by the arrows in the following figure, and lift the probe adaptor cap off the probe adaptor.

Figure 3–5: Probe adaptor cap release



2. For ESI probe adaptors, remove the protective cap, if fitted, from the probe tip.

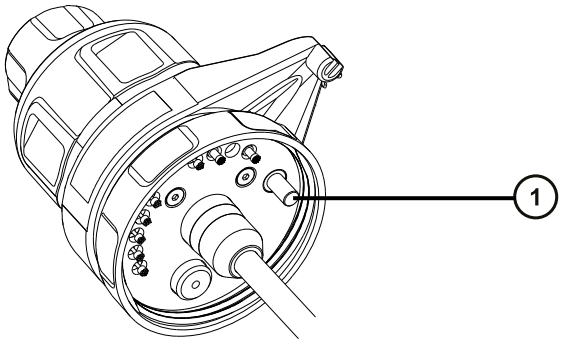
Figure 3–6: ESI probe protective cap



1 Protective cap

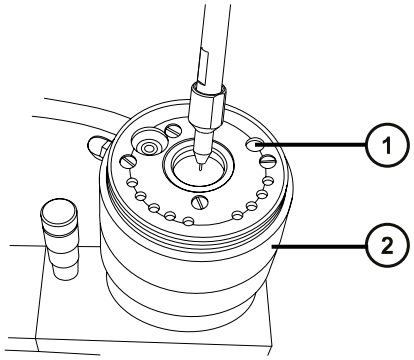
3. Carefully slide the probe adaptor into the hole in the probe adjuster assembly, ensuring that the probe location dowel aligns with the location hole in the probe adjuster assembly.

Figure 3–7: Probe location dowel



1 Probe location dowel

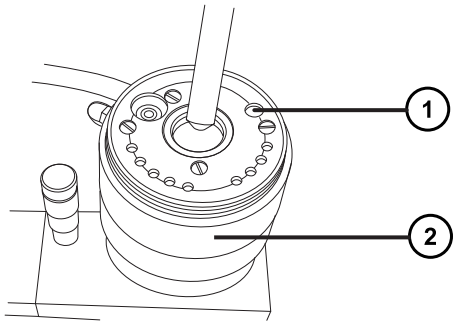
Figure 3–8: Locating the ESI probe adaptor



1 Location hole for probe location dowel

2 Probe adjuster assembly

Figure 3–9: Locating the APCI probe adaptor

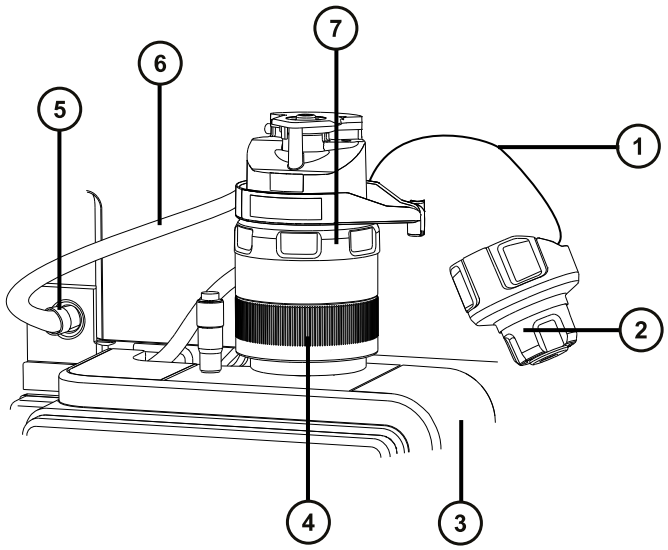


1 Location hole for probe location dowel

2 Probe adjuster assembly

4. Rotate the probe adaptor locking ring clockwise to secure the probe adaptor in place.

Figure 3–10: Probe adaptor, mounted on the source enclosure:



1. Probe adaptor cap tether
2. Probe adaptor cap
3. Source enclosure
4. Probe adjuster assembly
5. High voltage connector
6. ESI probe adaptor cable (ESI probe adaptor only)
7. Probe adaptor locking ring

5. For ESI probe adaptors, connect the ESI probe adaptor's cable to the high voltage connector.
6. Install the probe assembly, see Installing the new probe assembly.

3.2.6 Installing the probe assembly

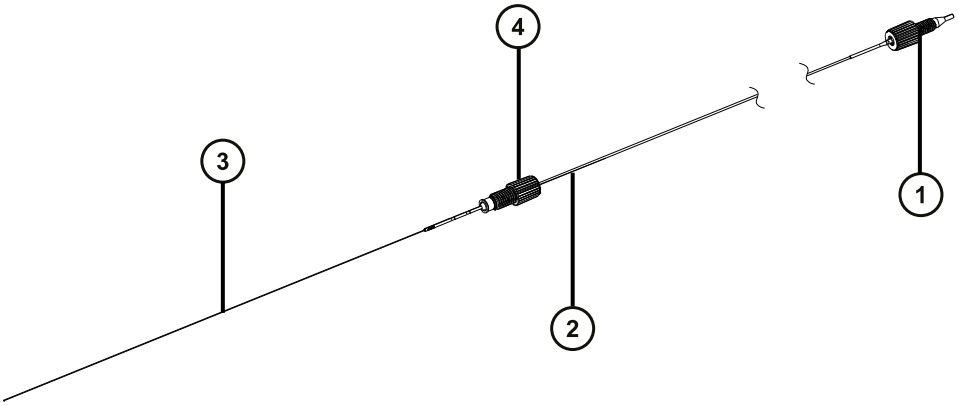
Requirements:

- Ensure that you use a probe assembly appropriate for your application. For example, using an ESI probe assembly with an APCI probe adaptor compromises instrument performance. You can use the part number on the identification label to verify the probe assembly type.
- Ensure that the probe adaptor is installed on the source, with the probe adaptor cap removed. See Installing the probe adaptor.
- Select the shortest probe assembly that can connect the diverter valve to the probe. Doing so minimizes delays and dispersion.

Recommendation: To connect the probe assembly directly to the fluidics valve, use the 500-mm ESI or APCI probe assembly.

Notice: Do not adjust the length of the probe assembly. Cutting the PEEKsil tubing renders the probe assembly unusable.

Figure 3–11: Probe assembly



1. Probe inlet fitting
2. Identification label showing part number
3. Capillary
4. Probe adaptor fitting

Required materials

- Chemical-resistant, powder-free gloves

To install the probe assembly:

Warning: To avoid personal contamination with biohazards or compounds that are toxic, wear clean, chemical-resistant, powder-free gloves when performing this procedure.

Warning: To avoid electric shock, do not insert any item into the probe cap aperture when the probe cap is fitted to the instrument.

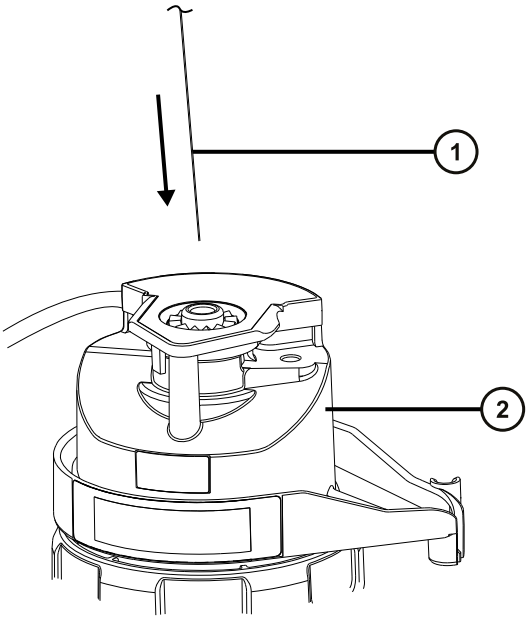
Notice: To avoid damaging the probe assembly, take care when inserting the capillary into the probe adaptor. Do not use force.

Warning: To avoid harmless, static-like electric shock, ensure the mass spectrometer is in Standby mode before you touch any of its external surfaces that are marked with this high voltage warning symbol.

1. Carefully insert the probe assembly capillary into the probe adaptor.

   Tip: To aid insertion, turn the capillary gently as you insert it, feeding the entire capillary in to the probe adaptor.

Figure 3–12: Inserting the probe assembly

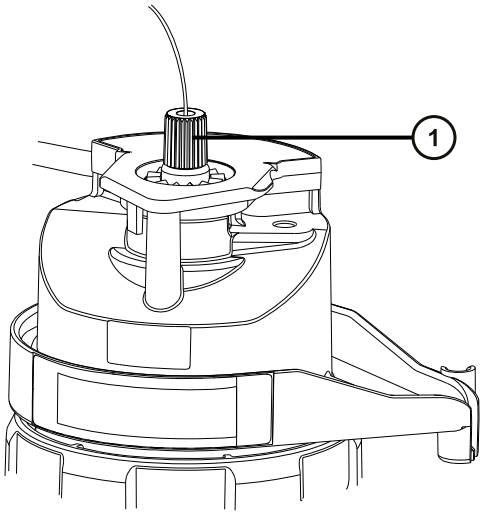


1 Probe assembly capillary

2 Probe adaptor

2. Screw the probe adaptor fitting into the probe adaptor, finger-tight only, until you hear a click.

Figure 3–13: Probe assembly fitted to the probe adaptor

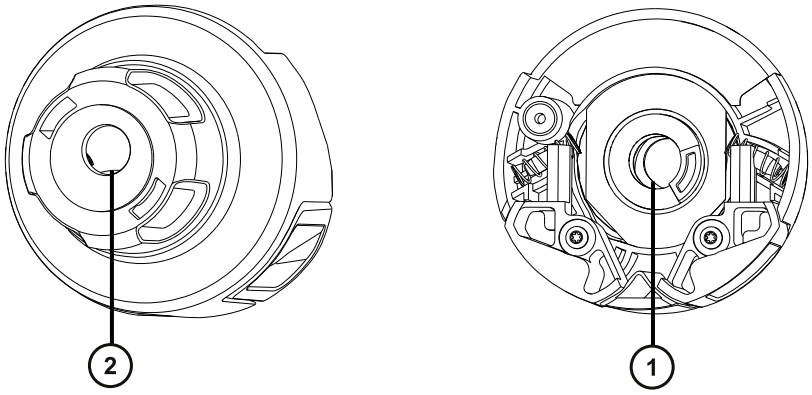


1 Probe adaptor fitting

Tip: The probe adaptor fitting on the UniSpray probe assembly is not compatible with the probe adaptor. If you cannot fit the probe adaptor cap, ensure that you are installing the correct probe assembly.

3. Tilt the probe adaptor cap, so that the ball-bearing is located in the recess at the bottom of the aperture, and insert the probe assembly tubing through the aperture.

Figure 3–14: Probe adaptor cap

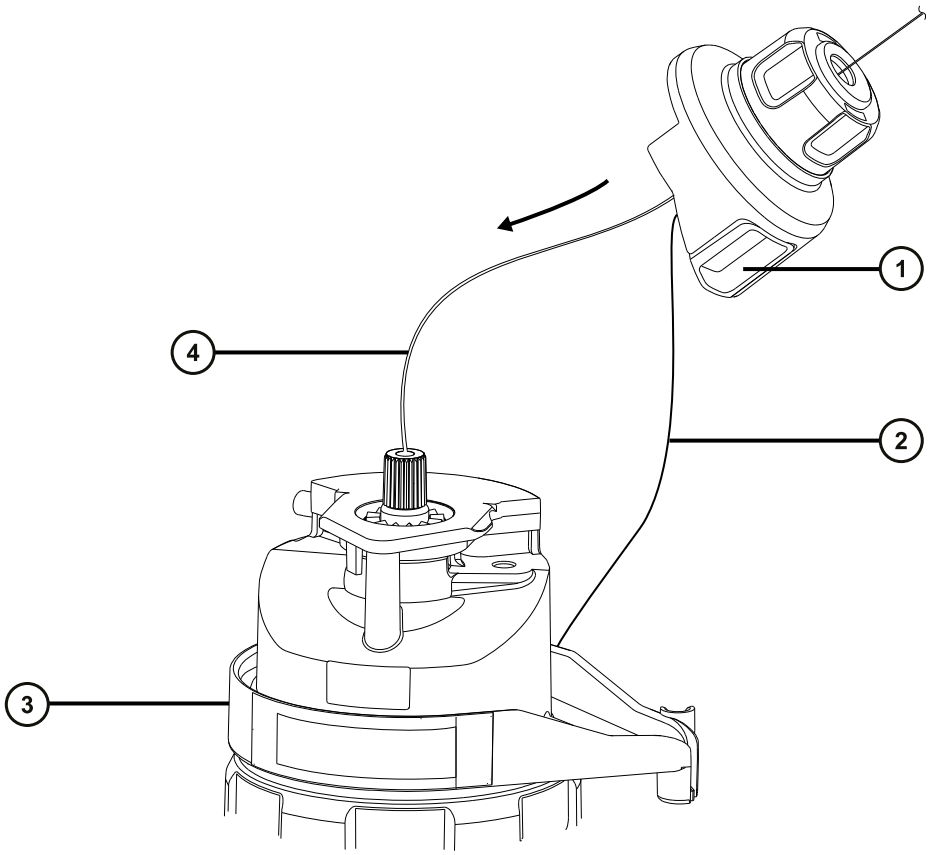


1 Probe cap aperture from the underside

2 Probe cap aperture from the top

Tip: The probe assembly tubing can pass through the aperture only when the ball-bearing is located in the recess at the bottom and does not block the aperture.

Figure 3–15:



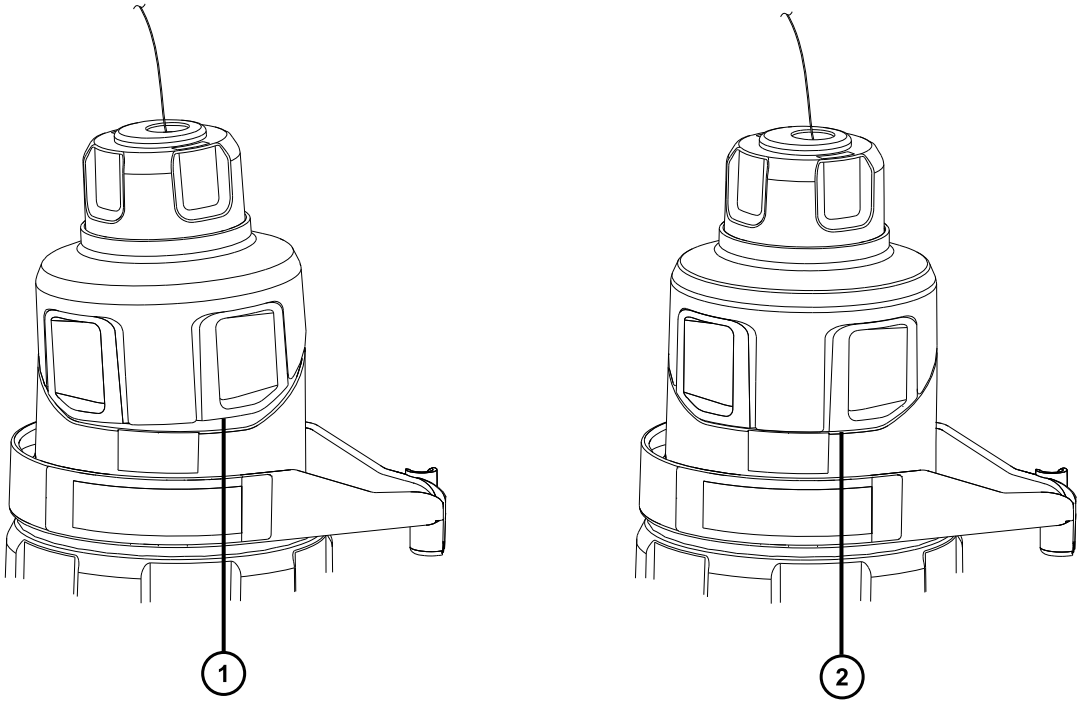
1. Probe adaptor cap
2. Probe adaptor cap tether
3. Probe adaptor
4. Probe assembly tubing

4. Slide the probe adaptor cap along the probe assembly, over the probe adaptor PEEK fitting.
5. Push the probe adaptor cap on to the probe adaptor until it clicks.

Tips:

- Do not squeeze the probe adaptor cap release buttons when fitting the probe adaptor cap.
- Ensure that the probe adaptor cap is correctly seated, and that both release buttons engage with the probe adaptor, producing a click.

Figure 3–16: Seating the probe adaptor cap

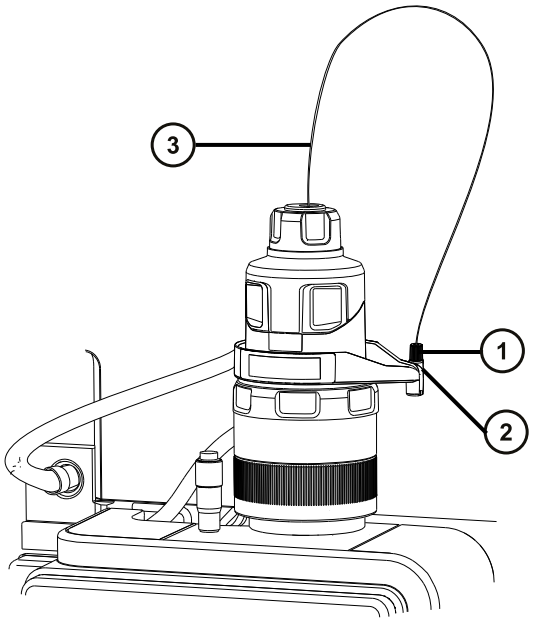


1. Probe adaptor cap seated incorrectly; edge does not align with the edge of the probe adaptor

2. Probe adaptor cap seated correctly; edge aligns with the edge of the probe adaptor

6. If you are not immediately connecting the probe assembly to the fluidics, insert the probe inlet PEEK fitting in to the PEEK fitting holder.

Figure 3–17: PEEK fitting holder



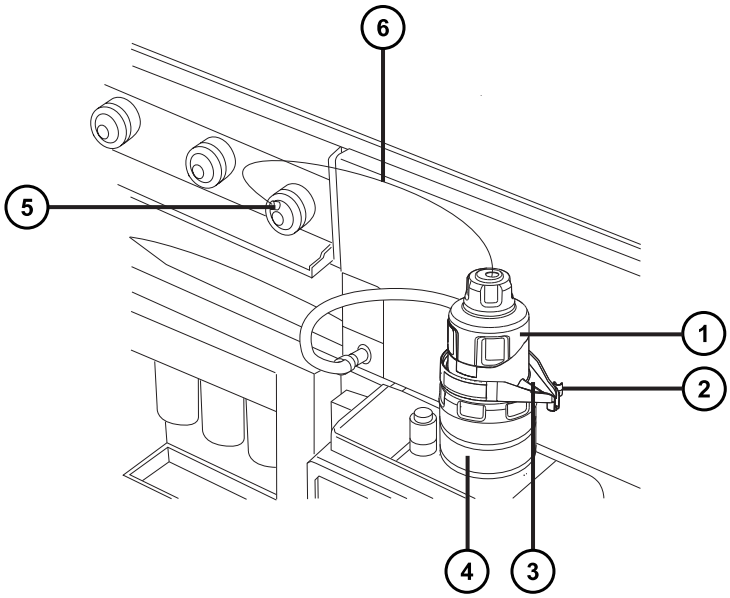
1. Probe inlet PEEK fitting
2. PEEK fitting holder
3. Probe assembly tubing

Warning: To avoid electric shock or solvent ignition, when connecting ESI or UPC^2 source probes directly to non-Waters equipment, ensure that the liquid outlet connection is grounded.

7. To connect the probe inlet PEEK fitting to the IntelliStart Fluidics system:
   a. Open the access door to the IntelliStart Fluidics system (see Waters ACQUITY Xevo TQ-S UPLC/MS system).
   b. Screw the probe inlet PEEK fitting into port 2 (the top port) of the diverter valve, finger-tight only, until you hear a click.

Figure 3–18: Tubing connection between the diverter valve and the ESI probe

Tip: The other plumbing connections are omitted for clarity.



1. Probe adaptor cap
2. PEEK fitting holder
3. Leak tray
4. Probe adaptor
5. Probe inlet PEEK fitting connected to diverter valve
6. Tubing

c. Close the access door to the IntelliStart Fluidics system.

Tip: If fluid collects in the leak tray, inspect the connection at the diverter valve.

3.2.7 Removing the probe adaptor

Remove the probe adaptor before performing any of the following actions:

- Switching between ESI and APCI modes (see Installing the probe adaptor).
- Installing the Low-flow ESI probe (see the *Low-flow ESI Probe Operator's Guide*).
- Replacing the ESI probe tip or gasket (see Replacing the ESI probe tip or gasket).

You can remove the probe adaptor with or without the probe assembly installed. To remove the probe assembly, see Removing the existing probe assembly.

Required materials

Chemical-resistant, powder-free gloves

To remove the ESI probe adaptor:

Warning: To avoid personal contamination with biohazards or compounds that are toxic, wear clean, chemical-resistant, powder-free gloves when performing this procedure.

Warning: To avoid harmless, static-like electric shock, ensure the mass spectrometer is in Standby mode before you touch any of its external surfaces that are marked with this high voltage warning symbol.

Warning: To avoid burn injuries, take great care while working with the probe and source; these components can be hot.

1. Prepare the instrument for working on the source (see Preparing the instrument for working on the source).

   Warning: To avoid electric shock or solvent ignition, when connecting ESI or UPC^2 source probes directly to non-Waters equipment, ensure that the liquid outlet connection is grounded.

2. If the probe assembly is fitted, open the access door to the IntelliStart Fluidics system (see Waters ACQUITY Xevo TQ-XS UPLC/MS system), and disconnect the fluidics tubing from the diverter valve.
3. For ESI probes, disconnect the probe adaptor cable from the high voltage connector.
4. Unscrew the probe adaptor locking ring.

   Warning: To avoid puncture wounds, handle sharp parts and materials with care.

5. Carefully remove the probe adaptor from the probe adjustor assembly.
6. For ESI probe adaptors, if available, fit the protective cap to the probe tip.

3.2.8 Installing and removing the corona pin

For APCI, ESCi, and dual-mode APPI/APCI operation, you must fit a corona pin to the source.

3.2.8.1 Installing the corona pin in the source

Required materials

Chemical-resistant, powder-free gloves

To install the corona pin in the source:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid harmless, static-like electric shock, ensure the mass spectrometer is in Standby mode before you touch any of its external surfaces that are marked with this high voltage warning symbol.

1. Prepare the instrument for working on the source (see Preparing the instrument for working on the source).

   Warning: To avoid burn injuries, take great care while working with the source enclosure open.

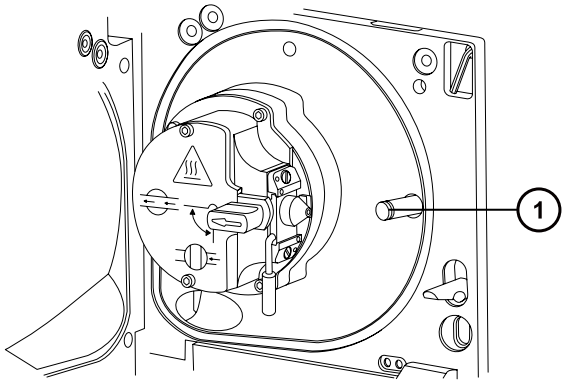
   

   Warning: To avoid puncture wounds, handle sharp parts and materials with care.

2. Pull the source enclosure release (located at the bottom, right-hand side) outward, and swing open the enclosure.
3. Remove the blanking plug from the corona pin mounting contact.

   Tip: Store the blanking plug in a safe location.

Figure 3–19: Corona pin mounting contact:

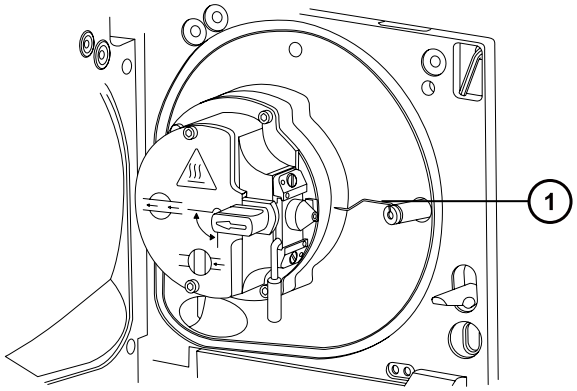


1 Corona pin mounting contact blanking plug

Warning: To avoid puncture wounds, handle sharp parts and materials with care.

4. Fit the corona pin to the corona pin mounting contact, ensuring that the corona pin is securely mounted and that its tip aligns with the sample cone orifice.

Figure 3–20: Corona pin:

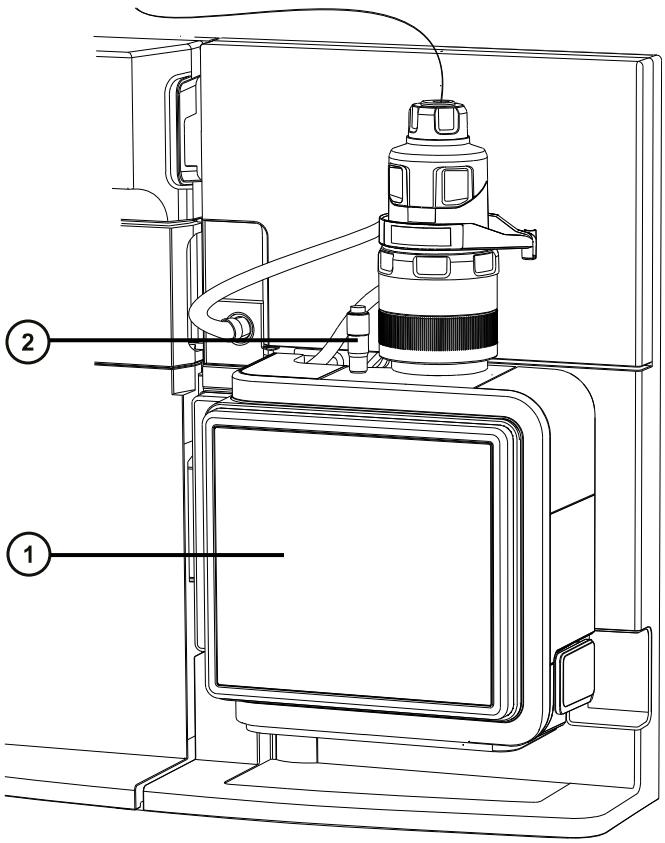


1 Corona pin

5. Close the source enclosure.

6. Look through the source window, and use the vernier probe adjuster to position the probe tip so that it is pointing approximately midway between the tips of the sample cone and the corona pin.

Figure 3–21: Source enclosure



1. Source window
2. Vernier probe adjuster

3.2.8.2 Removing the corona pin from the source

Required materials

Chemical-resistant, powder-free gloves

To remove the corona pin from the source:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid electric shock, ensure that the instrument is prepared for working on the source before commencing this procedure.

1. Prepare the instrument for working on the source (see Prepare the instrument for working on the source).

   Warning: To avoid burn injuries, take great care while performing this procedure.

   Warning: To avoid puncture wounds, take great care while working with the source enclosure open if an ESI probe is fitted; the ESI probe tip is sharp.

2. Pull the source enclosure release (located at the bottom, right-hand side) outwards, and swing open the enclosure.
3. Remove the corona pin from its mounting contact (see the figure in Installing the corona pin in the source).

   Tip: Store the corona pin in a safe location.
4. Fit the blanking plug to the corona pin mounting contact (see the figure in Installing the corona pin in the source).
5. Close the source enclosure.

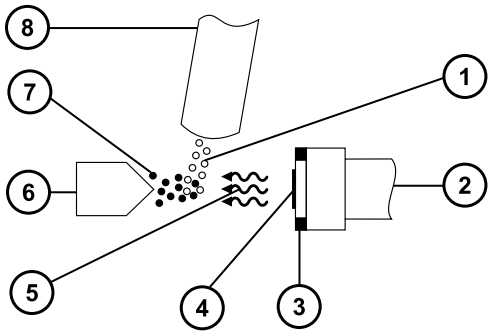
3.3 Combined APPI/APCI source

The combined APPI/APCI source uses an optional, replacement source enclosure. You can operate the source in APPI mode, APCI mode, or dual-mode APPI/APCI. Dual-mode APPI/APCI performs rapid switching between ionization modes.

3.3.1 APPI operation

In APPI mode, the source is fitted with an APCI probe adaptor, and the APPI lamp drive assembly is advanced into the source.

Figure 3–22: APPI mode:



1. Sample molecules
2. APPI lamp drive assembly
3. Repeller electrode
4. UV lamp
5. Photons from the UV lamp
6. Sample cone
7. Sample ions
8. APCI probe

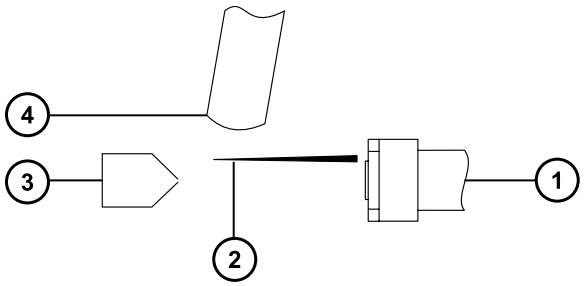
The APCI probe introduces vaporized sample into the source where photons generated by an ultra-violet (UV) lamp (mounted in the APPI lamp drive assembly) produce sample ions. Direct photoionization of a sample molecule occurs when the photon energy exceeds the ionization potential of the sample molecule.

A repeller electrode (mounted on the APPI lamp drive assembly) deflects and focuses the sample ions toward the sample cone.

3.3.2 APCI operation

APCI produces singly charged protonated or deprotonated molecules for a large range of nonvolatile analytes. In APCI mode, the source is fitted with an APCI corona pin. If unused, the APPI lamp drive assembly is retracted from the source.

Figure 3–23: APCI mode:



1. Retracted APPI lamp drive assembly
2. Corona pin

3 Sample cone

4 APCI probe

The APCI probe introduces vaporized sample into the source. The sample passes between the sample cone and the corona pin, which typically operates with a discharge current of 5 µA. The corona discharge generates ions that react with the mobile phase molecules to produce stable reagent ions. Analyte molecules in the mobile phase react with the reagent ions at atmospheric pressure and become protonated (in the positive ion mode) or deprotonated (in the negative ion mode). The sample and reagent ions pass through the sample cone.

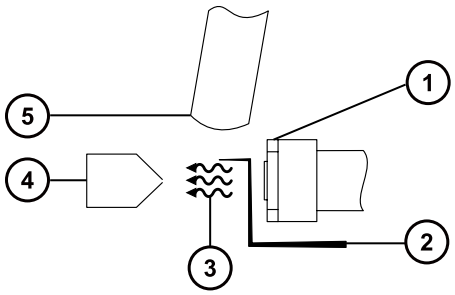
3.3.3 Dual-mode operation

Dual-mode operation enables rapid switching between APPI and APCI ionization modes and allows high-throughput operations (for example, for sample screening).

You replace the standard corona pin with a specially shaped APPI/APCI corona pin, so that the APPI lamp holder can be advanced into the source for dual operation.

When the source is configured for dual operation in APCI mode, current is applied to the corona pin, but the repeller electrode is inactive.

Figure 3–24: Dual operation in APCI mode:



1 Repeller electrode inactive

2 Corona pin with current applied

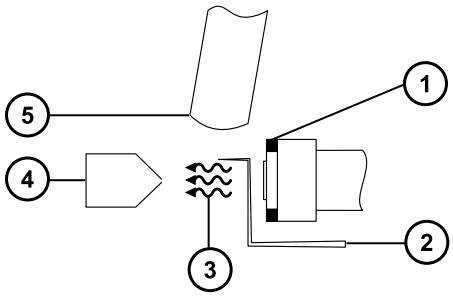
3 Photons from the UV lamp

4 Sample cone

5 APCI probe

When the source is configured for dual operation in APPI mode, the corona pin is inactive, and a voltage is applied to the repeller electrode.

Figure 3–25: Dual operation in APPI mode:

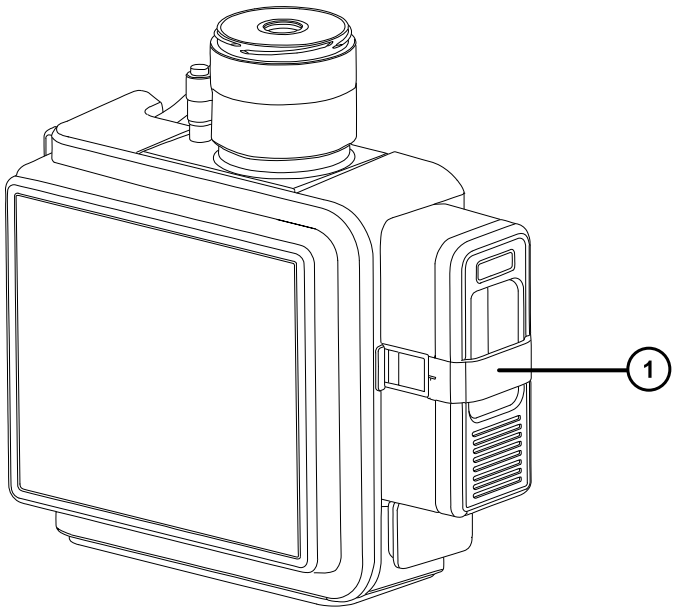


1. Repeller electrode with voltage applied
2. Corona pin inactive
3. Photons from the UV lamp
4. Sample cone
5. APCI probe

3.3.4 The combined APPI/APCI source components

The combined APPI/APCI source comprises the APCI probe adaptor and a source enclosure with an APPI lamp drive incorporated.

Figure 3–26: The combined APPI/APCI source enclosure:

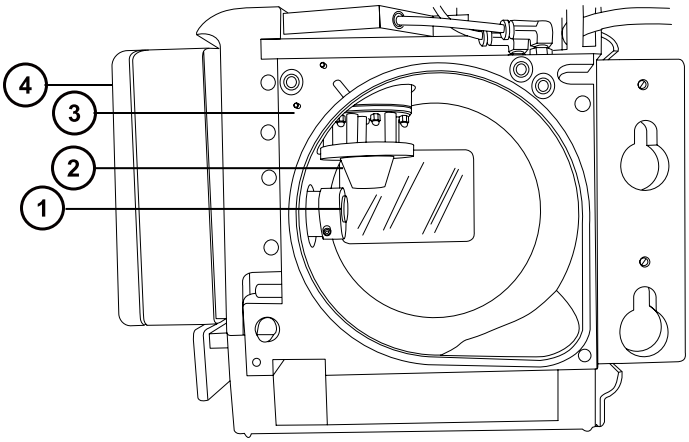


1 APPI lamp drive assembly

Notice: To prevent damage to the corona pin and lamp assembly, ensure that the lamp assembly does not touch the corona pin when the source enclosure door is closed.

The UV lamp, which you ignite via a control in the MassLynx software Tune window, provides a constant photon output. You vary the intensity of incident radiation upon the sample molecules by adjusting the distance between the UV lamp and probe tip.

Figure 3–27: APPI lamp drive assembly inside the source enclosure:



1 UV lamp and repeller electrode

2 Desolvation heater nozzle

3 Source enclosure

4 APPI lamp drive assembly

3.3.5 Installing the combined APPI/APCI source

Required materials

Chemical-resistant, powder-free gloves

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid electric shock, ensure that the instrument is suitably prepared before commencing this procedure.

To install the combined APPI/APCI source:

1. Prepare the instrument for working on the source (see Preparing the instrument for working on the source).

   Warning: To avoid burn injuries, take great care while working with the probe and source; these components can be hot.

2. Remove the probe adaptor from the currently installed source (see Removing the probe adaptor).
3. Remove the existing source enclosure (see Removing the source enclosure from the instrument).
4. Install the combined APPI/APCI source enclosure (see Fitting the source enclosure to the instrument).
5. Install the specially shaped corona pin (see Installing the corona pin in the source).
6. Slide open the instrument's source interface door (see the figure on Waters ACQUITY Xevo TQ-S UPLC/MS system).
7. Connect the APPI drive cable to the instrument's front panel connector.

   Tip: The front panel connectors and cables are color-coded. Ensure that the color of the connector and the cable match.

8. Connect the source enclosure cable to the instrument's front panel connector.

   Notice: To prevent damage to the corona pin and lamp assembly, ensure that the lamp assembly does not touch the corona pin when the source enclosure door is closed.

9. Close the instrument's source interface door.
10. Install the APCI probe adaptor to the source (see Installing the probe adaptor).
11. Install the APCI probe assembly (see Installing the probe assembly).

    Tip: An automatic pressure test is performed each time the source enclosure is closed and the probe cap is fitted, and when the instrument starts.

3.3.6 Removing the combined APPI/APCI source enclosure

Required materials

Chemical-resistant, powder-free gloves

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid electric shock, ensure that the instrument is prepared for working on the source before commencing this procedure.

Warning: To avoid burn injuries, before performing maintenance operations that involve handling components inside the mass spectrometer's ion source, allow the source interior to cool.

To remove the combined APPI/APCI source:

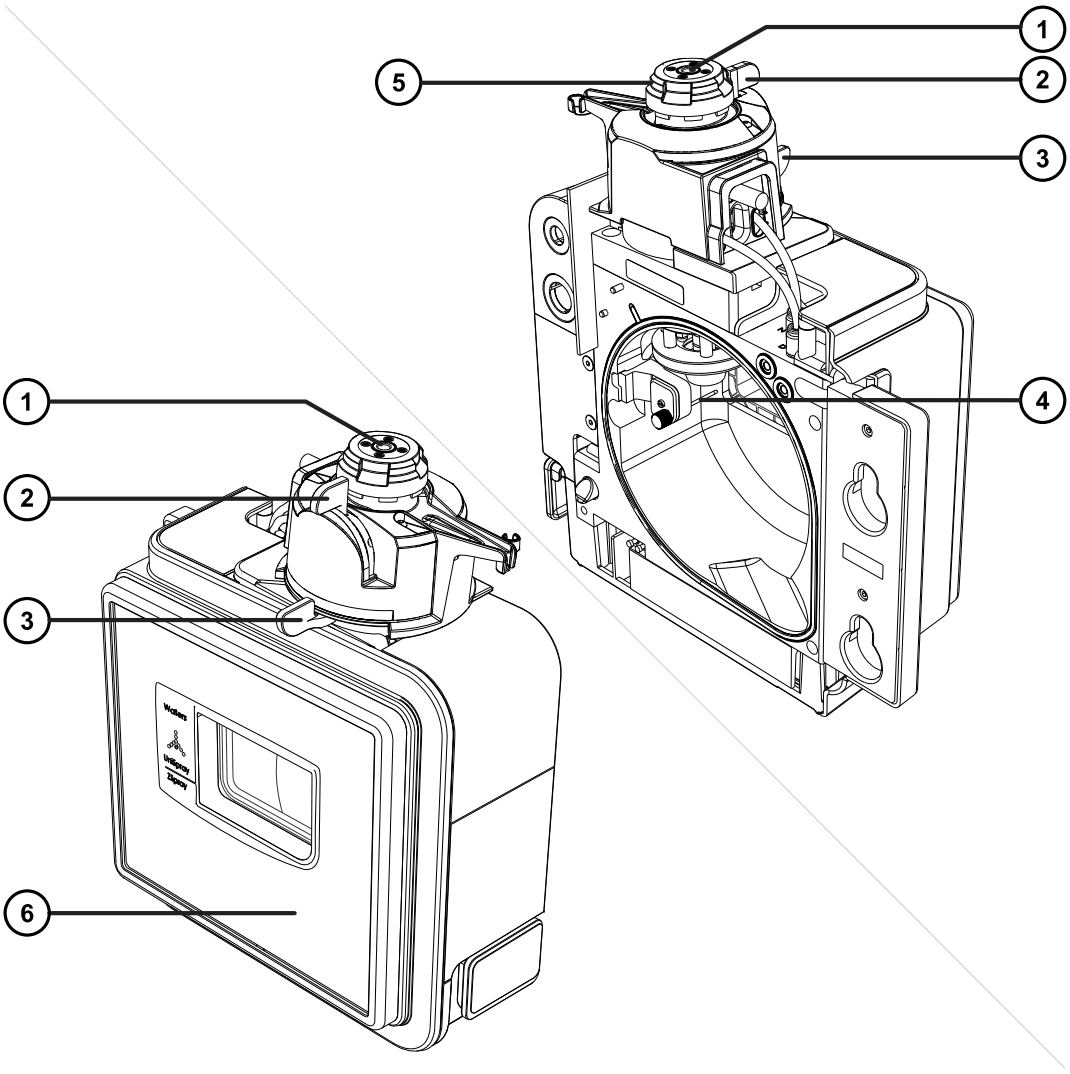
1. Prepare the instrument for working on the source (see Preparing the instrument for working on the source).
2. Remove the APCI probe adaptor (see Removing the probe adaptor).
3. Disconnect the source enclosure cable from the instrument’s front panel.
4. Disconnect the APPI drive cable from the instrument’s front panel.
5. Remove the source enclosure (see Removing the source enclosure from the instrument).
6. Remove the corona pin (see Removing the corona pin from the source).
7. Fit the blanking plug to the pin’s mounting contact.

3.4 UniSpray source

The UniSpray source enables the detection of a wide range of compounds in a single analysis.

The following sections explain how to install and remove the UniSpray source.

Figure 3–28: UniSpray source - front and rear view



1. Probe inlet shaft
2. Vertical probe adjuster
3. Horizontal probe adjuster
4. Impactor pin
5. Capillary adjuster
6. Source enclosure front panel

See also: For information about maintaining the source components:

- Replacing the UniSpray probe assembly
- Maintaining the UniSpray impactor pin

3.4.1 Installing the UniSpray source

Required materials

- Chemical-resistant, powder-free gloves

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

To install the UniSpray source:

1. Prepare the instrument for working on the source (see Preparing the instrument for working on the source).

   Warning: To avoid electric shock, ensure that the instrument is in Standby mode before commencing this procedure.

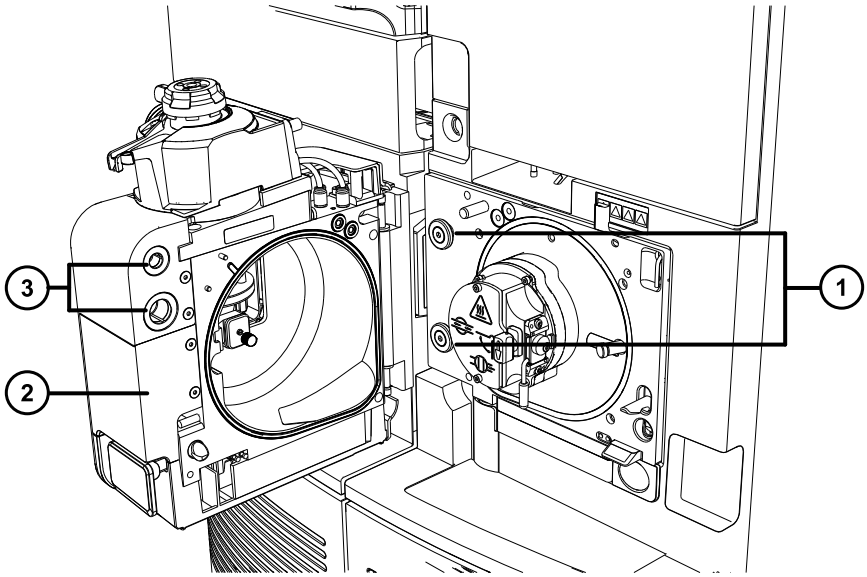
   Warning: To avoid burn injuries, exercise care when handling the components of the source enclosure heated to high temperatures. Wait until the hot components have sufficiently cooled before you handle them.

2. Remove the existing source enclosure (see Removing the source enclosure from the instrument).
3. Ensure that the probe assembly is connected to the UniSpray source before you fit the source to the mass spectrometer.

Tip: If you must fit the probe assembly, do so by inserting the probe assembly into the probe inlet shaft atop the source, and screwing the probe fitting into the probe inlet. See Fitting the UniSpray probe assembly.

4. Using two hands, fit the UniSpray source enclosure to the two supporting studs on the adaptor housing.

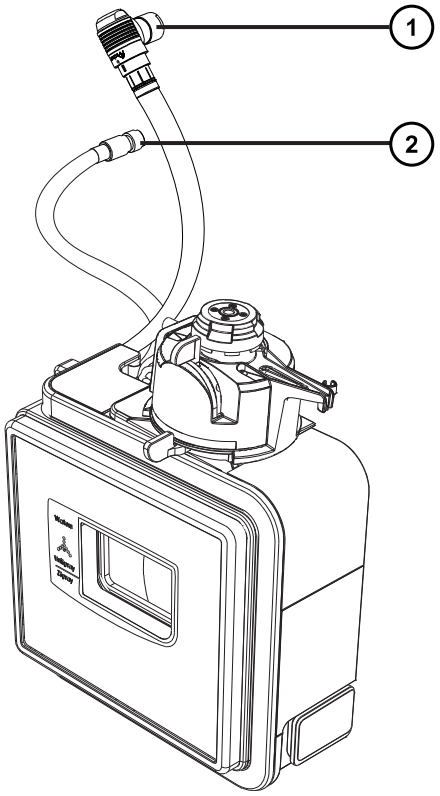
Figure 3–29: Fitting the source



1. Supporting studs
2. Source enclosure
3. Cable storage positions

5. Swing the source enclosure to the closed position, ensuring that it locks into place.

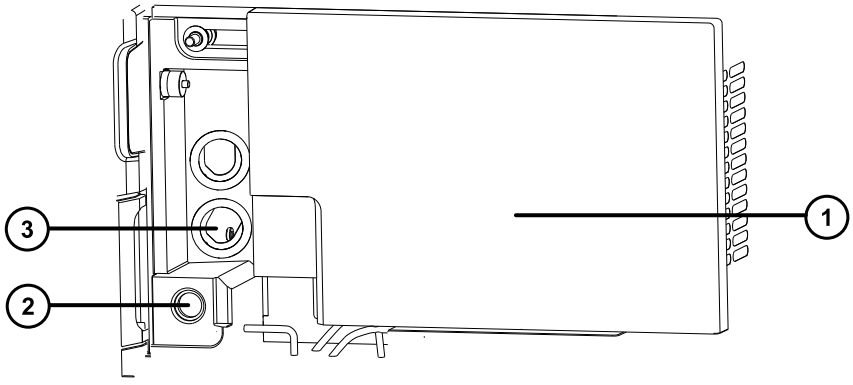
Figure 3–30: UniSpray source connections



1. Probe adjuster cable (yellow)
2. High-voltage connector

6. Slide open the instrument's source interface door.

Figure 3–31: UniSpray Source connections to mass spectrometer



① Instrument source interface door

② High-voltage cable socket

③ Probe adjuster cable socket (yellow)

7. Connect the high-voltage cable to the high-voltage cable socket on the mass spectrometer.
8. Connect the probe adjuster cable to the probe adjuster cable socket on the mass spectrometer.
9. Close the instrument's source interface door.
10. Screw the probe assembly's PEEK fitting into the LC flow or syringe pump.

3.4.2 Removing the UniSpray source

You can remove the UniSpray source, and replace it with another compatible interface.

Required materials

- Chemical-resistant, powder-free gloves

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid electric shock, ensure that the instrument is prepared for working on the source before commencing this procedure.

To remove the UniSpray source:

1. Prepare the instrument for working on the source (see Preparing the instrument for working on the source).

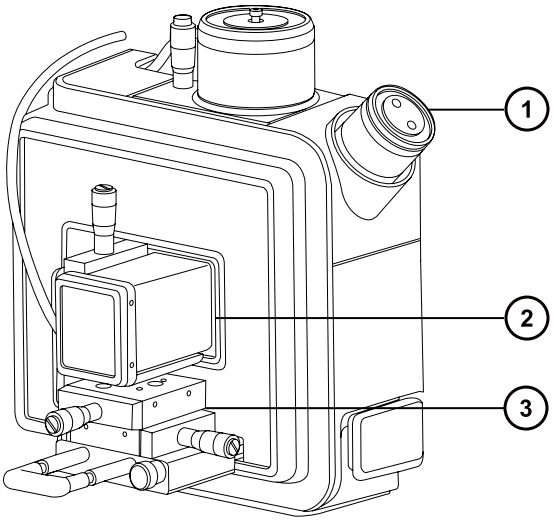
   Warning: To avoid burn injuries, exercise care when handling the components of the source enclosure heated to high temperatures. Wait until the hot components have sufficiently cooled before you handle them.

2. Disconnect the PEEK fitting connecting the probe assembly to the LC.
3. Swing open the UniSpray source enclosure unit from the source mounting on the mass spectrometer.
4. Disconnect the probe adjuster cable.
5. Disconnect the high-voltage cable.
6. Carefully remove the UniSpray source module, and store it safely.

3.5 NanoFlow ESI source

The NanoFlow source enclosure comprises the NanoFlow stage (for *x*-, *y*-, *z*-axis adjustment), the sprayer-enclosure, and a microscope camera.

Figure 3–32: NanoFlow source, stage and microscope camera:



1. Microscope camera
2. Sprayer enclosure
3. X, Y, Z stage

A sprayer is mounted on an X, Y, Z stage (three-axis manipulator), which slides on a pair of guide rails that allow its withdrawal from the source enclosure for maintenance and changes.

A light within the source provides illumination for the spray, which you can observe using the video camera mounted on the corner of the source housing.

The low flow rates involved with operating the NanoFlow source prohibit its use with the instrument's solvent delivery system.

3.5.1 Installing the NanoFlow source

Required materials

Chemical-resistant, powder-free gloves

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid electric shock, ensure that the instrument is prepared for working on the source before commencing this procedure.

Warning: To avoid burn injuries, before performing maintenance operations that involve handling components inside the mass spectrometer's ion source, allow the source interior to cool.

To install the NanoFlow source:

1. Prepare the instrument for working on the source (see Preparing the instrument for working on the source).

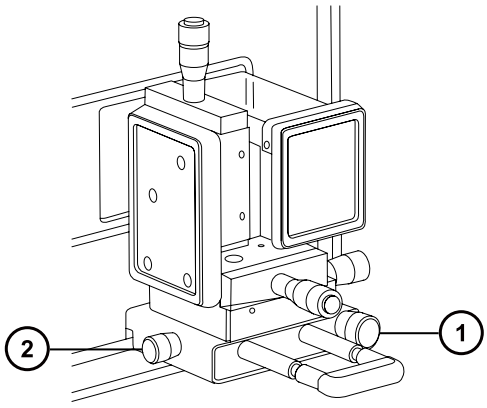
   Warning: To avoid burn injuries, exercise care when handling the components of the source enclosure heated to high temperatures. Wait until the hot components have sufficiently cooled before you handle them.

2. Remove the existing source enclosure (see Removing the source enclosure from the instrument).

   Notice: To prevent damage to the instrument, always retract the stage before installing the source enclosure or closing the door.

3. On the NanoFlow source, release the stage retaining screw, pull the stop screw, and slide the stage fully out of the enclosure.

   Figure 3–33:



1. Retaining screw
2. Stop screw

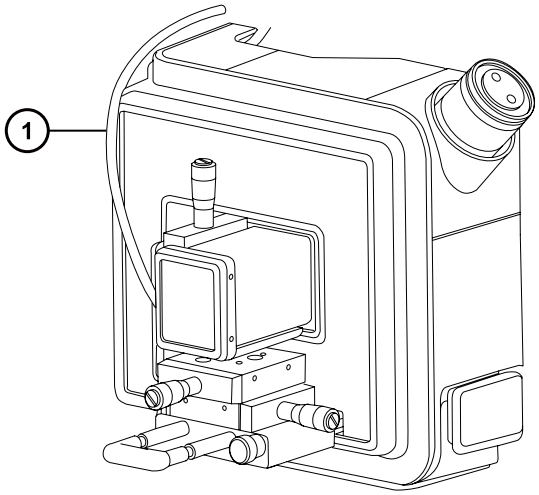
4. Using both hands, fit the NanoFlow source enclosure to the two supporting studs on the source adaptor housing.
5. Close the source enclosure door.
6. Connect a 1/16-inch PTFE tube between the mass-flow controller output (mounted beneath the stage on the front of the NanoFlow source) and your sprayer.

   Tip: For instructions on how to fit each sprayer, see the corresponding reference:

   - *Universal NanoFlow Sprayer Installation and Maintenance Guide* (part number 71500110107)
   - Fitting a borosilicate glass capillary (nanovial)
   - *Capillary Electrophoresis and Capillary Electrochromatography Sprayer Operator's Guide* (part number 6666522)
7. Open the instrument's source interface door (see Waters ACQUITY Xevo TQ-XS UPLC/MS system).
8. Connect the probe cable to the instrument's PROBE connection.
9. Connect the high-voltage cable to the instrument's HV connection.

   Note: The NanoFlow stage contains a high-voltage interlock, so that unless the sprayer is pushed fully forward in the source, the capillary voltage (the voltage applied to the sprayer assembly) and the sampling cone voltage are disabled.

   Figure 3–34:



   (1) High-voltage cable
10. Close the instrument's source interface door.

3.5.2 Fitting a borosilicate glass capillary (nanovial)

Required materials:

- Chemical-resistant, powder-free gloves
- Needle-nose pliers
- Borosilicate glass capillary
- Fused silica syringe needle or GELoader tip
- Fused silica tubing cutter

To fit a borosilicate glass capillary (nanovial):

Warning: To avoid lacerations, puncture injuries, and possible contamination with biohazardous and toxic samples, do not touch the sharp end of the capillary.

Warning: To avoid eye injury from broken fused silica lines, use eye protection when performing this procedure.

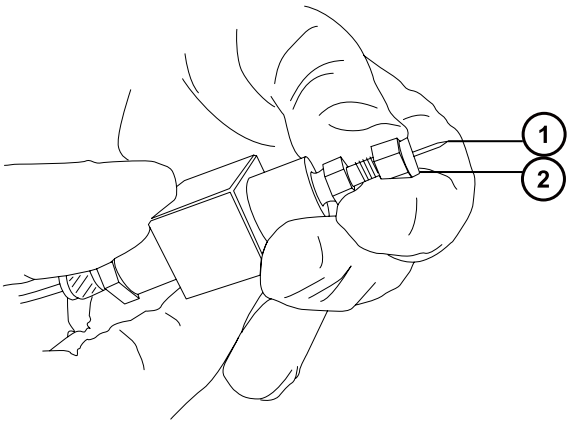
Notice: To avoid damaging capillaries, take great care when handling them; they are extremely fragile. Always hold the blunt end, never the sharp end.

Warning: To avoid electric shock, ensure that the NanoFlow stage is fully retracted from the source before beginning this procedure.

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

1. Loosen the stage retaining screw.
2. Pull the stop screw to release the stage.
3. Slide the stage out of the NanoFlow source enclosure, and remove the magnetic cover.
4. Unscrew the retaining screw, and lift the sprayer from the stage.
5. Unscrew the union from the end of the sprayer assembly.

Figure 3–35:

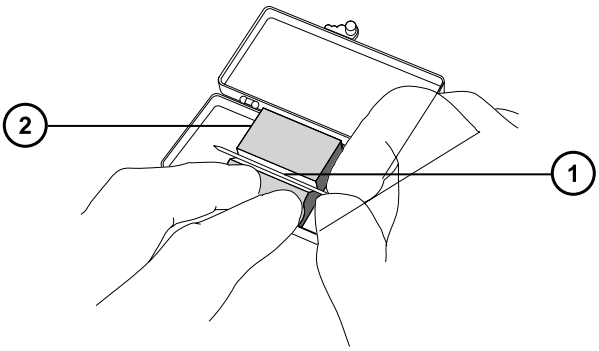


1 Capillary

2 Union

6. Remove the existing capillary from the sprayer.
7. Carefully remove the new borosilicate glass capillary from its case by lifting it vertically while pressing on the foam with two fingers.

Figure 3–36:



1 Capillary

2 Foam

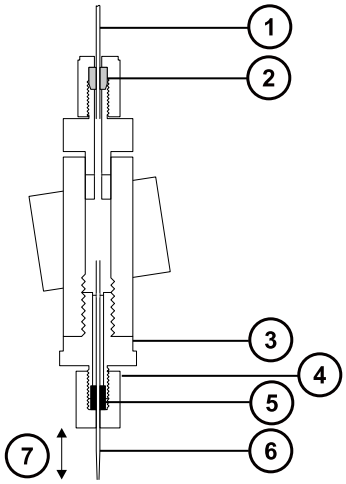
8. Load sample into the capillary using a fused silica syringe needle or a GELoader tip, minimizing any bubbles between the capillary tip and the sample.

   Recommendation: When using a GELoader tip, break the glass capillary in half, scoring it with a fused silica cutter so that the GELoader can reach the capillary's tip.
9. Thread the knurled nut and approximately five mm of conductive elastomer over the blunt end of the capillary.
10. Fit the capillary into the holder (probe).

11. Finger-tighten the nut so that five mm of glass capillary protrudes from its end.

    Tip: Measure the protrusion from the end of the nut to the shoulder of the glass capillary.

    Figure 3–37: Sprayer Assembly:



    1. PTFE tubing
    2. Ferrule
    3. Union
    4. Knurled nut
    5. Blue conductive elastomer
    6. Glass capillary
    7. 5-mm protrusion

12. Screw the sprayer back into the assembly.
13. Replace the sprayer cover.
14. On the MassLynx MS Tune window, ensure that the Capillary parameter on the ES+/- Source tab is set to 0 kV.

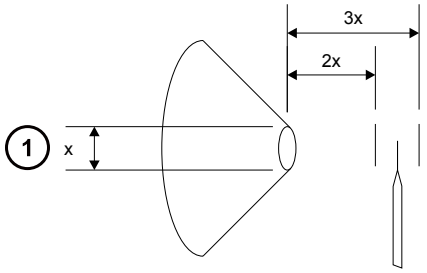
    Notice: To avoid damage to the capillary tip, adjust the sprayer tip position before you push the sprayer inside the NanoFlow source enclosure. Ensure that the capillary tip does not collide with the cone or the side of the source.

15. Carefully push the stage back into the NanoFlow source enclosure, using the stop and handle.

3.5.3 Positioning the borosilicate glass capillary tip

Having obtained a signal, you must adjust the tip position to maximize it. Using the three-axis manipulator, you can adjust the tip position up and down, left and right, forward and backward. As a starting point, set the tip so that it is on the center line of the sampling cone and at a distance between two and three times the diameter of the cone aperture. Typically this distance is approximately 2 mm.

Figure 3–38: Capillary tip position:



1 Cone aperture diameter

For tuning instructions, see the MassLynx, Xevo TQ-XS online help, “Tuning manually for NanoFlow operation”.

3.5.4 Restarting a stalled borosilicate glass capillary electrospray

Should the spray stop, you can restart it. To do so, in the Tune window, set **Capillary** to 0 kV. Then adjust the three-axis manipulator so that, viewed under magnification, the capillary tip touches the sample cone, and a small piece of the borosilicate glass capillary shears off.

If necessary, you can also apply some NanoFlow gas pressure, to force a drop of liquid from the capillary. Apply as much as 1.4 bar (20 psi). Doing so induces the drop’s appearance unless the capillary is blocked.

3.6 ionKey source

The ionKey source integrates UPLC separation into the source of the mass spectrometer. For a complete description, see ionKey source.

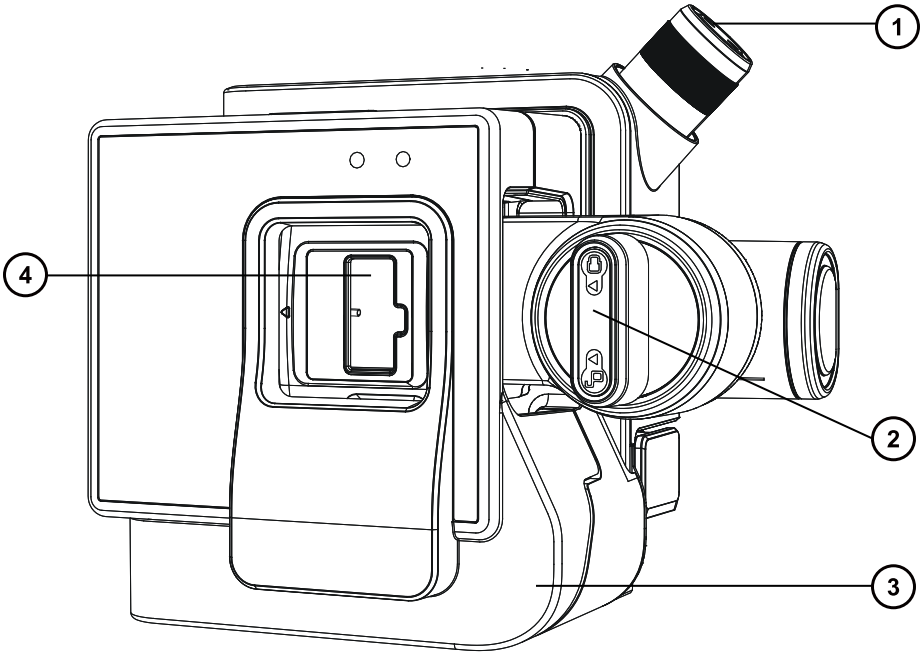
The following sections explain how to install or remove an ionKey source.

For additional information, see the *ACQUITY UPLC M-Class System Guide* (part number 715003588) and the *ionKey/MS System Guide* (part number 715004028).

3.6.1 Installing the ionKey source

The ionKey source enclosure comprises the iKey docking port, the iKey locking handle, the sprayer-enclosure, and a microscope camera.

Figure 3–39: ionKey source:



1. Microscope camera
2. Handle for locking and unlocking the iKey separation device
3. Front cover
4. Docking port for the iKey separation device

Required materials:

- Chemical-resistant, powder-free gloves
- Flat-blade screwdriver
- 1/4-inch open-end wrench

To install the ionKey source:

1. Prepare the instrument for working on the source (see Preparing the instrument for working on the source).

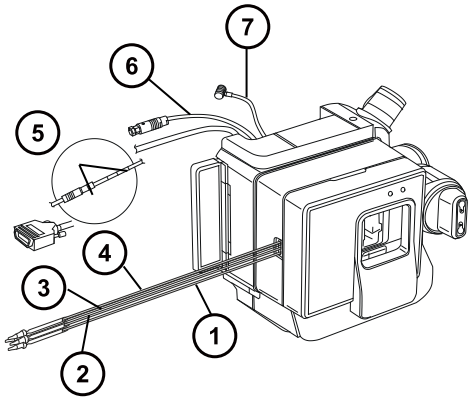
Warning: To avoid burn injuries, exercise care when handling the components of the source enclosure heated to high temperatures. Wait until the hot components have sufficiently cooled before you handle them.

2. Remove the existing source enclosure (see Removing the source enclosure from the instrument).
3. Using two hands, fit the ionKey source enclosure to the two supporting studs on the source adaptor housing.
4. Swing the source enclosure to the closed position, ensuring that it locks into place.

Notice: To avoid damaging the µSample manager or mass spectrometer,

- ensure the µSample manager's power is off before connecting the data/power cable;
- ensure that the mass spectrometer is in Standby mode before beginning any installation or maintenance.

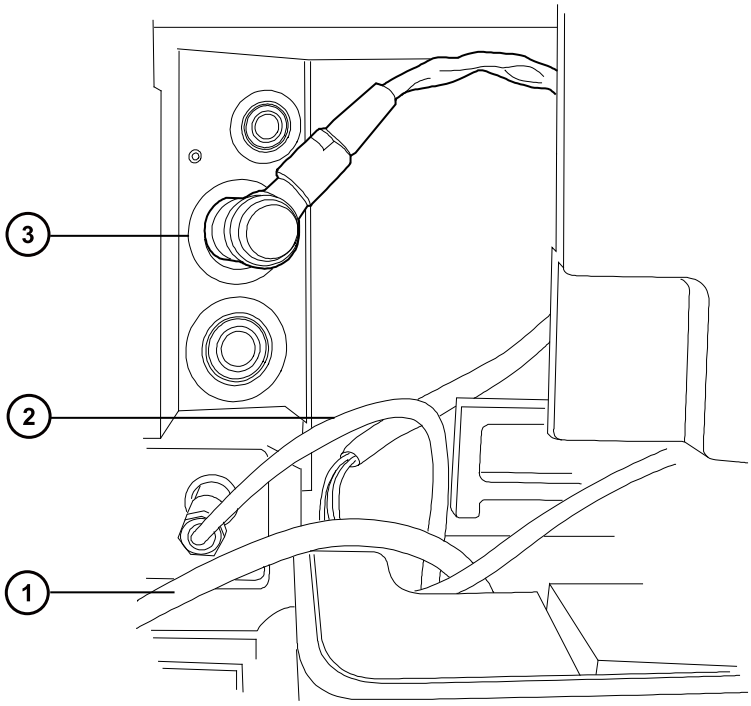
Figure 3–40: ionKey source connections:



1. Fluid waste line
2. Optional post-column addition line
3. Fluid infusion line
4. Fluid inlet line
5. Data/power cable to PSPI connector on µSample manager
6. High-voltage cable
7. Options cable

5. Connect the data/power cable to the PSPI connector on the rear of the µSample manager, and use a screwdriver to firmly tighten the connector screws.

Figure 3–41: Source connections to mass spectrometer:



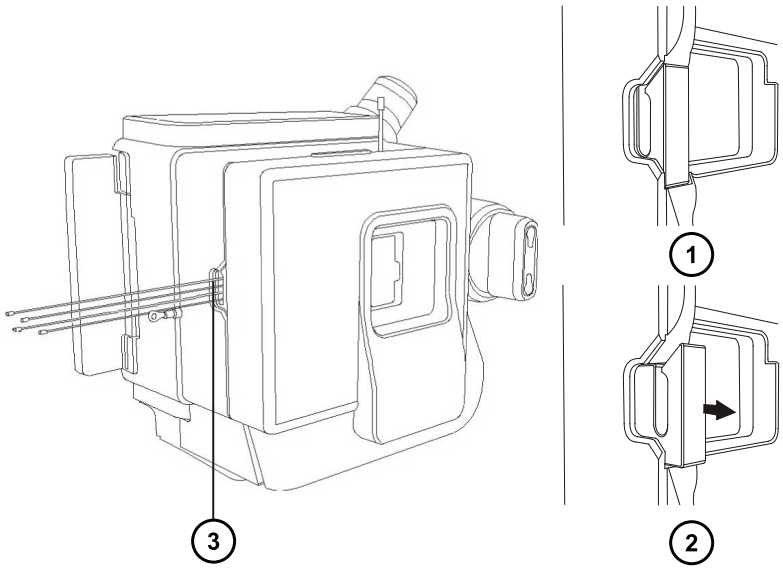
1. Data/power cable to PSPI µSample manager
2. High-voltage cable
3. Options cable

6. Connect the high-voltage cable (white) to the high-voltage supply outlet on the mass spectrometer.
7. Connect the options cable (blue) to the options port on the mass spectrometer.
8. Identify the three fluid lines by the part numbers printed on their shrink-wrap tubing.

Table 3–2: ionKey tubing assemblies:

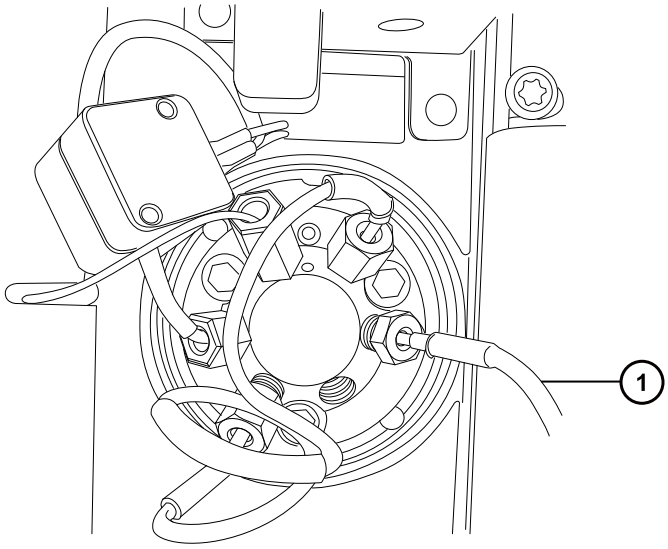
Part Number	Order Number	Description
430004188	700010399	Inlet tube
430004190	700010400	Infusion tube
430004212	700010401	Waste tube
430004476	700010470	Optional, post-column addition tube

Figure 3–42: Fluid line aperture:



1. Aperture closed
2. Aperture open (spring-loaded)
3. Fluid line aperture

Figure 3–43: µSample manager injection valve:



1. Fluid inlet line connected to injection valve port 6

9. Connect the fluid inlet line to port 6 on the injection valve of the µSample manager.
10. Connect the fluid infusion line to port 2 on the fluidics divert valve.

3.6.2 Installing ionKey source software

If you are installing an ionKey source on your Xevo TQ-XS for the first time, you must install the appropriate MassLynx software SCN and the ACQUITY UPLC M-Class driver pack. For further details, see the following documents:

- *ACQUITY UPLC M-Class System Guide* (part number 715003588) for detailed installation procedures, and information on using the ACQUITY Inlet Switch Utility.
- MassLynx software v4.2 and related SCN release notes for detailed information about installing MassLynx software and SCNs.

3.6.3 Installing the camera in the ionKey source

To install the camera in the ionKey source:

1. Connect the camera cable from the video output connector on the mass spectrometer's rear panel to the video-to-USB converter box.

   Notice: To avoid damaging the video converter, make sure the workstation is powered-off before connecting the converter to the workstation in the next step.

2. Connect the video-to-USB converter box to a USB port on the mass spectrometer's workstation.

3. On the Tune page, click **Camera Viewer**  .

4. In Device settings dialog box, specify the parameter settings according to the following table, and then click **OK**.

   Tip: After you install the camera software, when you select the ionKey camera viewer for the first time, the device settings dialog box opens. To subsequently open the device settings dialog box, in the camera viewer, click **View** > **Camera Options**.

Table 3–3: Device settings for the camera:

Parameter	Setting
Video norm	PAL_B
Video format	Y800 (768 x 576)
Frame rate (FPS)	25
Input channel	00 Video: Composite

3.6.4 Removing an ionKey source

You can remove the ionKey source, and replace it with a conventional interface.

Alternative: If you are using the ionKey source with an ACQUITY UPLC M-Class system mounted on an M-Class cart fitted with an ionKey or universal source holder, you can secure the source enclosure to the holder. Doing so keeps the enclosure close to the Xevo TQ-XS, for when it is next needed. Securing the source enclosure also assists with managing the ionKey source's fluid lines and helps prevent contamination of the fluid lines.

See the ACQUITY M-Class documentation for additional information about installing the ionKey source holder on the M-Class cart, and securing the source enclosure to the holder.

See *Installing and Using the Universal Source Holder* (part number 715004884) for additional information about installing and using the universal source holder on the M-Class cart, and securing the source enclosure to the holder.

See also: The *ionKey/MS System Guide* (part number 715004028).

Required materials

- Chemical-resistant, powder-free gloves
- 1/4-inch open-end wrench

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid electric shock, ensure that the instrument is prepared for working on the source before commencing this procedure.

To remove the ionKey source:

1. Prepare the instrument for working on its source (see Preparing the instrument for working on the source).

   Warning: To avoid burn injuries, exercise care when handling the column or other components heated to high temperatures. Wait until the hot components have sufficiently cooled before you handle them.

2. Remove the iKey from the docking port (see the *ionKey/MS System Guide*, part number 715004028).
3. Close the MassLynx software.
4. Power-off the µSample manager.
5. Disconnect the PSPI cable.
6. Using the ¼-inch open-end wrench, loosen and disconnect the fluid waste line and fluid inlet lines from the µSample manager.
7. Disconnect the optional post-column addition line from the flow control module of the auxiliary solvent manager.

8. Swing open the ionKey source enclosure unit from the source mounting on the mass spectrometer.
9. Disconnect the high-voltage cable (white) from the high-voltage supply outlet on the mass spectrometer.
10. Disconnect the reference probe power cable (green) from the reference probe power inlet on the mass spectrometer.
11. Disconnect the options cable (blue) from the options port on the mass spectrometer.
12. Disconnect the fluid infusion line from the onboard IntelliStart Fluidics system on the mass spectrometer.
13. Carefully remove the ionKey source module, and store safely.

4 Maintenance procedures

This section provides the maintenance guidelines and procedures necessary to maintain the mass spectrometer's performance.

Keep to a maintenance schedule, and perform maintenance as required and described in this section.

4.1 Maintenance schedule

The following table lists periodic maintenance schedules that ensure optimum instrument performance.

Table 4–1: Maintenance schedule:

Procedure	Frequency	For information...
Clean the instrument case.	As required.	See Cleaning the instrument case.
Empty the nitrogen exhaust trap bottle.	Check daily, empty as required.	See Emptying the nitrogen exhaust trap bottle.
Clean the source components.	When source components are visibly fouled, the background or high-peak contaminants are unacceptably high, or sensitivity decreases to unacceptable levels.	See Cleaning the source components.
Replace the ESI probe tip.	When sensitivity decreases to unacceptable levels, or if blocked or damaged.	See Replacing the ESI probe tip and gasket.
Replace the probe assembly.	When sensitivity decreases to unacceptable levels or signal is unstable due to inconsistent sample flow.	See Replacing the probe assembly.
Clean the APCI probe tip. (Options using the APCI probe adaptor only.)	When sensitivity decreases to unacceptable levels or when significant chemical interference is present.	See Cleaning the APCI probe tip.

Table 4–1: Maintenance schedule: (continued)

Procedure	Frequency	For information...
Clean or replace the corona pin (APCI and ESCi modes).	When the corona pin is corroded or black, or the sensitivity decreases to unacceptable levels.	See Cleaning or replacing the corona pin.
Replace the APCI probe heater. (Options using the APCI probe adaptor only.)	If the heater fails to heat when the instrument is switched to Operate.	See Replacing the APCI probe heater.
Replace the probe assembly (UniSpray mode).	When sensitivity decreases to unacceptable levels or signal is unstable due to inconsistent sample flow.	See Replacing the UniSpray probe assembly.
Clean or replace the impactor pin (UniSpray mode).	When the impactor pin is corroded or black, or the sensitivity decreases to unacceptable levels.	See Maintaining the UniSpray impactor pin.
Replace the ion block heater cartridge.	If the heater fails to heat when the instrument is pumped down (evacuated).	See Replacing the ion block source heater.
Replace the source assembly seals.	Annually.	See Replacing the source assembly seals.
Replace the roughing pump.	Every 3 years.	Contact Waters.
Replace the air filters.	Annually.	See Replacing the air filter inside the front door.
Clean the APPI/APCI source UV lamp window.	When the window becomes visibly dirty, or when the sensitivity decreases to unacceptable levels.	See APPI/APCI source—cleaning the lamp window.
Change the APPI/APCI source UV lamp bulb.	When the bulb fails.	See APPI/APCI source -- changing the UV lamp bulb.
Replace the APPI lamp drive assembly O-rings.	Annually.	See APPI/APCI source—replacing the APPI lamp drive seals.
Replace an ionKey source fluid line.	As required or during periodic maintenance.	See Replacing the fluidic lines of the ionKey source.
Clean the ionKey source surface, fluid connectors, or electronic connectors.	As required or during periodic maintenance.	See Cleaning the ionKey source and connectors.

4.2 Spare parts

Waters recommends that you replace only the parts mentioned in this document. For spare parts details, see the Waters Quality Parts Locator on the Waters Web site's Services & Support page (http://www.waters.com/waters/en_US/Spare-Parts/nav.htm?cid=511444).

4.3 Troubleshooting with Connections INSIGHT

Connections INSIGHT is an intelligent device management (IDM) Web service that enables Waters to provide proactive service and support for the ACQUITY UPLC system. To use Connections INSIGHT, you must install its service agent software on your workstation. In a client/server system, the service agent must also be installed on the computer from which you control the system. The service agent software automatically and securely captures and sends information about the support needs of your system directly to Waters.

If you encounter a performance issue when using the Instrument Console, you can manually submit a Connections INSIGHT request to Waters customer support. Alternatively, you can use Remote Desktop, a real-time collaboration option that controls the two-way connection with the ACQUITY UPLC system by enabling the Connections INSIGHT iAssist service level.

Consult these sources for more information about Connections INSIGHT and Connections INSIGHT iAssist:

- http://www.waters.com
- *Connections INSIGHT User's Guide* (part number 715003036)
- Your sales representative
- Your local Waters subsidiary
- Waters Customer Support

To submit a Connections INSIGHT request:

1. Select **Troubleshoot** > **Submit Connections INSIGHT Request**.
2. In the Connections INSIGHT Request dialog box, type your name, telephone number, e-mail address, and a description of the problem.
3. Click **Submit**, and allow approximately five minutes to save the service profile.

   Recommendation: A `.ZIP` file containing your Connections INSIGHT profile is forwarded to Waters customer support for review. Saving a service profile or plot file from the Instrument Console can require as much as 150 MB of file space.

4.4 Safety and handling

Bear in mind the following safety considerations when performing maintenance procedures:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: Observe Good Laboratory Practice (GLP) at all times, particularly when working with hazardous materials. Consult the Material Safety Data Sheets regarding the solvents you use. Additionally, consult the safety representative for your organization regarding its protocols for handling such materials.

Warning: To avoid electric shock, observe these precautions:

- Do not remove the mass spectrometer's protective panels. The components they cover are not user-serviceable.
- When the instrument is in Operate mode, avoid touching the areas marked with the high voltage warning symbol. To touch external areas marked with the symbol, first put the instrument in Standby mode.

Warning: To avoid burn injuries, take great care while working with the probe and source; these components can be hot.

Warning: To avoid puncture wounds, take great care working with the source enclosure open if one or both of these conditions apply:

- An ESI probe is fitted (the probe's tip is sharp).
- A corona pin is fitted (the pin's tip is sharp).

Warning: To avoid injury, ensure that these criteria are met when performing maintenance operations inside the source enclosure:

- The instrument is in Standby mode.
- LC flow is diverted to waste or set to Off.
- Desolvation gas flow is stopped.

Notice: To avoid damaging the iKey:

- Handle it with care. The component parts are fragile.
- For recommendations regarding the maximum pressure to subject the device to, see the *iKey Separation Device Care and Use Manual* (part number 720004897EN).
- Do not apply electrospray potential to the emitter without flow.
- Do not drop it.
- Do not immerse it in liquid.
- Do not freeze or overheat it. Keep the iKey within the allowed temperature ranges during operation and in storage.
- Use the iKey sheath to protect the device when it is not in use.
- Do not bend or pull the capillary connection tubing at the ionKey source module coupling.
- Avoid excess voltage, which can erode the emitter over time.
- Do not touch the electrospray emitter, for it can bend.
- Decompress the iKey before you remove it from the source.

See Safety advisories for safety advisory information.

4.5 Preparing the instrument for working on the source

For safety reasons, you must follow this procedure before working on the source (for example, when changing the probe, installing or removing the corona pin, or operating the source isolation valve), and when maintaining the source.

Follow the procedure for the software that controls your mass spectrometer:

4.5.1 Using MassLynx software to prepare the instrument for operations on or inside its source

To use MassLynx software to prepare the instrument for operations on or inside its source:

1. In the Instrument Console, click **Stop Flow**  , to stop the LC flow.

Note: If column flow is required, divert the LC flow to waste:

1. 1. In the Instrument Console system tree, expand Xevo TQ-XS Detector, Interactive Fluidics.
   2. Click **Control**  .
   3. Select **Waste** as the flow state.
2. In the Instrument Console, click **Standby**  , and confirm that the **Operate** indicator is not illuminated.
3. Wait three minutes, to allow the desolvation gas flow to cool the probe and source.
4. In the Instrument Console, click **API**  , to stop the desolvation gas flow.

4.6 Removing and refitting the source enclosure

Before performing certain maintenance procedures, or fitting the optional sources to the instrument, you must remove the source enclosure that is currently fitted to the instrument.

Note: The following procedures apply to both the standard and optional source enclosures.

4.6.1 Removing the source enclosure from the instrument

Required materials

Chemical-resistant, powder-free gloves

To remove the source enclosure:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

1. Prepare the instrument for working on the source (see Prepare the instrument for working on the source).

   Warning: To avoid burn injuries, exercise care when handling the components of the source enclosure heated to high temperatures. Wait until the hot components have sufficiently cooled before you handle them.
2. Remove the probe adaptor from the source (Removing the probe adaptor).
3. Slide open the instrument's source interface door (see Waters ACQUITY Xevo TQ-S UPLC/MS system).

4. Disconnect the probe adjuster and options cables from the instrument's connectors.

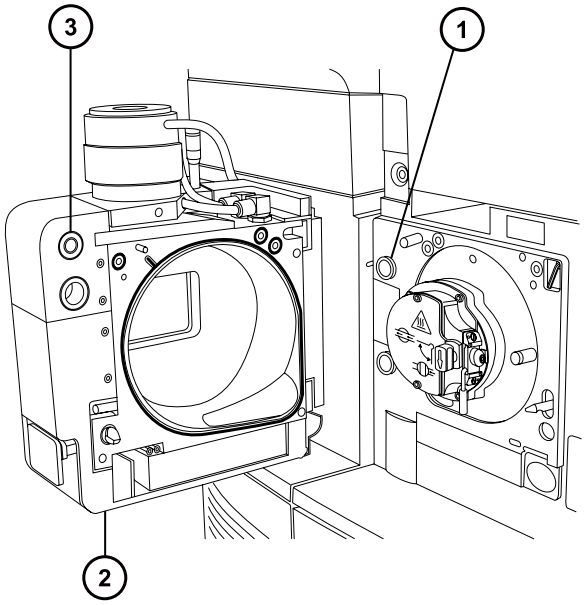
Warning: To avoid puncture wounds, handle sharp parts and materials with care.

Notice: To avoid damaging the sample inlet, when removing a NanoLockSpray source enclosure, you must slide the sprayer platform out of the source enclosure before you open the enclosure.

5. Pull the source enclosure release (located at the bottom, right-hand side) outwards, and swing open the enclosure.

6. Using both hands, grasp the source enclosure, and lift it vertically off the two supporting studs on the source adaptor housing.

Figure 4–1:



1. Supporting stud
2. Source enclosure
3. Cable storage positions

7. Store the cables neatly by plugging them into the cable-storage positions on the rear of the source enclosure.

4.6.2 Fitting the source enclosure to the instrument

Required materials

Chemical-resistant, powder-free gloves

To fit the source enclosure to the instrument:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid puncture injuries, handle sample needles, syringes, fused silica lines, and borosilicate tips with extreme care.

1. Using both hands, fit the source enclosure to the two supporting studs on the source adaptor housing.

   Notice: To avoid damaging the sample inlet, when removing a NanoLockSpray source enclosure, you must slide the sprayer platform out of the source enclosure before you open the enclosure.

2. Close the source enclosure.
3. Connect the probe adjuster and options cables to the instrument's connectors.

   Tip: The cables and connectors are color coded; the blue-sleeved cable connects to the blue connector and the yellow-sleeved cable to the yellow connector.

4. Slide closed the instrument's source interface door.

4.7 Operating the source isolation valve

You must close the source isolation valve to isolate the source from the instrument vacuum system for certain maintenance procedures.

Required materials

Chemical-resistant, powder-free gloves

4.7.1 Closing the source isolation valve

To close the source isolation valve before starting a maintenance procedure:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

1. Prepare the instrument for working on the source (see Preparing the instrument for working on the source).

   Warning: To avoid burn injuries, take great care while working with the source enclosure open.

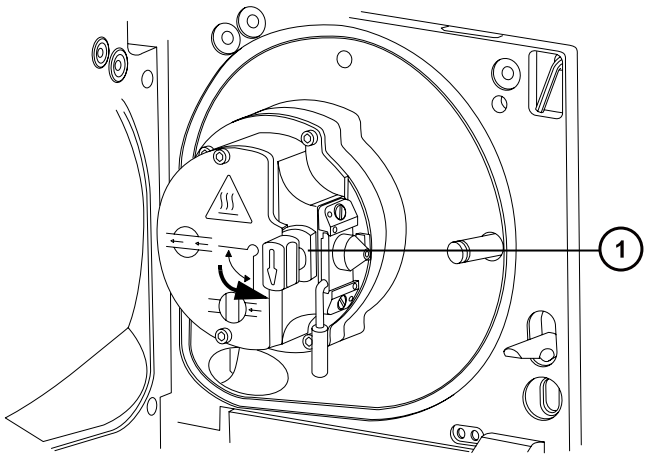
   

   Warning: To avoid puncture wounds, take great care working with the source enclosure open if one or both of these conditions apply:

   - An ESI probe is fitted (the probe's tip is sharp).
   - A corona pin is fitted (the pin's tip is sharp).

2. Pull the source enclosure release (located at the bottom, right-hand side) outwards, and swing open the enclosure.
3. Close the source isolation valve by turning its handle counterclockwise, to the vertical position.

Figure 4–2:



1 Isolation valve handle in closed position

4.7.2 Opening the source isolation valve

To open the source isolation valve after completing a maintenance procedure:

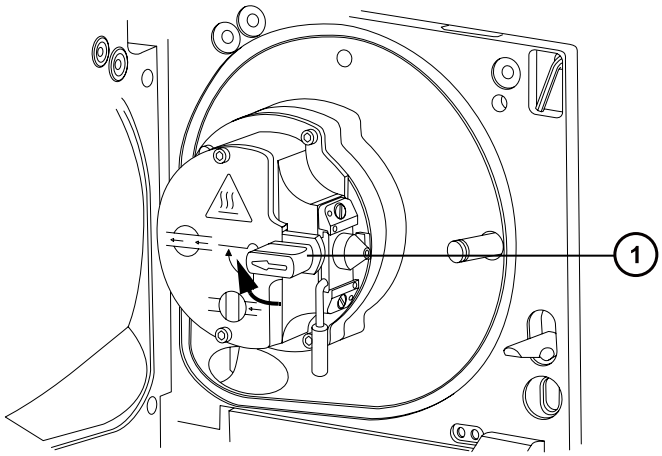
Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid puncture wounds, take great care working with the source enclosure open if one or both of these conditions apply:

- An ESI probe is fitted (the probe's tip is sharp).
- A corona pin is fitted (the pin's tip is sharp).

1. Open the source isolation valve by moving its handle clockwise to the horizontal position.

   Figure 4–3:



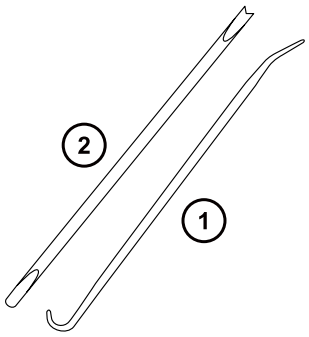
   (1) Isolation valve handle in open position

2. Close the source enclosure.

4.8 Removing O-rings and seals

When performing certain maintenance procedures, you must remove O-rings or seals from instrument components. An O-ring removal kit is provided with the instrument.

Figure 4–4: O-ring removal kit:



1 Tool 1

2 Tool 2

To remove an O-ring:

Note: To avoid damaging the component when removing an O-ring or seal from it, ensure that you do not scratch the component with the removal tool.

Use the tools as aids to pull the O-ring or seal from its groove.

Tip: If the O-ring or seal will not be reused, you can use the forked end of tool 2 to impale the O-ring or seal, aiding its removal.

4.9 Cleaning the instrument case

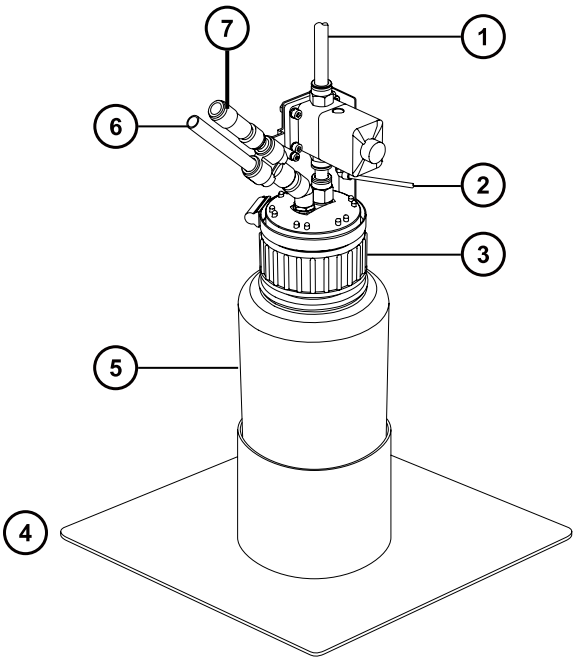
Notice: To avoid abrading the surfaces of the instrument, do not use abrasives or solvents when cleaning them.

Use a soft cloth, dampened with water, to clean the outside surfaces of the mass spectrometer.

4.10 Emptying the nitrogen exhaust trap bottle

Inspect the nitrogen exhaust trap bottle in the instrument exhaust line daily, and empty it before it is more than approximately 10% full.

Figure 4–5: Nitrogen exhaust trap bottle:



1. To laboratory exhaust port
2. From instrument pilot valve port
3. Cap
4. Bottle support
5. Nitrogen exhaust trap bottle
6. From instrument exhaust connection
7. One-way valve

Required materials

Chemical-resistant, powder-free gloves

To empty the nitrogen exhaust trap bottle:

1. In the instrument console, click **Stop Flow**  .
2. Pull the source enclosure release (located at the bottom, right-hand side) outward, and swing open the enclosure.

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

3. Unscrew and remove the nitrogen exhaust trap bottle from the cap and associated fittings.

   Warning: To avoid contaminating uncontaminated surfaces with biologically hazardous, toxic, or corrosive materials, dispose of all waste materials according to local environmental regulations.

4. Dispose of the waste liquid in accordance with local environmental regulations.
5. Fit and tighten the nitrogen exhaust trap bottle to the cap.
6. Secure the nitrogen exhaust trap bottle in the upright position.
7. Close the source enclosure.

   Tip: An automatic pressure test is performed.

8. In the instrument console, click **Start Flow** .

4.11 Maintaining the roughing pump

There are no user maintenance procedures for the EBARA EV-SA30 pump.

To replace the pump, contact Waters Technical Support.

4.12 Cleaning the source components

Clean the sample cone and cone gas nozzle when these conditions apply:

- The sample cone and cone gas nozzle are visibly fouled.
- LC and sample-related causes for decreased signal intensity are dismissed.

See Cleaning the sampling cone assembly.

If cleaning the sample cone and cone gas nozzle fails to increase signal sensitivity, clean the ion block and isolation valve (see Cleaning the ion block assembly).

If cleaning the ion block and isolation valve fails to increase signal sensitivity, clean the StepWave assembly (see Cleaning the StepWave ion guide assembly).

4.13 Cleaning the sampling cone assembly

You can remove the sampling cone assembly (comprising the sample cone, O-ring, and cone gas nozzle) for cleaning without venting the instrument.

4.13.1 Removing the sampling cone assembly from the source

Required materials

Chemical-resistant, powder-free gloves

To remove the sampling cone assembly from the source:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid electric shock, ensure that the instrument is in Standby mode before commencing this procedure.

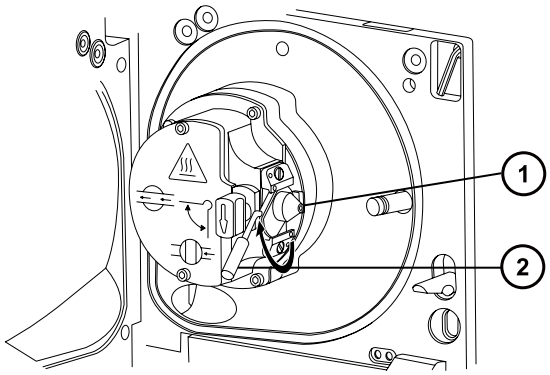
Warning: To avoid puncture wounds, take great care working with the source enclosure open if one or both of these conditions apply:

- An ESI probe is fitted (the probe's tip is sharp).
- A corona pin is fitted (the pin's tip is sharp).

Warning: To avoid burn injuries, take great care while working with the source enclosure open.

1. Close the source isolation valve (see Closing the source isolation valve).
2. Grasp the cone gas nozzle handle, and use it to rotate the sampling cone assembly 90 degrees, moving the handle from the vertical position to the horizontal position.

   Figure 4–6:

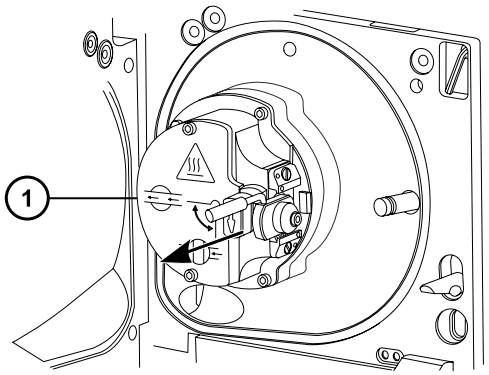
   

   (1) Sampling cone assembly, comprising the cone gas nozzle, sampling cone, and O-ring

   (2) Cone gas nozzle handle

3. Slide the sampling cone assembly out of the ion block assembly.

Figure 4–7:



1 Ion block assembly

Notice: To avoid damaging the StepWave assembly, do not switch the instrument into Operate mode when the isolation valve is closed.

Notice: To avoid damage, do not open the source isolation valve before fitting the sampling cone assembly to the ion block assembly

4.13.2 Disassembling the sampling cone assembly

Required materials

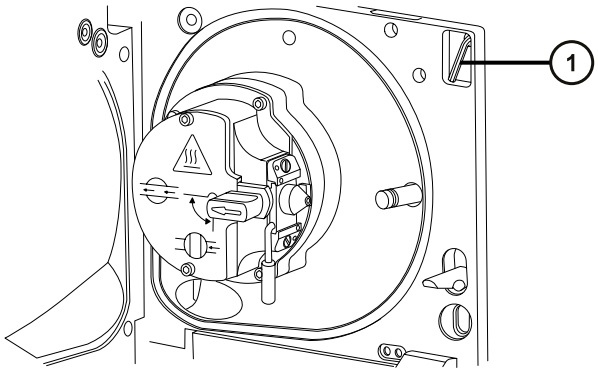
- Chemical-resistant, powder-free gloves
- Combined 2.5-mm hex wrench and cone extraction tool

To disassemble the sampling cone assembly:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

1. Retrieve the combined 2.5-mm hex wrench and cone extraction tool from its storage location behind the source enclosure.

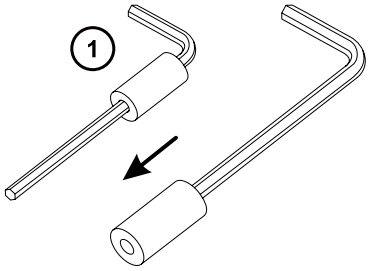
Figure 4–8: Cone extraction tool location



1 Combined 2.5-mm hex wrench and cone extraction

2. Slide the collar to the end of the tool.

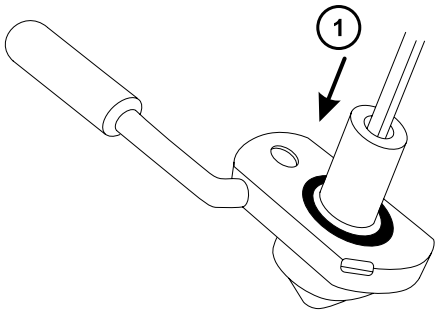
Figure 4–9: Cone extraction tool



1 Collar

3. Insert the collar in the sample cone.

Figure 4–10: Inserting the cone extraction tool

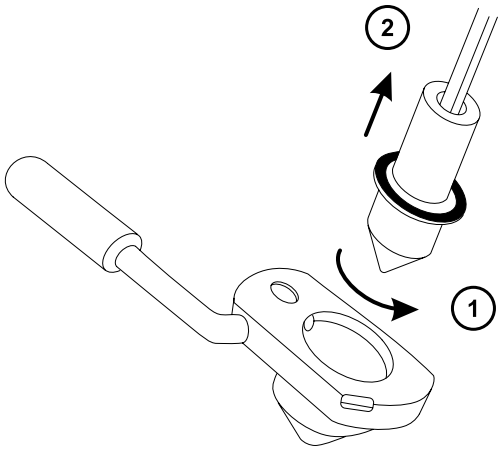


1 Insert the collar

Notice: To avoid damaging the sampling cone, which is fragile, do not place it on its tip; always place it on its flanged base

4. Rotate and lift the tool and collar to remove the sample cone from the cone gas nozzle.

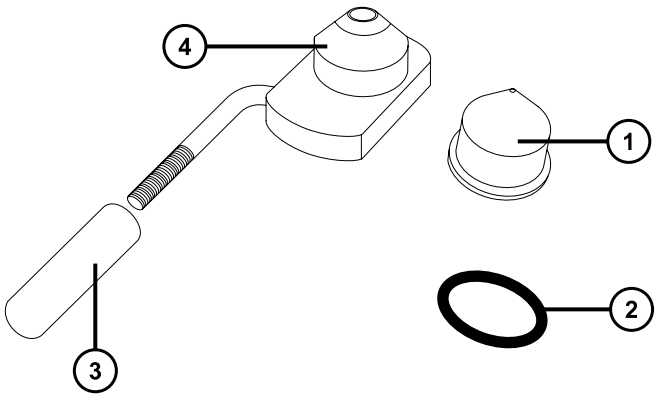
Figure 4–11: Removing the sample cone



1. Rotate the tool
2. Remove the sample cone

5. Remove the O-ring from the sample cone.

Figure 4–12: O-ring removed from the sample cone



1. Sample cone
2. O-ring
3. Cone gas nozzle handle
4. Cone gas nozzle

Warning: To avoid spreading contamination, dispose of all waste materials according to local environmental regulations.

6. If the O-ring shows signs of deterioration or damage, dispose of it in accordance with local environmental regulations.
7. Unscrew and remove the PEEK cone gas nozzle handle from the cone gas nozzle.

4.13.3 Cleaning the sample cone and cone gas nozzle

Required materials

- Chemical-resistant, powder-free gloves
- Appropriately sized glass vessels in which to completely immerse components when cleaning. Use only glassware not previously cleaned with surfactants.
- HPLC-grade (or better) methanol
- HPLC-grade (or better) water
- Formic acid
- Ultrasonic bath
- Oil free, argon gas or Oil free, nitrogen gas
- Wash bottle containing HPLC-grade (or better) 1:1 methanol/water
- Large beaker

To clean the sample cone and cone gas nozzle:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid injury when working with formic acid, which is extremely corrosive and toxic, take extreme care handling it, and use a fume hood and suitable protective equipment.

Notice: To avoid damaging the sampling cone, which is fragile, do not place it on its tip; always place it on its flanged base

1. If the sample cone contains debris, place a drop of formic acid on its orifice.
2. Immerse the sample cone, cone gas nozzle, and cone gas nozzle handle in separate glass vessels containing 1:1 methanol/water.

   Tip: If the components are obviously contaminated, use 45:45:10 methanol/water/formic acid.

3. Place the vessels in the ultrasonic bath for 30 minutes.
4. If you used formic acid in the cleaning solution, do as follows:
    a. Rinse the components by immersing them in separate glass vessels containing water and then placing the vessels in the ultrasonic bath for 20 minutes.
    b. Remove any residual water from the components by immersing them in separate glass vessels containing methanol and then placing the vessels in the ultrasonic bath for 10 minutes.

    Notice: To avoid recontaminating the components, wear clean, chemical-resistant, powder-free gloves for the rest of this procedure.
5. Carefully remove the components from the vessels, and blow dry them with inert, oil-free gas.
6. Inspect each component for persisting contamination. If contamination is present, do as follows:
    a. Use the wash bottle containing 1:1 methanol/water to rinse the component over the large beaker.
    b. Blow dry the component with inert, oil-free gas.

    Warning: To avoid spreading contamination, dispose of all waste materials according to local environmental regulations.
7. Inspect each component for persisting contamination.

    Requirement: If contamination is present, clean the component again. If contamination is still present, dispose of the component, according to local environmental regulations, and obtain a new one before reassembling the sampling cone assembly.

4.13.4 Assembling the sampling cone assembly

Required materials

Chemical-resistant, powder-free gloves

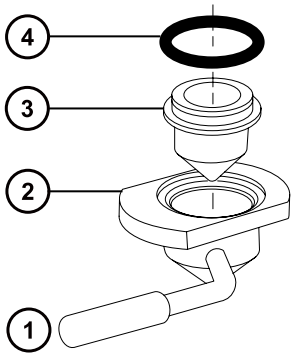
To assemble the sampling cone assembly:

Note: To avoid recontaminating the components, wear clean, chemical-resistant, powder-free gloves for the rest of this procedure.

Notice: To avoid damaging the sampling cone, which is fragile, do not place it on its tip; always place it on its flanged base

1. Fit the cone gas nozzle handle to the cone gas nozzle and turn the handle clockwise to tighten.

Figure 4–13:



1. Cone gas nozzle handle
2. Cone gas nozzle
3. Sample cone
4. O-ring

2. Carefully fit the sample cone into the cone gas nozzle.
3. Fit the O-ring (a new one, if you disposed of the old O-ring) into the groove created between the sample cone and cone gas nozzle.

4.13.5 Fitting the sampling cone assembly to the source

Required materials

Chemical-resistant, powder-free gloves

To fit the sampling cone assembly to the source:

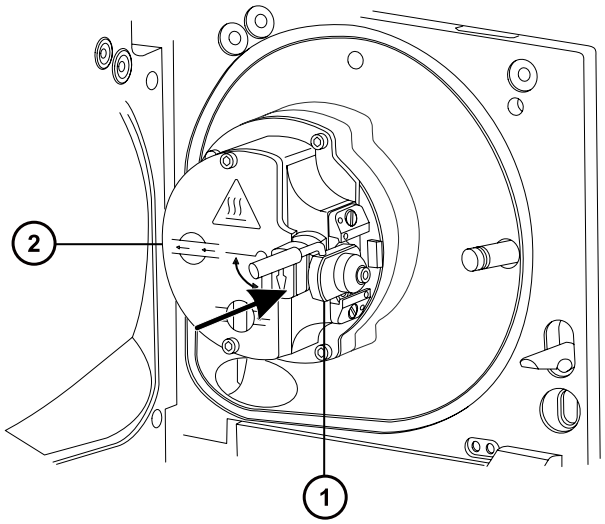
Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid puncture injuries, handle sample needles, syringes, fused silica lines, and borosilicate tips with extreme care.

Notice: To avoid damage, do not open the source isolation valve before fitting the sampling cone assembly to the ion block assembly

1. Ensure that the source isolation valve is in the closed position (see Closing the source isolation valve).
2. Hold the sampling cone assembly so that the cone gas nozzle handle is oriented horizontally and at the top, and then slide the sampling cone assembly into the ion block assembly.

Figure 4–14:



1 Sampling cone assembly

2 Ion block assembly

3. Grasp the cone gas nozzle handle, and use it to rotate the sampling cone assembly 90 degrees, moving the handle downward from the horizontal to the vertical position.
4. Open the source isolation valve (see Opening the source isolation valve).
5. Close the source enclosure.

4.14 Cleaning the ion block assembly

Clean the ion block assembly if cleaning the sample cone and cone gas nozzle fails to increase signal sensitivity.

4.14.1 Removing the ion block assembly from the source assembly

Required materials

- Chemical-resistant, powder-free gloves
- Combined 2.5-mm hex wrench and cone extraction tool

To remove the ion block assembly:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

1. Vent and shut down the mass spectrometer (see the mass spectrometer's online Help for details).

   Warning: To avoid personal injury, as well as damage to the roughing pump and mass spectrometer, disconnect the power cords for the mass spectrometer and roughing pump from the main power source.

2. Disconnect the power cords for the mass spectrometer and the roughing pump from the main power source.

   Warning: To avoid burn injuries, exercise care when handling the column or other components heated to high temperatures. Wait until the hot components have sufficiently cooled before you handle them.

   Warning: To avoid puncture wounds, take great care working with the source enclosure open if one or both of these conditions apply:

   - An ESI probe is fitted (the probe's tip is sharp).
   - A corona pin is fitted (the pin's tip is sharp).

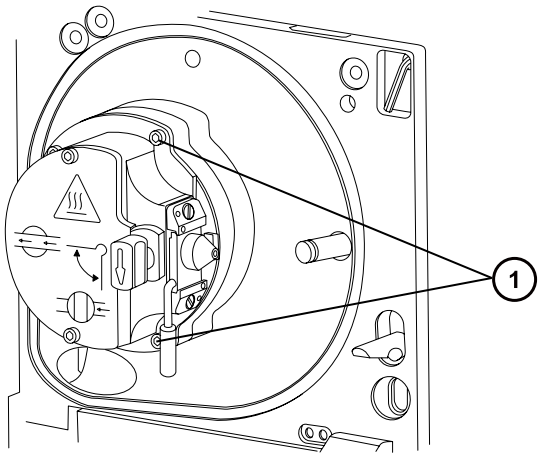
3. Remove the source enclosure (see Removing the source enclosure from the instrument).

   Rationale: Removing the source enclosure aids access to the ion block assembly.

4. Close the source isolation valve (see Closing the source isolation valve).

5. Use the combined 2.5-mm Allen wrench and cone extraction tool to unscrew the four, captive, ion block assembly securing screws.

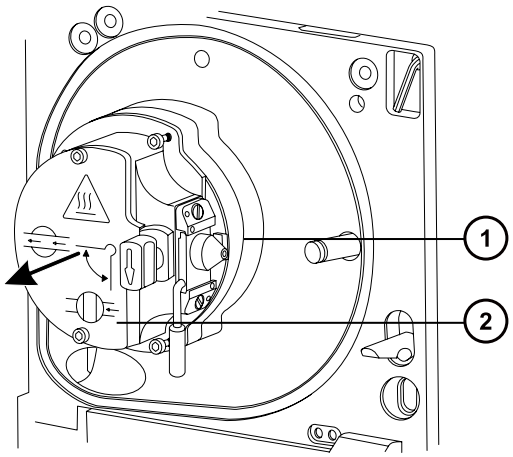
Figure 4–15:



1 Ion block assembly securing screws

6. Remove the ion block assembly from the PEEK ion block support.

Figure 4–16:



1 PEEK ion block support

2 Ion block assembly

4.14.2 Disassembling the source ion block assembly

Required materials

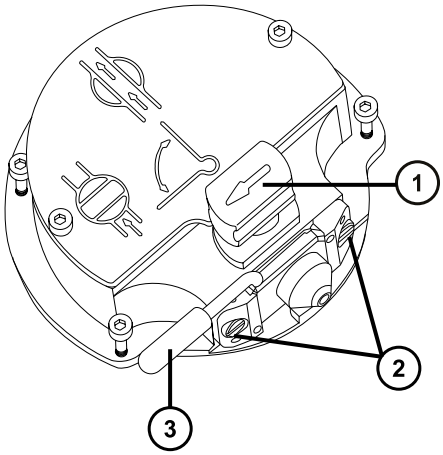
- Chemical-resistant, powder-free gloves
- Combined 2.5-mm hex wrench and cone extraction tool
- O-ring removal kit

To disassemble the ion block assembly:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

1. Ensure that the source isolation valve is closed.

Figure 4–17: Source ion block assembly



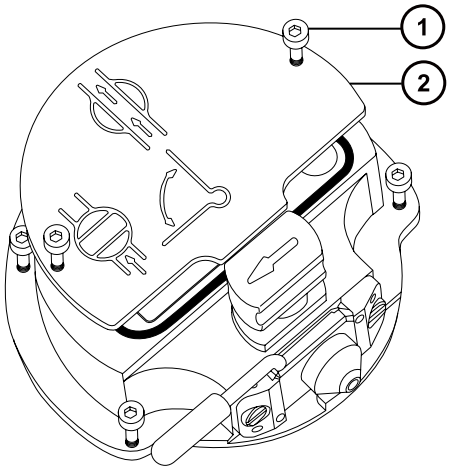
1. Source isolation valve handle in closed position
2. Sampling cone assembly retaining blocks
3. Cone gas nozzle handle

2. Grasp the cone gas nozzle handle, and use it to rotate the sampling cone assembly through 90 degrees.
3. Slide the sampling cone assembly out of the ion block assembly.
4. Use the combined 2.5-mm Allen wrench and cone extraction tool to loosen the two captive screws securing the ion block cover plate.

Important: To ensure correct operation of the ion block assembly after reassembly,

- do not remove the sampling cone assembly retaining blocks.
- do not adjust the screws securing the sampling cone assembly retaining blocks.

Figure 4–18: Source ion block cover plate

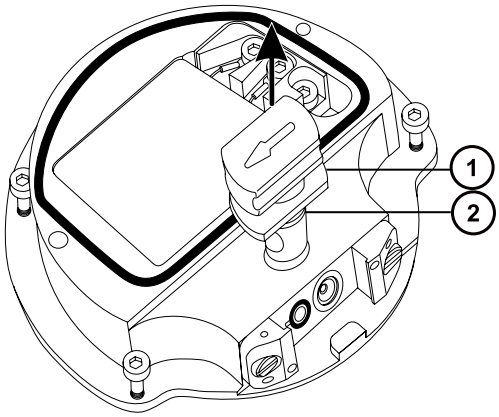


1 Ion block cover plate securing screw

2 Ion block cover plate

5. Remove the ion block cover plate.
6. Grasp the isolation valve, and pull it out of the ion block.

Figure 4–19: Removing the isolation valve from the ion block



1 Isolation valve

2 O-ring

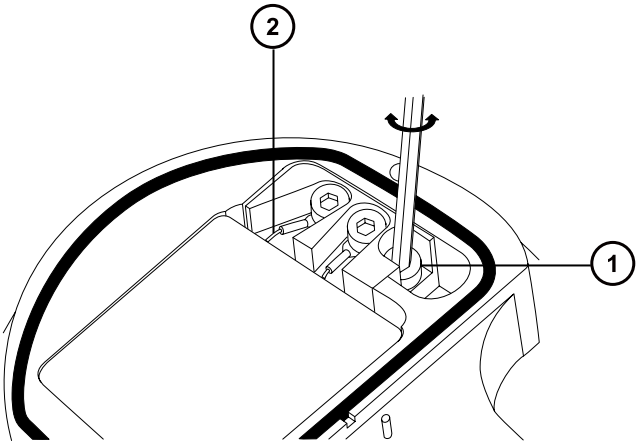
7. Use the O-ring removal kit to carefully remove the isolation valve O-ring (see Removing O-rings and seals).

Warning: To avoid spreading contamination, dispose of all waste materials according to local environmental regulations.

8. If the isolation valve O-ring shows signs of deterioration or damage, dispose of it in accordance with local environmental regulations.

9. Use the combined 2.5-mm Allen wrench and cone extraction tool to loosen the captive PEEK terminal block securing screw.

Figure 4–20: Loosening the PEEK terminal block securing screw



(1) PEEK terminal block securing screw

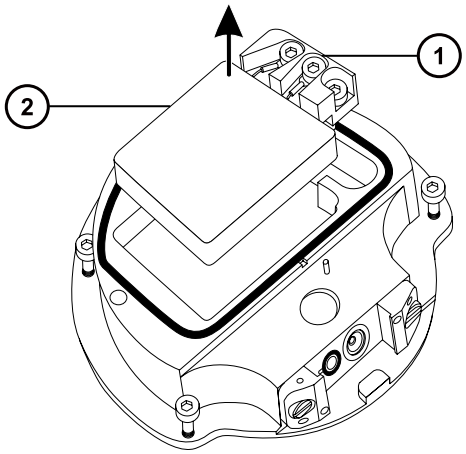
(2) Heater cartridge assembly wires

Notice: To avoid damaging the heater cartridge assembly wires, do not bend or twist them when removing the assembly and ceramic heater mounting block from the ion block.

10. Carefully remove the PEEK terminal block and ceramic heater mounting block, complete with heater cartridge assembly, from the ion block.

Tip: You can invert the ion block assembly to facilitate this process.

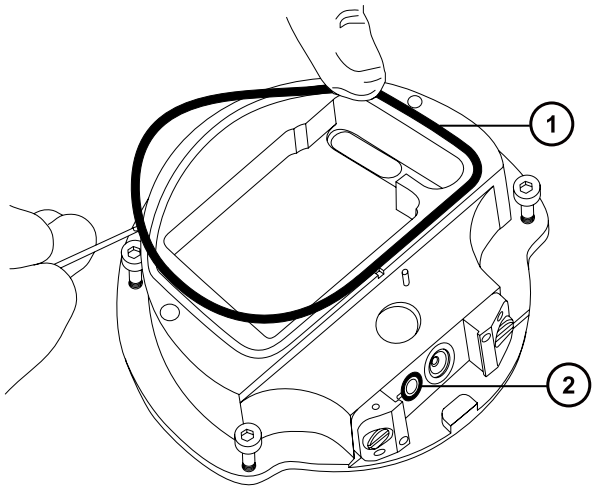
Figure 4–21: Removing the PEEK terminal block and ceramic heater mounting block



1. PEEK terminal block
2. Ceramic heater mounting block

11. Use the O-ring removal kit to carefully remove the cover seal from the ion block (see also Removing O-rings and seals).

Figure 4–22: Removing the cover seal from the ion block



1. Cover seal
2. Cone gas O-ring

12. Use the O-ring removal kit to carefully remove the cone gas O-ring from the ion block.

Warning: To avoid spreading contamination, dispose of all waste materials according to local environmental regulations.

13. If the cover seal or cone gas O-ring shows signs of deterioration or damage, dispose of it in accordance with local environmental regulations.

4.14.3 Cleaning the ion block components

Required materials

- Chemical-resistant, powder-free gloves
- Appropriately sized glass vessels in which to completely immerse components when cleaning. Use only glassware not previously cleaned with surfactants.
- HPLC-grade (or better) methanol
- HPLC-grade (or better) water
- Formic acid
- Ultrasonic bath
- Oil free, nitrogen gas for drying (air-drying optional).
- Wash bottle containing HPLC-grade (or better) 1:1 methanol/water
- Large beaker

To clean the ion block components:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid injury when working with formic acid, which is extremely corrosive and toxic, take extreme care handling it, and use a fume hood and suitable protective equipment.

1. Immerse the ion block and isolation valve in separate glass vessels containing 1:1 methanol/water.

   Tip: If the components are obviously contaminated, use 45:45:10 methanol/water/formic acid.

2. Place the vessels in the ultrasonic bath for 30 minutes.
3. If you used formic acid in the cleaning solution, do as follows:

a. Rinse the components by immersing them separately in glass vessels containing water and then placing the vessels in the ultrasonic bath for 20 minutes.

b. Dry the components by immersing them in separate glass vessels containing methanol and then placing the vessels in the ultrasonic bath for 10 minutes.

Notice: To avoid recontaminating the components, wear clean, chemical-resistant, powder-free gloves for the rest of this procedure.

4. Carefully remove the components from the vessels, and blow-dry them using inert, oil-free gas.
5. Inspect each component for persisting contamination.

   Requirement: If contamination is present, do as follows:

   a. Use the wash bottle containing 1:1 methanol/water to rinse the component over the large beaker.

   b. Blow-dry the component using inert, oil-free gas.

   Warning: To avoid spreading contamination, dispose of all waste materials according to local environmental regulations.
6. Inspect each component for persisting contamination. If contamination is present, dispose of the component, and obtain a new one before reassembly.

4.14.4 Assembling the source ion block assembly

Required materials

- Chemical-resistant, powder-free gloves
- Combined 2.5-mm hex wrench and cone extraction tool
- Isopropyl alcohol in small container
- HPLC-grade (or better) 1:1 methanol/water
- Lint-free cloth

To assemble the ion block assembly:

Note: To avoid recontaminating the components, wear clean, chemical-resistant, powder-free gloves for the rest of this procedure.

Notice: To avoid damaging the heater cartridge assembly wires, do not bend or twist them when removing the assembly and ceramic heater mounting block from the ion block.

1. Carefully fit the PEEK terminal block and ceramic heater mounting block, complete with heater cartridge assembly, to the ion block.
2. Use the combined 2.5-mm Allen wrench and cone extraction tool to tighten the captive PEEK terminal block securing screw.
3. Ensure that the grooves for the cover seal, cone gas O-ring, and isolation valve O-ring are free from dirt and debris.

   Tip: If contamination is present, use 1:1 methanol/water, applied to a lint-free cloth, to carefully clean the grooves.
4. Fit the cover seal (a new one if you disposed of the old seal) to the ion block, ensuring that it is correctly seated.
5. Fit the cone gas O-ring (a new one if you disposed of the old O-ring) to the ion block, ensuring that it is correctly seated.
6. Fit the O-ring to the isolation valve.

   Tip: If you use a new O-ring, first soak it for several minutes in isopropyl alcohol, so that it better fits the isolation valve.
7. Fit the isolation valve to the ion block assembly, so that it is in the closed position.
8. Fit the ion block cover plate to the ion block assembly, and then use the combined 2.5-mm Allen wrench and cone extraction tool to tighten the two captive securing screws for the ion block cover plate.
9. Hold the sampling cone assembly so that the cone gas nozzle handle is oriented horizontally and at the top, and then slide the sampling cone assembly into the ion block assembly.
10. Grasp the sampling cone assembly handle, and use it to rotate the sampling cone assembly through 90 degrees.

4.14.5 Fitting the ion block assembly to the source assembly

Required materials

- Chemical-resistant, powder-free gloves
- Combined 2.5-mm hex wrench and cone extraction tool

To fit the ion block assembly to the source assembly:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid puncture wounds, take great care working with the source enclosure open if one or both of these conditions apply:

- An ESI probe is fitted (the probe's tip is sharp).
- A corona pin is fitted (the pin's tip is sharp).

Notice: To avoid recontaminating the components, wear clean, chemical-resistant, powder-free gloves for the rest of this procedure.

1. Fit the ion block assembly to the PEEK ion block support.
2. Use the combined 2.5-mm hex wrench and cone extraction tool to fit, and then slowly tighten, the four ion block assembly securing screws sequentially and in small increments.
3. Open the source isolation valve (see Opening the source isolation valve).
4. Fit the source enclosure (see Fitting the source enclosure to the instrument).
5. Close the source enclosure.
6. Connect the power cords for the mass spectrometer and the roughing pump to the main power source.

4.15 Cleaning the StepWave ion guide assembly

Clean the StepWave ion guide assembly if cleaning the ion block and isolation valve fails to increase signal sensitivity.

4.15.1 Handling the StepWave ion guide assembly

Notice: To avoid damaging the StepWave ion guide assembly, handle it and its components carefully throughout the cleaning procedure.
In particular, to avoid damaging the wiring on assemblies fitted with an externally wired printed circuit board (PCB), do not touch the wiring.

4.15.2 Removing the ion block support from the source assembly

Required materials

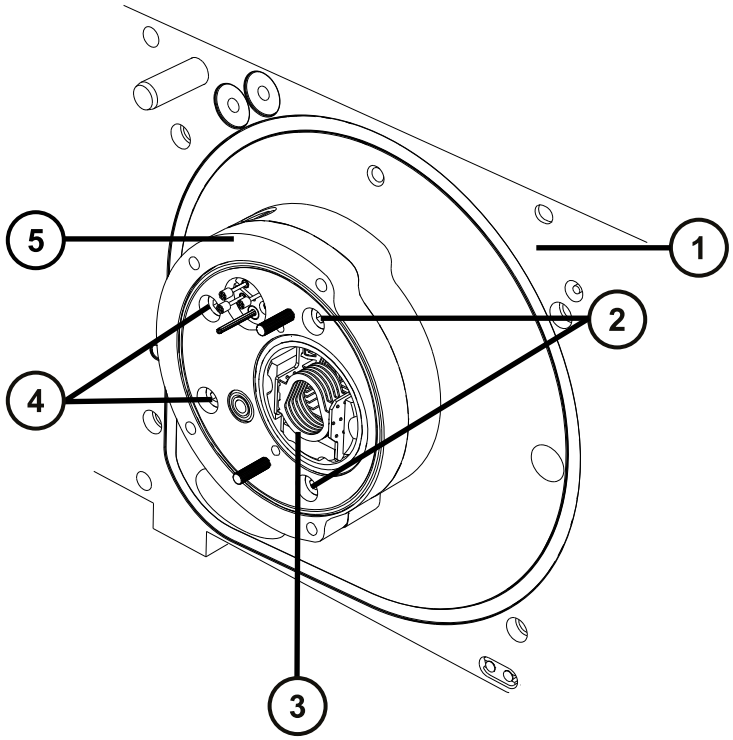
- Chemical-resistant, powder-free gloves
- 3-mm hex wrench
- O-ring removal kit

To remove the ion block support from the source assembly:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

1. Remove the source enclosure from the instrument (see Removing the source enclosure from the instrument).
2. Remove the ion block assembly from the PEEK ion block support (see Removing the ion block assembly from the source assembly).
3. Use the 3-mm hex wrench to unscrew and remove the four screws securing the PEEK ion block support to the adaptor housing.

Figure 4–23: PEEK ion block support



1. Housing
2. Securing screws
3. StepWave assembly
4. Securing screws
5. PEEK ion block support

4. Remove the PEEK ion block support from the adaptor housing.
5. Use the O-ring removal kit to carefully remove all the O-rings from the PEEK ion block support (see Removing o-rings and seals).

Warning: To avoid spreading contamination, dispose of all waste materials according to local environmental regulations.

6. If any of the O-rings show signs of deterioration or damage, dispose of them in accordance with local environmental regulations.

4.15.3 Removing the StepWave assembly from the source assembly

Required materials

- Chemical-resistant, powder-free gloves
- Seal breaker and locator tool
- StepWave assembly removal and insertion tool

Recommendation: When not in use, store the seal breaker and locator tool on the end of the StepWave assembly removal and insertion tool.

To remove the StepWave assembly from the source assembly:

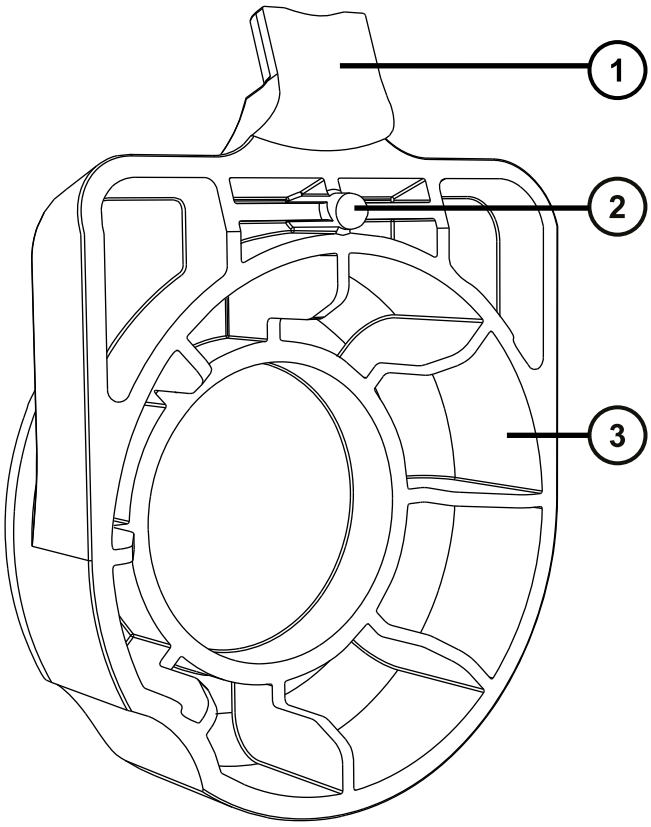
Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Notice: To avoid damaging the StepWave ion guide assembly when removing it from the source assembly, use only these tools:

- Seal breaker and locator tool
- StepWave assembly removal and insertion tool

1. Position the seal breaker and locator tool so that it engages as follows:
   - Its pin with the hole on the adaptor housing directly under the end of the StepWave ion guide assembly.
   - Its lip behind the StepWave ion guide assembly's ion guide cap.

Figure 4–24: Seal breaker and locator tool:

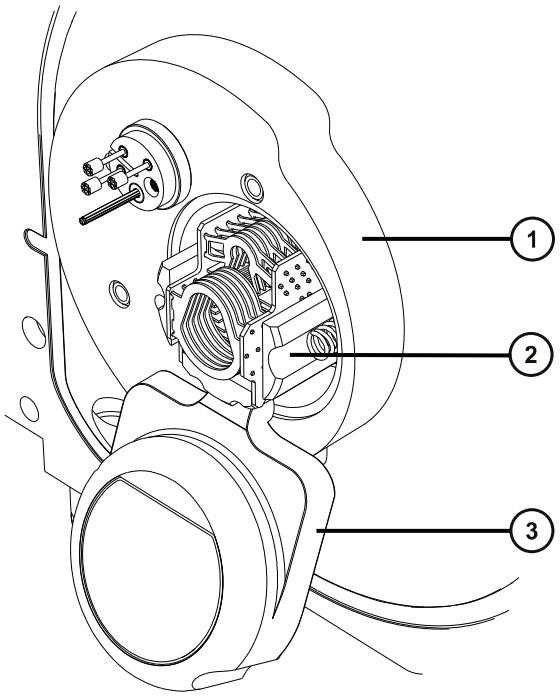


1 Lip

2 Pin

3 Handle

Figure 4–25: Seal breaker and locator tool positioned on the adaptor housing:



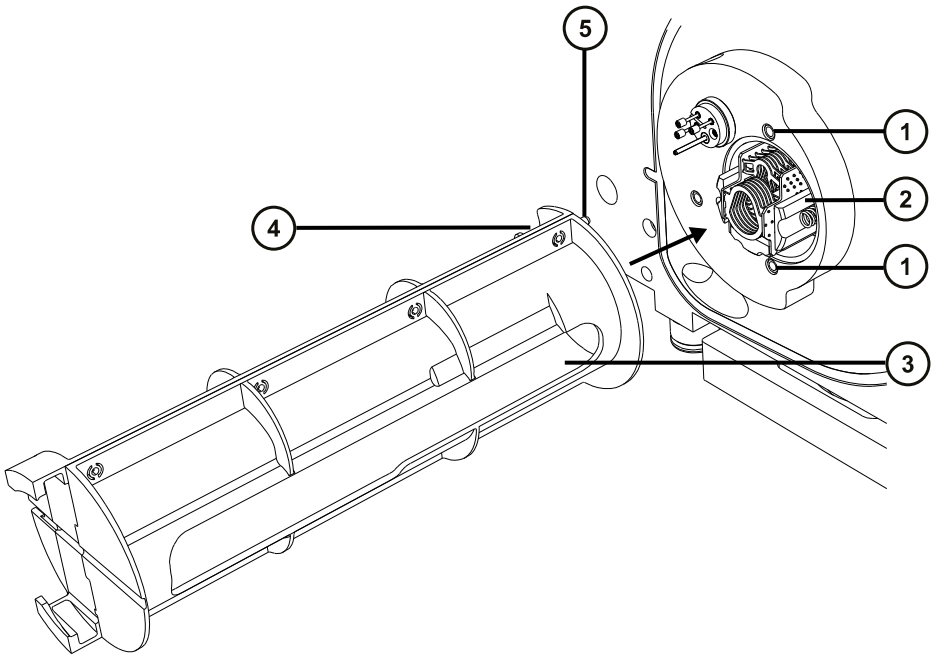
1. Adaptor housing
2. Ion guide cap
3. Seal breaker and locator tool

2. Push firmly on the seal breaker and locator tool's handle, to lever the StepWave assembly slightly out of the adaptor housing.

   Rationale: Moving the assembly in this manner releases it from a seal located inside the instrument.

3. With the StepWave removal and insertion tool's cutout uppermost, insert the tool's pins into the ion block support screw holes above and below the aperture in the pumping block assembly.

Figure 4–26: StepWave assembly removal and insertion tool



1. Ion block support screw holes (2)
2. Brown PEEK ion guide cap
3. Slot
4. Cutout
5. Pins

> **Notice:** To avoid damage when removing the StepWave ion guide assembly from the adaptor housing, handle only the brown PEEK ion guide cap

4. Inserting your thumbs through the slots in the StepWave removal and insertion tool, pull the StepWave ion guide assembly from the pumping block assembly and into the StepWave removal and insertion tool.

> **Notice:** To avoid damaging the StepWave ion guide assembly, handle it and its components carefully throughout the cleaning procedure.
> In particular, to avoid damaging the wiring on assemblies fitted with an externally wired printed circuit board (PCB), do not touch the wiring.

5. Remove the StepWave ion guide assembly from the StepWave removal and insertion tool.

6. Using both hands, fit the source enclosure to the two supporting studs on the source adaptor housing.
7. Close the source enclosure.

   Rationale: Fitting and closing the source enclosure prevents debris entering the instrument while you are working on the StepWave ion guide assembly.

4.15.4 Disassembling the StepWave ion guide assembly

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

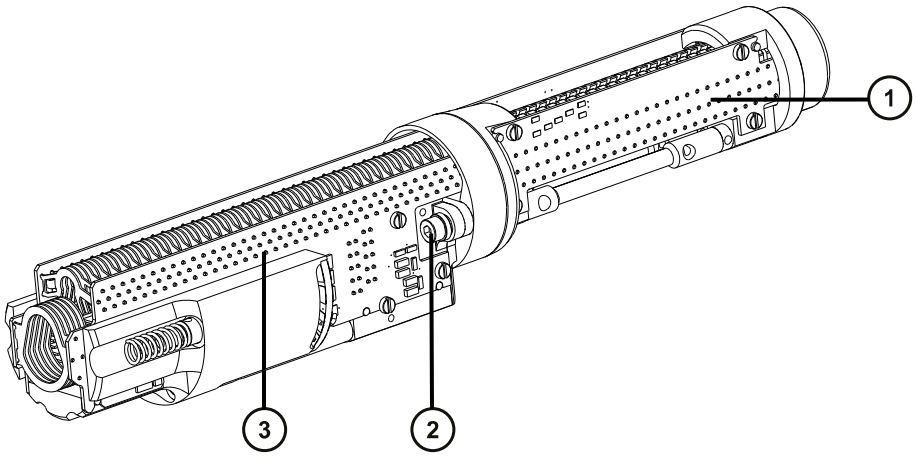
Required materials

- Chemical-resistant, powder-free gloves
- Combined 2.5-mm hex wrench and cone extraction tool
- O-ring removal kit

To disassemble the StepWave ion guide assembly:

1. Use the combined 2.5-mm hex wrench and cone extraction tool to remove the two screws securing the first ion guide assembly to the second ion guide assembly.

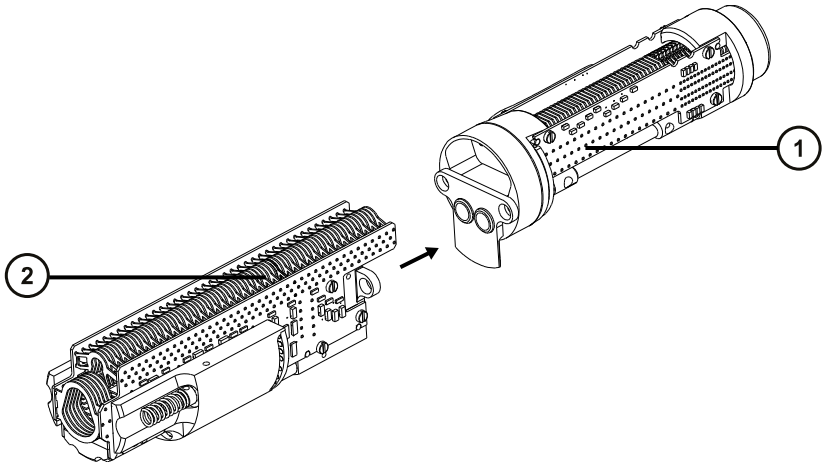
   Figure 4–27: StepWave ion guide assembly



1. Second ion guide assembly
2. Securing screw
3. First ion guide assembly

2. Separate the first and second ion guide assemblies.

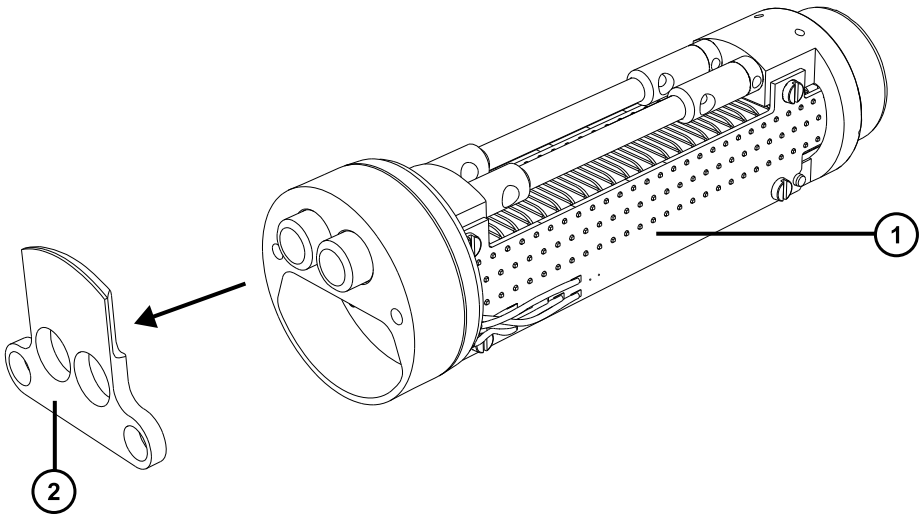
Figure 4–28: StepWave ion guide assembly separated



1. Second ion guide assembly
2. First ion guide assembly

3. Remove the brown PEEK gasket from the second ion guide assembly.

Figure 4–29: StepWave second ion guide assembly

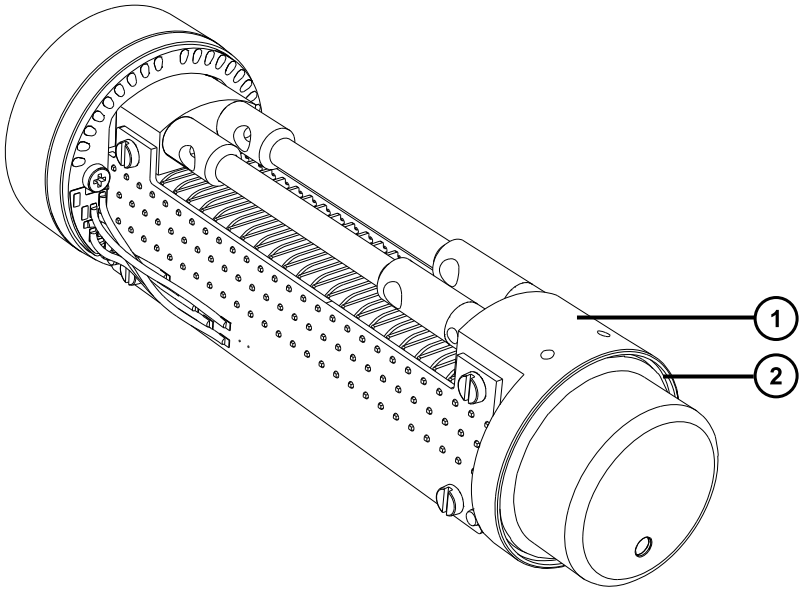


1. Second ion guide assembly

2. Brown PEEK gasket

4. Remove the O-ring from the differential pumping aperture on the second ion guide assembly (see Removing O-rings and seals).

Figure 4–30: StepWave second ion guide assembly



1. Differential pumping aperture

2. O-ring

Warning: To avoid spreading contamination, dispose of all waste materials according to local environmental regulations.

5. If the O-ring shows signs of deterioration or damage, dispose of it in accordance with local environmental regulations.

Notice: To avoid misalignment of the StepWave ion guide, do not remove the differential pumping aperture or any further components from the assembly.

4.15.5 Cleaning the StepWave ion guide assembly

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Notice: To avoid damaging the StepWave ion guide assembly, handle it and its components carefully throughout the cleaning procedure.
In particular, to avoid damaging the wiring on assemblies fitted with an externally wired printed circuit board (PCB), do not touch the wiring.

Notice: To avoid damaging the StepWave ion guide assembly, do not use acetone, chlorinated solvents, or acid as solvents when cleaning it. Use only the solvents specified in this procedure.

Required materials

- Chemical-resistant, powder-free gloves
- Appropriately sized glass vessels in which to completely immerse components when cleaning. Use only glassware not previously cleaned with surfactants.
- Two lengths of PEEK, PTFE, or stainless-steel tubing, appropriately sized for suspending the first ion guide and second ion guide assemblies in the glass vessels when cleaning.
- HPLC-grade deionized water
- Waters MS Cleaning Solution (186006846)
- Waste container
- HPLC-grade isopropyl alcohol
- Ultrasonic bath
- Source of Oil free, argon gas or Oil free, nitrogen gas for drying.

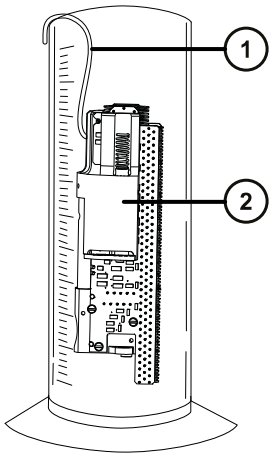
To clean the first ion guide and second ion guide PCB assemblies:

1. Bend the PEEK, PTFE, or stainless-steel tubing into a hook shape.

   Notice: To avoid damage to the ion guide caused by vibration, ensure that the bottom of the ion guide does not touch the bottom of the glass vessel.

2. Use the hook to carefully suspend the first ion guide PCB assembly in the glass vessel so that the bottom of the assembly does not touch the bottom of the vessel.

Figure 4–31: Cleaning the first ion guide PCB assembly

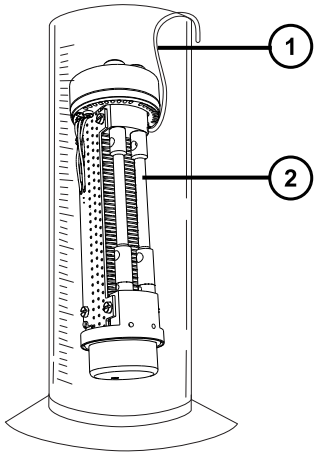


1 First ion guide PCB assembly

2 Hook

3. Add Waters MS Cleaning Solution to the glass vessel until the first ion guide PCB assembly is immersed completely.
4. Repeat step 1 through step 3 for the second ion guide PCB assembly, placing the hook through one of the support rod holes.

Figure 4–32: Cleaning the second ion guide PCB assembly



1 Hook

2 Second ion guide PCB assembly

5. Place the vessels containing the first ion guide and second ion guide PCB assemblies in the ultrasonic bath for 20 minutes.

6. Carefully pour the cleaning solution from the vessel holding the first ion guide PCB assembly into the holding container, retaining the ion guide in the vessel.

   Tip: You can reuse the cleaning solution for one subsequent cleaning.

7. Fill the vessel with deionized water, to rinse the first ion guide PCB assembly, and then discard the water.
8. Refill the vessel with deionized water, to rinse the first ion guide PCB assembly a second time, and then discard the water.

   Note: Ensure that you remove all of the cleaning solution.

9. Repeat step 6 through step 8 for the second ion guide PCB assembly.
10. Fill both vessels with deionized water, ensuring that each ion guide PCB assembly is immersed completely.
11. Place the vessels containing the first ion guide and second ion guide PCB assemblies in the ultrasonic bath for 20 minutes.
12. Carefully pour out and discard the deionized water from both vessels, retaining the ion guide PCB assemblies in each vessel.
13. Fill both vessels with isopropyl alcohol, ensuring that each ion guide PCB assembly is immersed completely.
14. Place the vessels containing the first ion guide and second ion guide PCB assemblies in the ultrasonic bath for 20 minutes.
15. Carefully remove each ion guide PCB assembly from its vessel, and blow-dry each assembly using inert, oil-free gas.
16. Discard the used isopropyl alcohol, using an appropriate waste container.

4.15.6 Assembling the StepWave ion guide assembly

Required materials

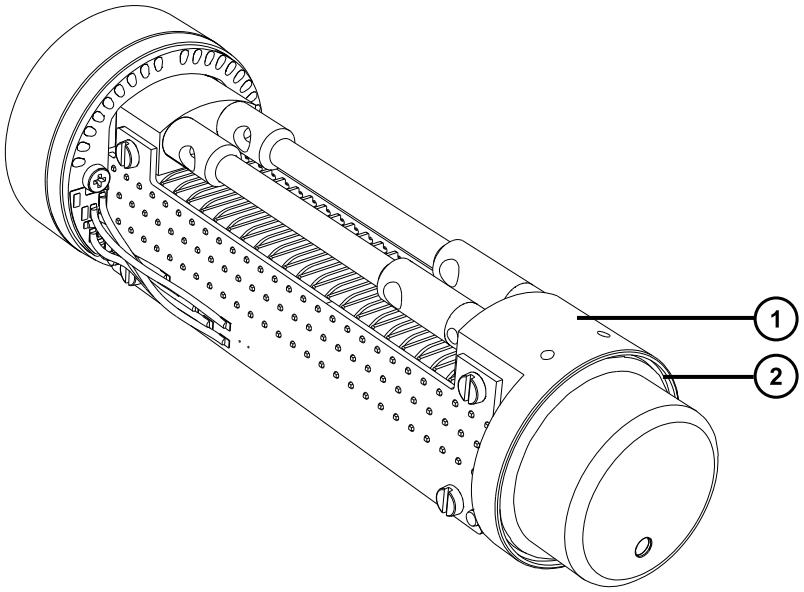
- Chemical-resistant, powder-free gloves
- Combined 2.5-mm hex wrench and cone extraction tool
- New O-ring
- PEEK gasket
- StepWave assembly securing screws (2)

To assemble the StepWave ion guide assembly:

Notice: To avoid damaging the StepWave ion guide assembly, handle it and its components carefully throughout the cleaning procedure.
In particular, to avoid damaging the wiring on assemblies fitted with an externally wired printed circuit board (PCB), do not touch the wiring.

1. Fit the new O-ring to the differential pumping aperture on the second ion guide assembly.

   Figure 4–33:



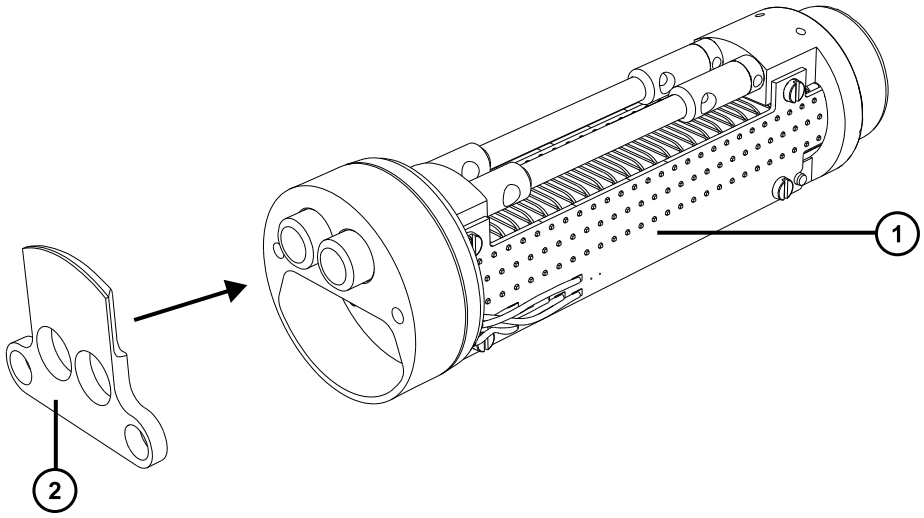
   1 Differential pumping aperture

   2 O-ring

2. Fit the brown PEEK gasket to the second ion guide assembly.

   Important: Ensure that the gasket is orientated correctly.

Figure 4–34:



1 Second ion guide assembly

2 Brown PEEK gasket

3. Align the first ion guide assembly with the second ion guide assembly.
4. Use the combined, 2.5-mm, Allen wrench and cone extraction tool to fit and tighten the two screws securing the first ion guide assembly to the second ion guide assembly.

4.15.7 Fitting the StepWave assembly to the source assembly

Required materials

- Chemical-resistant, powder-free gloves
- Seal breaker and locator tool
- StepWave assembly removal and insertion tool

To fit the StepWave assembly to the source assembly:

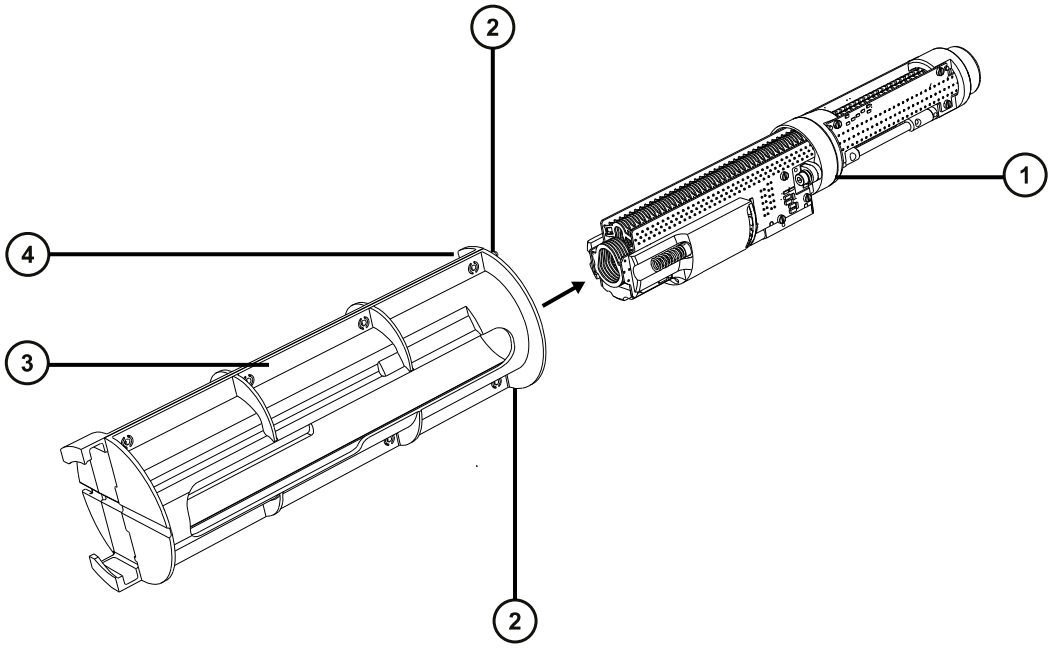
Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Notice: To avoid damage to the StepWave ion guide assembly when fitting it to the source assembly, use only the seal breaker and locator, and the assembly's removal and insertion tools.

1. Pull the source enclosure release (located at the bottom, right-hand side) outwards, and swing open the enclosure.
2. Using both hands, grasp the source enclosure, and lift it vertically off the two supporting studs on the source adaptor housing.
3. Slide the first ion guide assembly end of the StepWave assembly into the StepWave removal and insertion tool.

   Tip: The StepWave assembly can only be inserted in the correct orientation in the StepWave removal and insertion tool.

Figure 4–35: Sliding the StepWave assembly into the StepWave removal and insertion tool



1. StepWave assembly
2. Pins (2)
3. StepWave assemby removal and insertion tool
4. Cutout

4. With the StepWave removal and insertion tool's cutout uppermost, insert the StepWave removal and insertion tool's pins into the ion block support screw holes above and below the aperture in the pumping block assembly.

Notice: To avoid damage when removing the StepWave ion guide assembly from the adaptor housing, handle only the brown PEEK ion guide cap

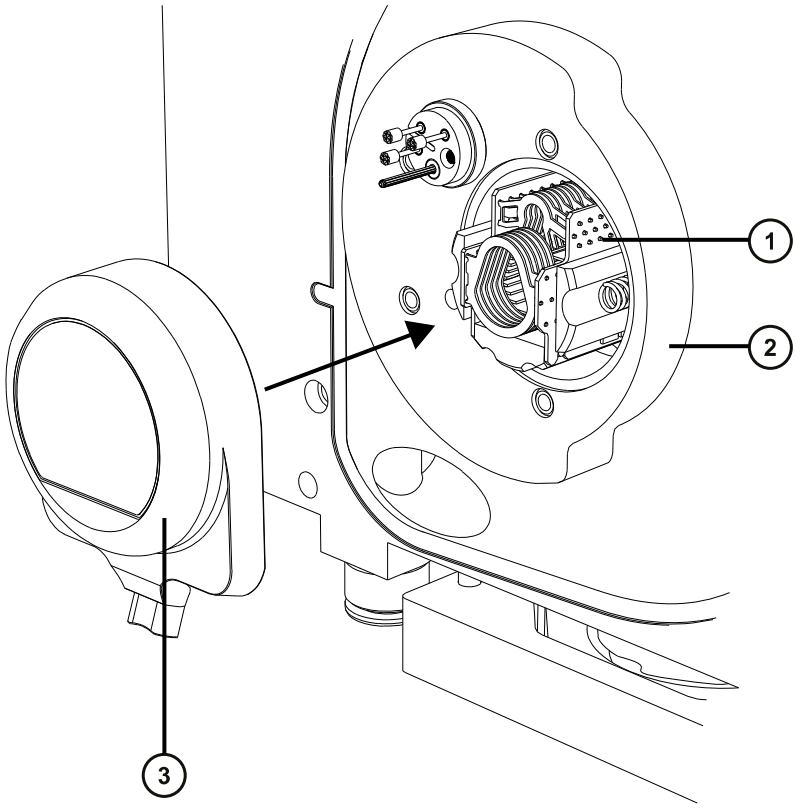
5. Inserting your thumbs through the slots in the StepWave removal and insertion tool, firmly push the StepWave ion guide assembly into the pumping block assembly.

   Tip: You will detect some resistance to motion when the StepWave assembly encounters the seal inside the instrument; continue pushing until you detect further resistance.

6. Remove the StepWave removal and insertion tool.

7. Invert the seal breaker and locator tool, and locate it over the end of the StepWave assembly.

   Figure 4–36:



   1 StepWave assembly

   2 Adaptor housing

   3 Inverted seal breaker and locator tool

8. Push firmly on the seal breaker and locator tool until the tool's face contacts the adaptor housing.

   Rationale: This fully locates the StepWave assembly in the adaptor housing.

9. Remove the seal breaker and locator tool.

4.15.8 Fitting the ion block support to the source

Required materials

- Chemical-resistant, powder-free gloves
- 3-mm hex wrench
- New seals and O-rings

To fit the PEEK ion block support to the source:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

1. Ensure that the grooves for the PEEK ion block support O-rings are free from dirt and debris.

   Tip: If contamination is present, use 1:1 methanol/water, applied to a lint-free cloth, to carefully clean the grooves.

2. Fit the O-rings (new ones if you disposed of the old) to the PEEK ion block support.

   Tip: To fit an O-ring in its groove, start fitting the O-ring at the notch in the groove, and then progressively work the ring into the groove, in either direction from the notch.

3. Fit the PEEK ion block support to the instrument's housing.
4. Use the 3-mm Allen wrench to fit and tighten the four PEEK ion block support securing screws.
5. Fit the ion block assembly to the PEEK ion block support (see Fitting the ion block assembly to the source assembly).
6. Fit the source enclosure to the instrument (see Fitting the source enclosure to the instrument).

4.16 Replacing the probe assembly

Replace probe assembly if it becomes irreversibly blocked, or if it becomes contaminated or damaged.

4.16.1 Removing the probe assembly

Required materials

- Chemical-resistant, powder-free gloves

To remove the probe assembly:

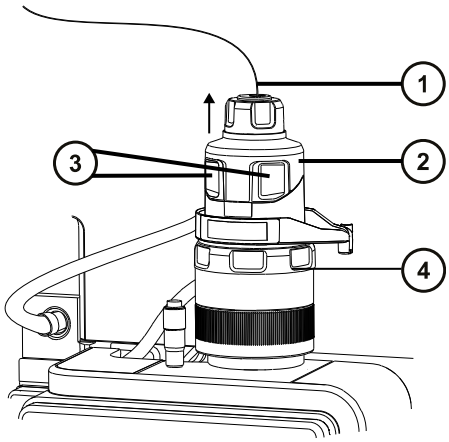
Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid puncture wounds, handle sharp parts and materials with care.

Warning: To avoid electric shock or solvent ignition, when connecting ESI or UPC^2 source probes directly to non-Waters equipment, ensure that the liquid outlet connection is grounded.

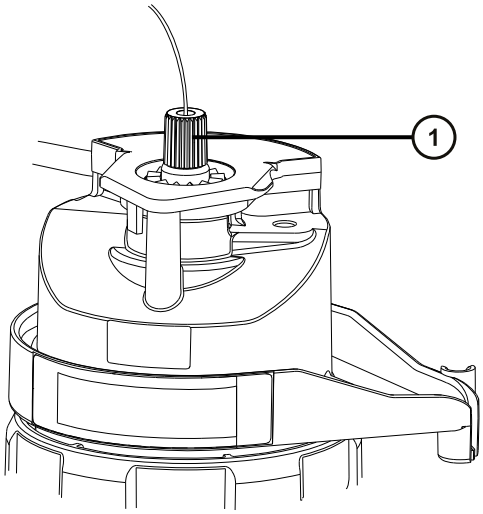
1. If the probe assembly is connected to the fluidics, open the access door to the IntelliStart Fluidics system (see Waters ACQUITY Xevo TQ-S UPLC/MS system), and disconnect the PEEK fitting from the diverter valve.
2. Squeeze the probe adaptor cap release buttons together and lift the probe cap off the probe adaptor, sliding it over the probe assembly.

Figure 4–37: Removing the probe adaptor cap



1. Probe assembly
2. Probe adaptor cap
3. Probe adaptor cap release buttons
4. Probe adaptor

3. Unscrew the finger-tight PEEK fitting.



1 PEEK fitting

4. Remove the probe assembly.

Warning: To avoid spreading contamination, dispose of all waste materials according to local environmental regulations.

5. Dispose of the probe assembly in accordance with local environmental regulations.
6. To install a new probe assembly, see Installing the probe assembly.

4.17 Replacing the ESI probe tip and gasket

Replace the ESI probe tip if a blockage occurs in the internal metal sheathing through which the stainless steel capillary passes or if the probe tip is damaged.

4.17.1 Removing the ESI probe tip and gasket

Required materials

- Chemical-resistant, powder-free gloves
- 7-mm open-end wrench
- 10-mm open-end wrench

To remove the ESI probe tip and gasket:

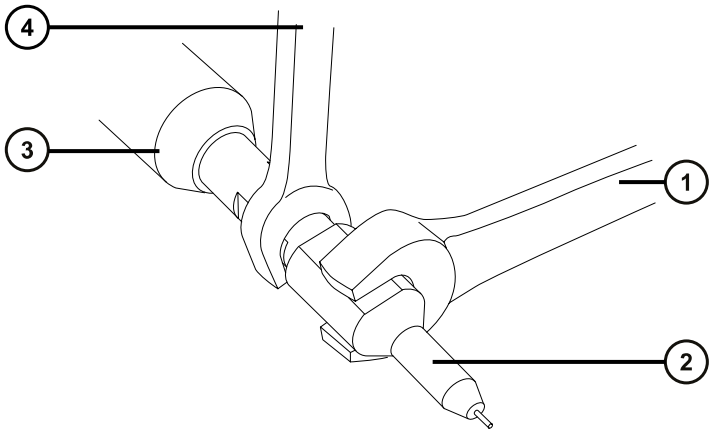
Warning: To avoid personal contamination with biohazards, wear clean, chemical-resistant, powder-free gloves when performing this procedure.

Warning: To avoid burn injuries, take great care while performing this procedure.

Warning: To avoid puncture injuries, handle sample needles, syringes, fused silica lines, and borosilicate tips with extreme care.

1. Remove the ESI probe adaptor from the source (see Removing the probe adaptor).
2. Use the 7-mm wrench in conjunction with the 10-mm wrench to remove the probe tip.

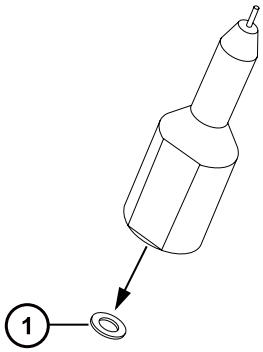
   Figure 4–38:



   1. 10-mm wrench
   2. Probe tip
   3. ESI probe adaptor
   4. 7-mm wrench

3. Remove the metal gasket from the probe tip.

Figure 4–39:



1 Metal gasket

Warning: To avoid contaminating uncontaminated surfaces with biologically hazardous, toxic, or corrosive materials, dispose of all waste materials according to local environmental regulations.

4. Dispose of the metal gasket in accordance with local environmental regulations.
5. If the probe tip is damaged, dispose of it in accordance with local environmental regulations.

4.17.2 Fitting the ESI probe tip and gasket

Required materials

- Chemical-resistant, powder-free gloves
- 10-mm open-end wrench
- 7-mm open-end wrench
- New metal gasket

To fit the ESI probe tip and gasket:

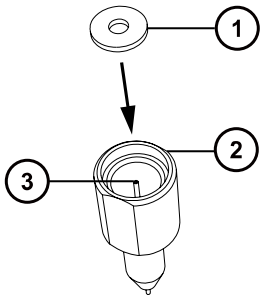
Warning: To avoid personal contamination with biohazards, wear clean, chemical-resistant, powder-free gloves when performing this procedure.

Warning: To avoid puncture injuries, handle sample needles, syringes, fused silica lines, and borosilicate tips with extreme care.

Notice: To avoid damage, do not reuse metal gaskets. Always fit a new gasket.

1. Fit the new metal gasket into the probe tip.

Figure 4–40: Inserting the gasket



1. Metal gasket
2. ESI probe tip
3. Stainless steel tube

2. Fit the probe tip, and screw the tip onto the probe assembly.
3. Use the 7-mm wrench in conjunction with the 10-mm wrench to tighten the probe tip.

   Important: To avoid gas leakage, fully tighten the probe tip.
4. Fit the ESI probe adaptor to the source (see Installing the probe adaptor).
5. If required, re-optimize the probe position (see the mass spectrometer's online Help).

4.18 Cleaning the APCI probe tip

Clean the APCI probe tip when you detect buffer buildup on the probe tip or when the signal intensity weakens. See the mass spectrometer's online Help for further details.

To clean the APCI probe tip:

1. On the Manual Optimization page, click **Stop fluidics** .
2. To start the API gas flow, click **Gas** .
3. Set Desolvation Gas to 650 L/h.
4. Set APCI probe Temp to 650 °C.
5. Click **Operate** .
6. Wait 10 minutes.

   Rationale: The high APCI probe heater temperature removes any chemical contamination from the probe tip.
7. Click **Standby** .

4.19 Replacing the APCI probe heater

Replace the APCI probe heater it fails to heat the probe.

4.19.1 Removing the APCI probe heater

Required materials

Chemical-resistant, powder-free gloves

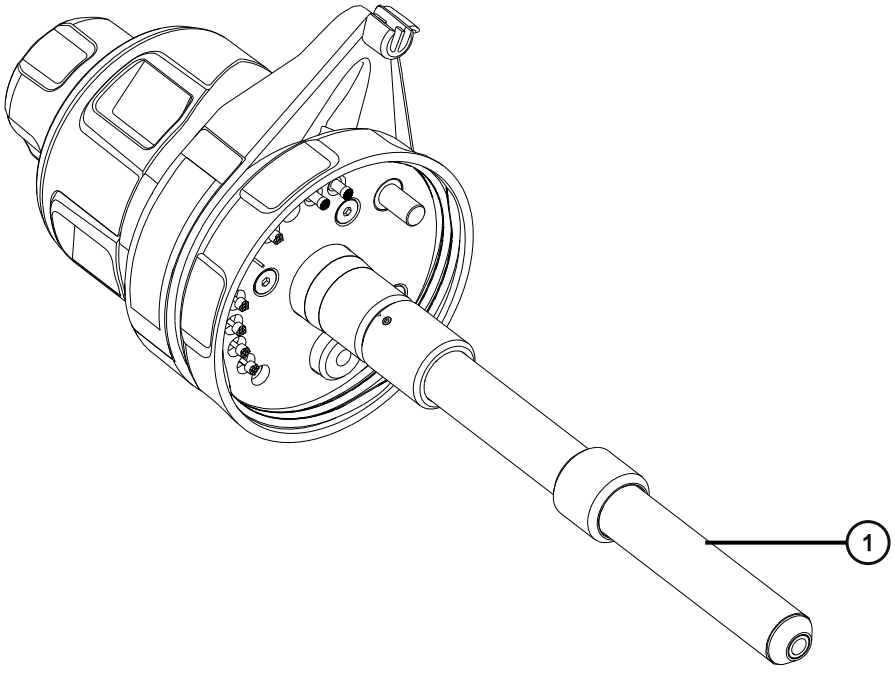
To remove the APCI probe heater:

Warning: To avoid burn injuries, take great care while working with the probe and source; these components can be hot.

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

1. Remove the probe adaptor from the source (see Removing the probe adaptor).

Figure 4–41:



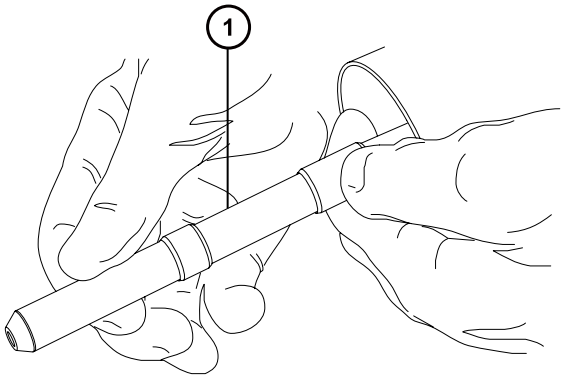
1 Probe heater

Notice: To avoid damaging the probe heater's electrical connections, do not twist the heater when removing it from or refitting it to the probe adaptor.

Warning: To avoid burn injuries, take great care while performing this procedure.

2. Gripping the probe heater as shown, carefully pull it off the probe adaptor.

Figure 4–42:



1 Probe heater

Warning: To avoid contaminating uncontaminated surfaces with biologically hazardous, toxic, or corrosive materials, dispose of all waste materials according to local environmental regulations.

3. Dispose of the probe heater in accordance with local environmental regulations.

4.19.2 Fitting the new APCI probe heater

Required materials

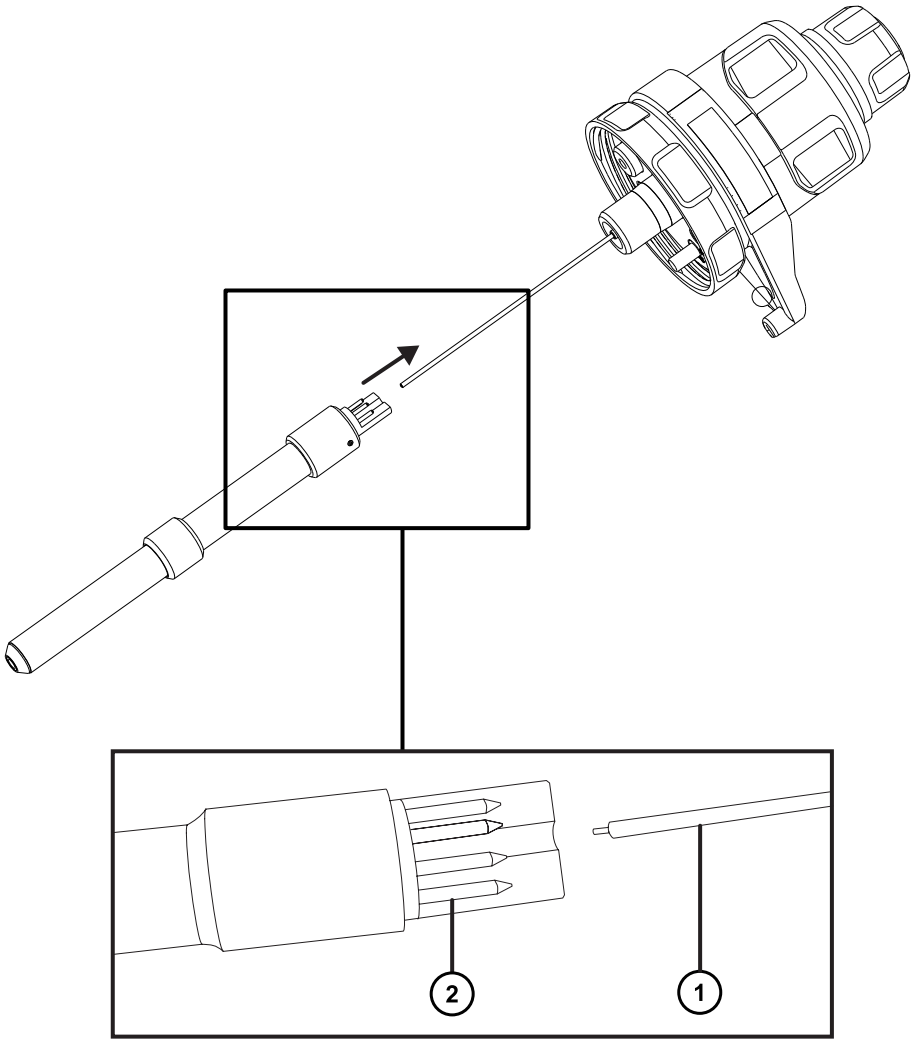
- Chemical-resistant, powder-free gloves
- APCI probe heater

To fit the new APCI probe heater:

Notice: Take great care not to damage the probe heater’s electrical connections, capillary sleeve, or capillary when fitting the heater over the capillary sleeve.

1. Carefully slide the probe heater over the capillary sleeve on the probe adaptor, ensuring that the heater is fully seated on the probe adaptor.

Figure 4–43: Fitting the probe heater



1. Capillary sleeve
2. Probe heater connections

Notice: To avoid damaging the probe heater's electrical connections, do not twist the heater when removing it from or refitting it to the probe adaptor.

2. Fit the probe adaptor to the instrument (see Installing the probe adaptor).

4.20 Cleaning or replacing the corona pin

Required materials

- Chemical-resistant, powder-free gloves
- Needle-nose pliers
- HPLC-grade methanol
- Lint-free tissue
- Lapping film
- Corona pin

To clean or replace the corona pin:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid burn injuries, exercise care when handling the column or other components heated to high temperatures. Wait until the hot components have sufficiently cooled before you handle them.

Warning: To avoid puncture injuries, handle sample needles, syringes, fused silica lines, and borosilicate tips with extreme care.

1. Remove the corona pin from the source (see Removing the corona pin from the source).
2. Replace the corona pin if it is deformed or damaged. Otherwise clean its tip with the lapping film, and then wipe it clean with a methanol-saturated tissue.

   Warning: To avoid contaminating uncontaminated surfaces with biologically hazardous, toxic, or corrosive materials, dispose of all waste materials according to local environmental regulations.
3. If you are replacing the corona pin, dispose of the old pin in accordance with local environmental regulations.
4. Install the corona pin in the source (see Installing the corona pin in the source).

4.21 Replacing the ion block source heater

Replace the ion block source heater if it fails to heat the ion block when the instrument is pumped-down (evacuated).

Required materials

- Chemical-resistant, powder-free gloves
- Needle-nose pliers
- Combined 2.5-mm hex wrench and cone extraction tool
- New ion block source heater assembly

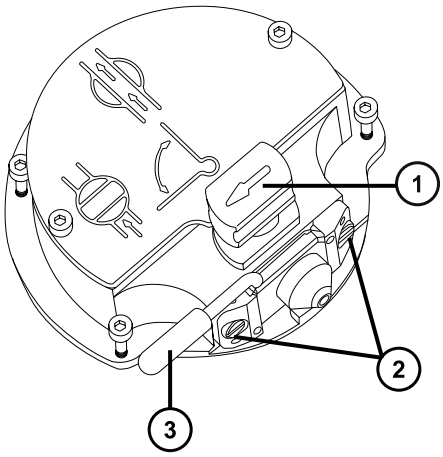
To replace the ion block source heater:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

1. Remove the ion block assembly from the instrument (see Removing the ion block assembly from the source assembly).
2. Ensure that the isolation valve is closed.

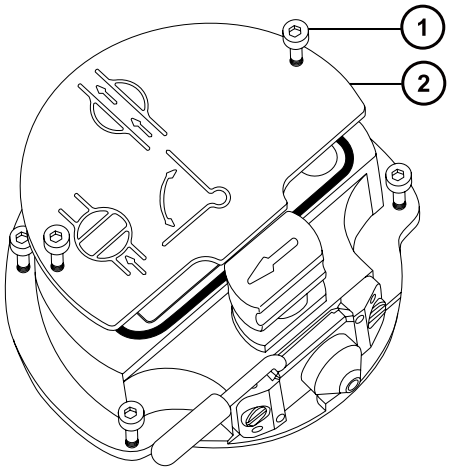
   Figure 4–44:

   1. Source isolation valve handle in closed position
   2. Sampling cone assembly retaining blocks
   3. Cone gas nozzle handle

3. Use the combined 2.5-mm Allen wrench and cone extraction tool to loosen the two captive screws securing the ion block cover plate.

Figure 4–45:

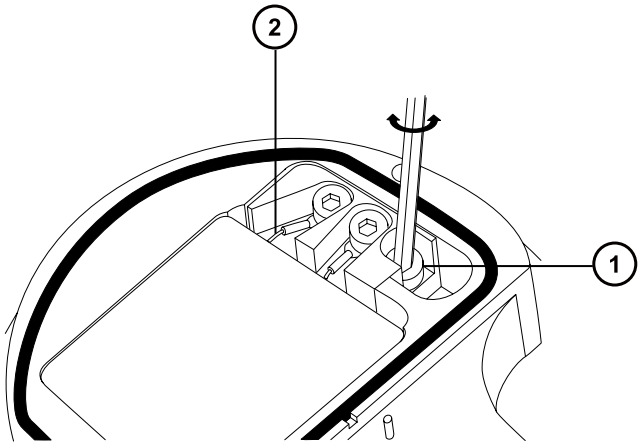


1 Ion block cover plate securing screw

2 Ion block cover plate

4. Remove the ion block cover plate.
5. Use the combined 2.5-mm Allen wrench and cone extraction tool to loosen the captive PEEK terminal block securing screw.

Figure 4–46:



1 PEEK terminal block securing screw

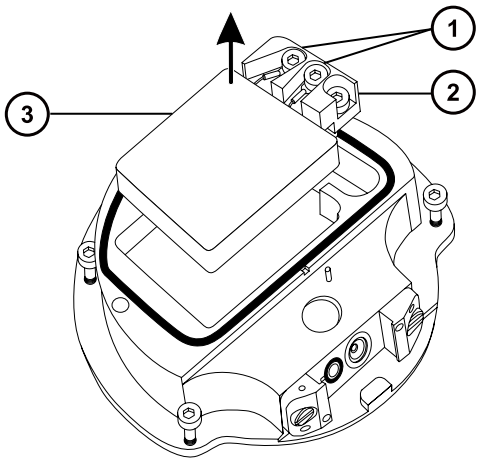
2 Heater cartridge assembly wires

Notice: To avoid damaging the heater cartridge assembly wires, do not bend or twist them when removing the assembly and ceramic heater mounting block from the ion block.

6. Carefully remove the PEEK terminal block and ceramic heater mounting block, complete with heater cartridge assembly, from the ion block.

   Tip: You can invert the ion block assembly to facilitate this process.

   Figure 4–47:



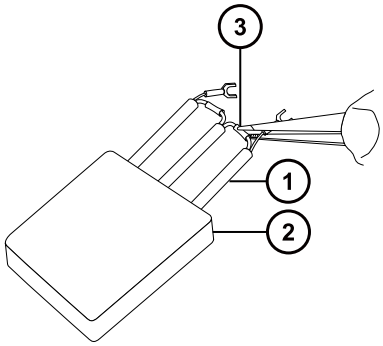
   1 Heater wire securing screws

   2 PEEK terminal block

   3 Ceramic heater mounting block

7. Use the combined 2.5-mm Allen wrench and cone extraction tool to loosen the two screws securing the heater wires to the PEEK terminal block.
8. Disconnect the heater cartridge wires from the PEEK terminal block.
9. Use the needle-nose pliers to gently grasp the heat-shrink tubing on the heater cartridge assembly, and slide the assembly out of the ceramic heater mounting block.

   Figure 4–48:



1. Heater cartridge assembly
2. Ceramic heater mounting block
3. Heat-shrink tubing

10. Dispose of the heater cartridge assembly.

> **Notice:** To avoid damaging the heater cartridge assembly wires, do not bend or twist them when removing the assembly and ceramic heater mounting block from the ion block.

11. Use the needle-nose pliers to gently grasp the heat-shrink tubing on the new heater cartridge assembly, and slide the assembly into the ceramic heater mounting block.
12. Use the needle-nose pliers to position the heater cartridge's wiring ring tags fully under their securing screws.
13. Use the combined 2.5-mm Allen wrench and cone extraction tool to tighten the two, wire-securing screws.
14. Fit the PEEK terminal block and ceramic heater mounting block, complete with heater cartridge assembly, to the ion block.
15. Use the combined 2.5-mm Allen wrench and cone extraction tool to tighten the captive, PEEK terminal block securing screw.
16. Fit the ion block cover plate to the ion block assembly, and then use the combined 2.5-mm Allen wrench and cone extraction tool to tighten the two captive screws securing ion block cover plate.
17. Fit the ion block assembly to the instrument (see Fitting the ion block assembly to the source assembly).

4.22 Replacing the source assembly seals

Warning: To avoid excessive leakage of solvent vapor into the laboratory atmosphere, the seals listed below must be renewed, at intervals of no greater than one year, exactly as described in this section.

To avoid excessive leakage of solvent vapor into the laboratory atmosphere, the following seals must be renewed at intervals of no greater than one year:

- Probe adjuster assembly probe seal
- Probe adjuster assembly nebulization gas seal

- Source enclosure seal
- Nebulizer gas seal
- Desolvation gas seal

4.22.1 Removing the probe adjuster assembly probe and source enclosure seals

Required materials

- Chemical-resistant, powder-free gloves
- O-ring removal kit

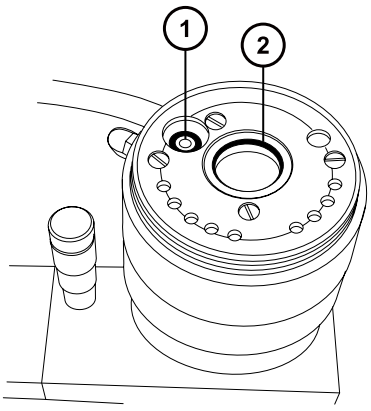
To remove the probe adjuster assembly probe and source enclosure seals:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

1. Remove the source enclosure from the instrument (see Removing the Source Enclosure from the Instrument).
2. Use the O-ring removal kit to carefully remove the following seals from the probe adjuster assembly:
   - Probe seal
   - Nebulizer gas seal

   See also: See Removing O-rings and seals.

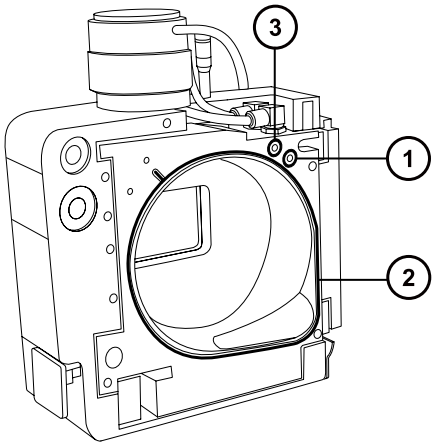
Figure 4–49: Probe adjuster assembly seals



1. Probe adjuster nebulizer gas seal
2. Probe adjuster assembly probe seal

3. Use the O-ring removal kit to carefully remove the following seals from the source enclosure:
   - Source enclosure seal
   - Nebulizer gas seal
   - Desolvation gas seal

Figure 4–50: Source enclosure seals



1. Desolvation gas seal
2. Source enclosure seal
3. Nebulizer gas seal

Warning: To avoid spreading contamination, dispose of all waste materials according to local environmental regulations.

4. Dispose of all the seals in accordance with local environmental regulations.

4.22.2 Fitting the new source enclosure and probe adjuster assembly probe seals

Required materials

- Chemical-resistant, powder-free gloves
- Wash bottle containing HPLC-grade (or better) 1:1 methanol/water
- New seals
- Lint-free cloth

To fit the new source enclosure and probe adjuster assembly probe seals:

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

1. Ensure that all the grooves for seals are free from dirt and debris.

   Tip: If contamination is present, use 1:1 methanol/water, applied to a lint-free cloth, to carefully clean the grooves.

2. Fit the new source enclosure seal to the source enclosure.

   Important: Ensure that the tails of the source enclosure seals are correctly located in the groove when fitting them to the source enclosure.

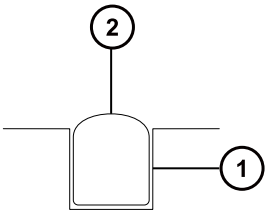
   Start by feeding the seal into the groove at the bottom right-hand corner, then work around the seal in the counterclockwise direction.

3. Fit the following new seals to the source enclosure:

   - Nebulizer gas seal
   - Desolvation gas seal

   Requirement: Fit the seals, which incorporate a special cross-section, into grooves, as shown.

   Figure 4–51:



1 Groove

2 Seal

4. Fit the following new seals to the probe adjuster assembly:
   - Probe seal
   - Nebulizer gas seal
5. Fit the source enclosure to the instrument (see Fitting the source enclosure to the instrument).

4.23 Replacing the air filter inside the front door

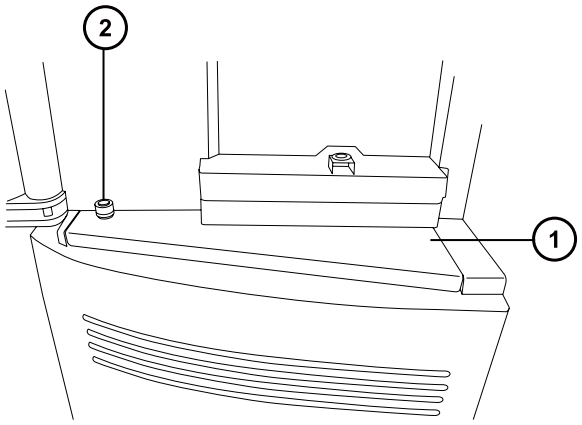
Required materials

- Needle-nose pliers
- New filter

To replace the air filter inside the front door:

1. Open the access door to the fluidics pump (see the figure on Waters ACQUITY Xevo TQ-S UPLC/MS system).
2. Unscrew the captive thumbscrew on the filter cover.

Figure 4–52:

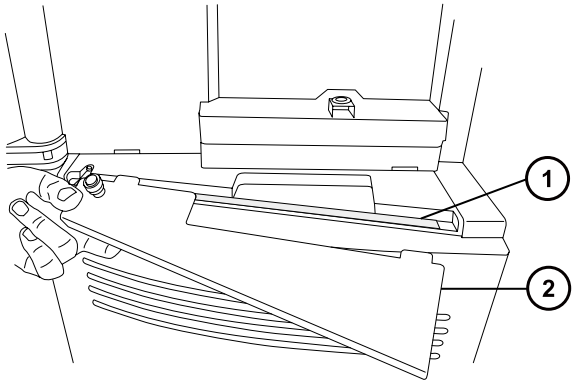


1 Filter cover

2 Thumbscrew

3. Remove the filter cover from the instrument.

Figure 4–53:



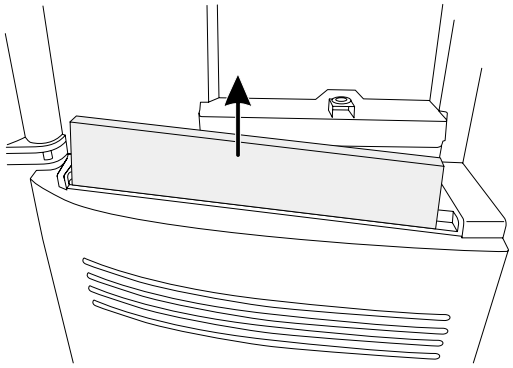
1 Filter

2 Filter cover

4. Lift the filter, vertically, from its slot in the instrument.

   Tip: If necessary, use the needle-nose pliers to grasp the filter.

Figure 4–54:



5. Dispose of the filter.
6. Fit the new filter into the instrument.
7. Fit the filter cover to the instrument.
8. Tighten the thumbscrew on the filter cover.
9. Close the access door to the fluidics pump.

4.24 APPI/APCI source - changing the UV lamp bulb

Required materials:

- Chemical-resistant, powder-free gloves
- Combined 2.5-mm hex wrench and cone extraction tool
- Phillips screwdriver
- 20-cm (8-inch) length of 4-mm nylon tube

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid electric shock, ensure that the instrument is prepared for working on the source before commencing this procedure.

To change the UV lamp bulb:

1. Prepare the instrument for working on the source (see Preparing the instrument for working on the source).

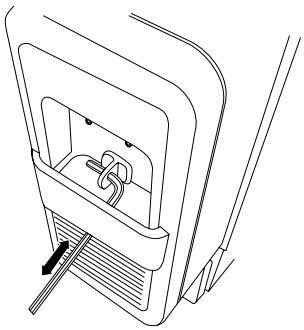
   

   Warning: To avoid burn injuries, take great care while working with the probe and source; these components can be hot.

   Note: To avoid eye injury from UV radiation, ensure that the APPI lamp is extinguished before carrying out this procedure.

2. Pull the source enclosure release (located at the bottom, right-hand side) outwards, and swing open the enclosure.
3. Retrieve the combined 2.5-mm Allen wrench and cone extraction tool from its storage location on the source adaptor housing.
4. Hook the short-end of the Allen wrench through the ring on the back of the bulb extraction plug, and tug to remove it.

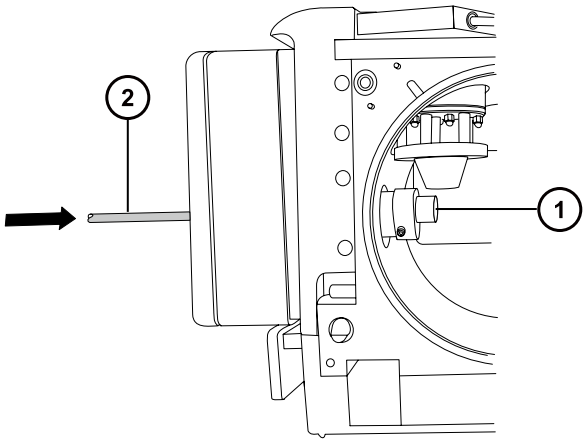
Figure 4–55:



Note: To avoid breaking the bulb, do not use a screwdriver to push the bulb forward in the lamp drive assembly.

5. Insert the length of 4-mm nylon tube through the back of the lamp drive assembly, and push the bulb forward.

Figure 4–56:



(1) APPI lamp bulb

(2) Nylon tube

6. Remove the bulb from the lamp drive assembly.
7. Insert the new bulb into the lamp drive assembly.

Tip: The lamp glass is magnesium fluoride. Avoid touching it because dirt or other contaminants on the window significantly reduce UV transmission.

8. Refit the lamp-bulb access plug.
9. Return the combined 2.5-mm Allen wrench and cone extraction tool to its storage location on the source adaptor housing.
10. Close the source enclosure.
11. Slide closed the instrument's source interface door.

4.25 APPI/APCI source—cleaning the lamp window

The transmission of the high-energy photons responsible for APPI relies on the cleanliness of the magnesium fluoride lamp window. Clean the window to keep the surface clear of contamination, and avoid reduced sensitivity.

Required materials

- Chemical-resistant, powder-free gloves
- Lint-free cloth
- Methanol or isopropyl alcohol

Warning: To avoid burn injuries, take great care while performing this procedure.

Note: To avoid eye injury from UV radiation, ensure that the APPI lamp is extinguished before carrying out this procedure.

To clean the lamp window:

1. Prepare the instrument for working on the source (see Preparing the instrument for working on the source).
2. Pull the source enclosure release (located at the bottom, right-hand side) outwards, and swing open the enclosure.
3. Use methanol or isopropyl alcohol, applied to the lint-free cloth, to carefully clean the lamp window.
4. Close the source enclosure.
5. Slide closed the instrument's source interface door.

4.26 APPI/APCI source - replacing the APPI lamp drive seals

Warning: To ensure the integrity of the source exhaust system, the APPI lamp drive assembly O-rings listed below must be renewed at intervals not exceeding one year, exactly as described in this section.

The following APPI lamp drive assembly O-rings must be renewed at intervals of no greater than one year:

- UV lamp bulb sealing O-ring
- Mounting shaft O-rings
- UV lamp mounting flange O-ring

Tip: An automatic pressure test is performed each time the source enclosure is closed and when the instrument starts.

4.26.1 Removing the APPI lamp drive assembly seals

Required materials

- Chemical-resistant, powder-free gloves
- Combined 2.5-mm hex wrench and cone extraction tool
- 3-mm hex wrench
- Phillips screwdriver
- #0 POZIDRIV screwdriver
- 20-cm (8-inch) length of 4-mm nylon tube.
- O-ring removal kit
- Mounting shaft insertion tool
- A suitable, clear working area on a bench
- A soft cloth or mat to protect the source enclosure window as it is laid on its face

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid electric shock, ensure that the instrument is in Standby mode before commencing this procedure.

To remove the APPI lamp drive assembly seals:

1. Remove the APCI probe and combined APPI/APCI source enclosure (see Removing the combined APPI/APCI source enclosure).

   Note: To avoid damaging the UV bulb, handle it with care; the bulb is fragile.

2. Remove the UV bulb from the lamp drive assembly, and store it in a secure place (see APPI/APCI soource -- changing the UV lamp bulb).
3. Retrieve the combined 2.5-mm Allen wrench and cone extraction tool from its storage location on the source adaptor housing.

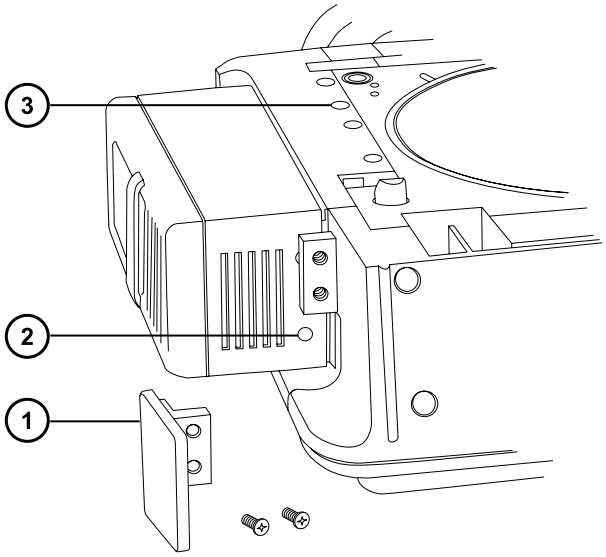
4. Use the combined 2.5-mm Allen wrench and cone extraction tool to remove the two lamp-drive cover screws (located above the bulb-extraction plug-aperture).

   Note: To avoid damaging the source enclosure, take care to lay it on a smooth surface. Laying the source enclosure face-first on a hard object or other protrusion can smash the glass window.

5. Clear an area, lay out the soft cloth or mat, and lay the source enclosure on its face.

6. Use the Phillips (cross-head) screwdriver to remove the source enclosure, release-handle screws, and remove the handle.

   Figure 4–57:



   (1) Release handle

   (2) Lamp drive cover screws

   (3) Source enclosure cover screws

7. Use the combined 2.5-mm Allen wrench and cone extraction tool to remove the remaining two lamp-drive cover screws, which were hidden by the release handle.

8. Slide the cover off the lamp drive.

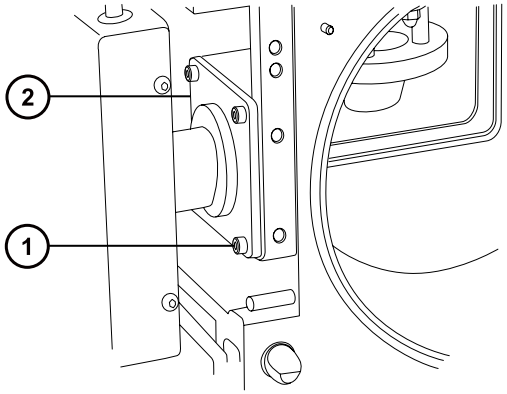
9. Use the 3-mm Allen wrench to remove the four source enclosure cover screws.

10. Ease the source enclosure cover over the lamp drive assembly.

11. Use the combined 2.5-mm Allen wrench and cone extraction tool to unscrew the four mounting-flange screws.

    Tip: Take care not to drop the screws inside the lower cover.

Figure 4–58:

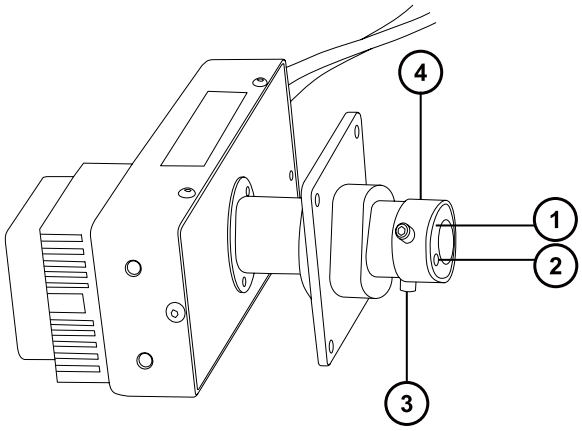


1. Mounting-flange screw
2. Lamp mounting flange

12. Slide the lamp assembly, shaft, and flange out of the APPI source enclosure.

    Tip: The cables remain attached to the shaft, which you fully withdraw and lay on the bench beside the source enclosure.

Figure 4–59:

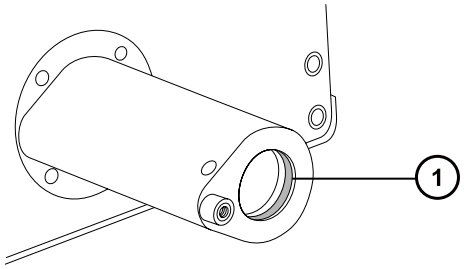


1. Repeller electrode
2. Electrode screw
3. Insulator retaining screw
4. PEEK insulator

13. Using the small Phillips screwdriver, remove the electrode screw and repeller electrode.

14. Use the combined 2.5-mm Allen wrench and cone extraction tool to remove the two insulator screws.
15. Remove the PEEK insulator from the end of the mounting shaft.
16. Slide the shaft mounting flange off the shaft, and note the correct orientation, for its reassembly.
17. Use the O-ring removal kit to carefully remove the O-ring sealing the lamp bulb from inside the bulb holder (see Removing O-rings and seals).

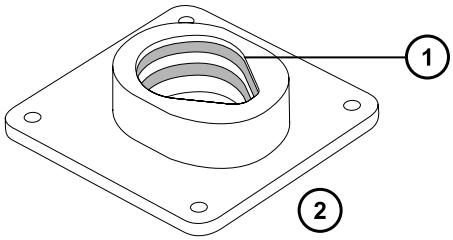
Figure 4–60:



1 Lamp bulb sealing O-ring

18. Use the O-ring removal kit to carefully remove the two O-rings from inside the lamp mounting flange.

Figure 4–61:

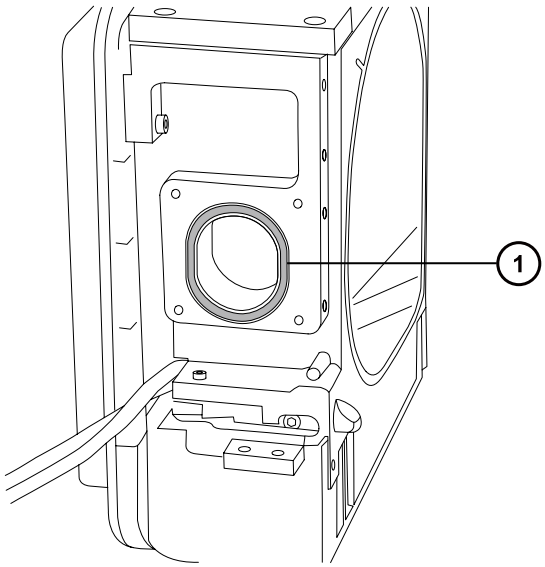


1 Mounting shaft O-rings

2 Lamp mounting flange

19. Use the O-ring removal kit to carefully remove the shaft mounting flange O-ring from the APPI source enclosure side.

Figure 4–62:



1 Lamp mounting flange O-ring

Warning: To avoid contaminating uncontaminated surfaces with biologically hazardous, toxic, or corrosive materials, dispose of all waste materials according to local environmental regulations.

20. Dispose of the O-rings in accordance with local environmental regulations.

4.26.2 Fitting the new APPI lamp drive assembly O-rings

Required materials

- Chemical-resistant, powder-free gloves
- 3-mm hex wrench
- Phillips screwdriver
- #0 POZIDRIV screwdriver
- HPLC-grade (or better) 1:1 methanol/water
- Lint-free cloth

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Note: To avoid damaging the APPI lamp drive assembly O-rings, take care when fitting them. Small nicks, tears, dirt, and dust can compromise their performance, leading to rapid deterioration in the assembly's operation.

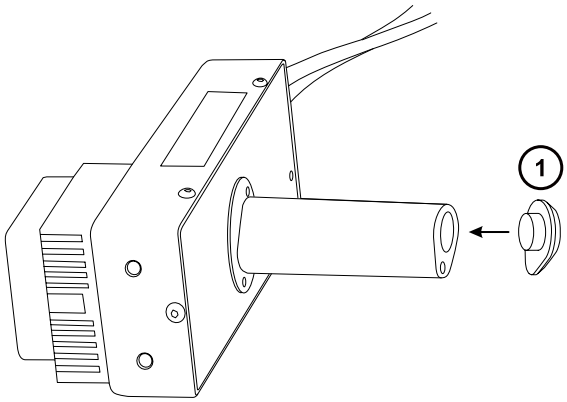
1. Ensure that all the grooves for the O-rings are free from dirt and hairs.

   Tip: If contamination is present, use 1:1 methanol/water, applied to the lint-free cloth, to carefully clean the grooves.

   Tip: For the asymmetric O-ring seals, first seat the O-ring in the small radius at the bottom of the groove. Then use a suitable tool, one with a circular cross-section, to roll the remainder of the O-ring into the groove.

2. Fit the lamp bulb sealing O-ring in the lamp aperture.
3. Fit the two new O-rings inside the lamp mounting flange.
4. Fit the new lamp mounting flange O-ring to the APPI source enclosure side.
5. Fit the mounting shaft insertion tool to the mounting shaft.

   Figure 4–63:



   (1) Mounting shaft insertion tool

   Note: To prevent damage to the mounting shaft O-rings, fit the mounting shaft insertion tool to the mounting shaft before fitting the shaft to the lamp mounting flange.

6. Slide the lamp mounting flange onto the shaft, taking care to align it correctly.
7. Reinsert the shaft through the side of the source enclosure, and fit the lamp mounting flange to the APPI source enclosure side.
8. Use the combined 2.5-mm Allen wrench and cone extraction tool to tighten the four mounting-flange securing screws.

   Note: Requirement: Tighten the securing screws sequentially and by small increments until they are all fully tight. Doing so ensures that the lamp mounting flange is uniformly seated on the APPI source enclosure side plate.

9. Remove the mounting shaft insertion tool from the mounting shaft.
10. Fit the PEEK insulator to the end of the mounting shaft.

11. Use the combined 2.5-mm Allen wrench and cone extraction tool to fit and tighten the two insulator retaining screws.
12. Fit the repeller electrode to the PEEK insulator.
13. Use the small Phillips screwdriver to fit and tighten the repeller electrode retaining screw.
14. Insert the UV bulb into the lamp drive assembly and push it fully home.
15. Fully retract the lamp mounting shaft from the source enclosure.
16. Refit the lamp-assembly collar-cover, and secure it on its base with the four screws.
17. Refit the lamp assembly cover, and secure it on its base (two screws) and above the bulb extraction aperture (two screws).
18. Refit the source enclosure release handle, and secure it with the two screws.
19. Refit and reconnect the source enclosure to the machine, refit the corona pin and probe. Refer to Installing the combined APPI/APCI source for instructions.

4.27 Replacing the UniSpray probe assembly

Replace the probe assembly in the UniSpray probe if it becomes irreversibly blocked, or if it becomes contaminated or damaged.

4.27.1 Removing the UniSpray probe assembly

Required Materials

- Chemical-resistant, powder-free gloves

To remove the UniSpray probe assembly:

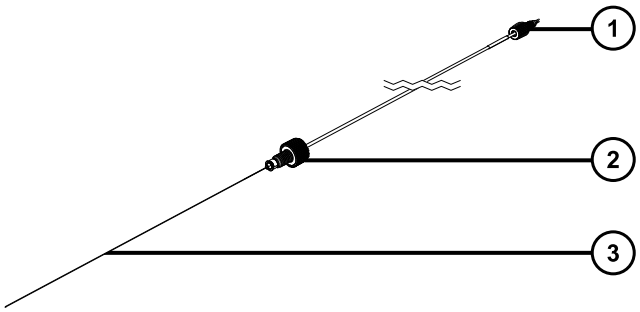
1. Prepare the instrument for working on the source (see Preparing the instrument for working on the source).

   Warning: To avoid burn injuries, take great care while working with the probe and source; these components can be hot.

2. Unscrew the probe's PEEK fitting to disconnect the probe assembly's input from the fluidics.

Figure 4–64: UniSpray probe assembly



1. PEEK fitting
2. Probe fitting
3. Probe capillary

3. Unscrew the probe fitting and pull the probe assembly out of the shaft inlet atop the source enclosure.

Warning: To avoid lacerations, puncture injuries, and possible contamination with biohazardous and toxic samples, do not touch the sharp end of the capillary.

4. Dispose of the tubes and fittings in accordance with local environmental regulations.
5. Install a replacement UniSpray probe assembly (see Fitting the UniSpray probe assembly).

4.27.2 Fitting the UniSpray probe assembly

Required Materials

- Chemical-resistant, powder-free gloves
- UniSpray probe assembly

Warning: To avoid lacerations, puncture injuries, and possible contamination with biohazardous and toxic samples, do not touch the sharp end of the capillary.

Notice: To avoid damaging capillaries, take great care when handling them; they are extremely fragile. Always hold the blunt end, never the sharp end.

Notice: Ensure that you install the correct probe capillary assembly for your probe type. Using the incorrect probe capillary assembly for the probe type can compromise instrument performance.

To replace the UniSpray probe assembly:

1. Prepare the instrument for working on the source (see Preparing the instrument for working on the source).

   Warning: To avoid burn injuries, exercise care when handling the components of the source enclosure heated to high temperatures. Wait until the hot components have sufficiently cooled before you handle them.

2. Remove the existing probe assembly from the source (see Removing the UniSpray probe assembly).

3. Carefully insert the probe assembly into the probe inlet shaft atop the source enclosure, and tighten the probe fitting.

   Notice: To avoid damaging the capillary on instruments where the source is situated above eye level, remove the source from the device and move it to a lower position before inserting the probe assembly into the probe.

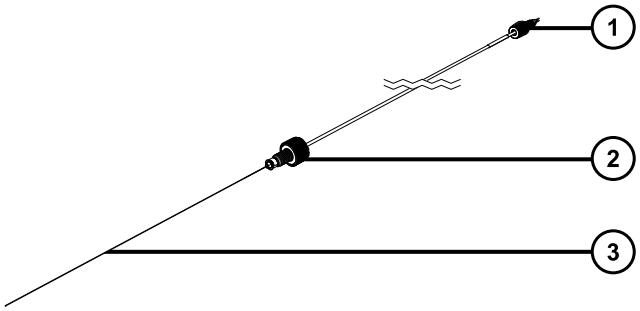
   See also: Removing a UniSpray source.

4. If you removed the source enclosure from the device to fit the probe assembly, reinstall the source enclosure.

   See also: Installing the UniSpray source.

5. Connect the PEEK fitting of the replacement probe assembly to the fluidics.

Figure 4–65: UniSpray probe assembly

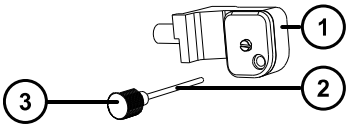


1. PEEK fitting
2. Probe fitting
3. Probe capillary

4.28 Maintaining the UniSpray impactor pin

UniSpray directs the spray at an impactor pin held at a voltage, creating smaller charged droplets, amenable to easy desolvation. This section provides details about removing, cleaning, and installing the UniSpray impactor pin.

Figure 4–66: UniSpray Impactor pin



1. Impactor pin mounting block
2. Impactor pin
3. Pin handle

4.28.1 Removing and installing the UniSpray impactor pin

Required materials

- Chemical-resistant, powder-free gloves
- UniSpray impactor pin

Warning: To avoid personal contamination with biohazards or compounds that are toxic, wear clean, chemical-resistant, powder-free gloves when performing this procedure.

To install the UniSpray impactor pin in the source:

1. Prepare the instrument for working on the source (see Preparing the instrument for working on the source).

   Warning: To avoid burn injuries, exercise care when handling the components of the source enclosure heated to high temperatures. Wait until the hot components have sufficiently cooled before you handle them.

   Warning: To avoid puncture wounds, handle sharp parts and materials with care.

2. Pull the source enclosure release (located at the bottom, right-hand side) outward, and swing open the enclosure.

3. Unscrew the pin handle and pull it to withdraw the pin from the mounting block.
4. Dispose of the used pin in accordance with local environmental regulations, or clean the pin, according to the procedure in Cleaning the UniSpray impactor pin.
5. Holding the handle of the pin you are installing, insert the pin through the inlet on the mounting block and screw the handle into the mounting block.
6. Close the source enclosure.
7. Refer to the online Help or the quick reference card supplied with the source for details about aligning and optimizing the source.

4.28.2 Cleaning or replacing the UniSpray impactor pin

Required materials

- Chemical-resistant, powder-free gloves
- Lapping film
- HPLC-grade (or better) methanol
- Lint-free tissue
- Impactor pin

Warning: To avoid personal contamination with toxic materials, wear clean, chemical-resistant, powder-free gloves when performing this procedure.

Warning: To avoid burn injuries, exercise care when handling the components of the source enclosure heated to high temperatures. Wait until the hot components have sufficiently cooled before you handle them.

Warning: To avoid puncture wounds, handle sharp parts and materials with care.

To clean the impactor pin:

1. Remove the impactor pin from the UniSpray source (see Removing and installing the UniSpray impactor pin).
2. Inspect the impactor pin, and replace it if it is deformed or damaged.
3. Clean the pin tip by wiping the lapping film along the length of the pin, and then wipe the pin clean with a methanol-saturated tissue.

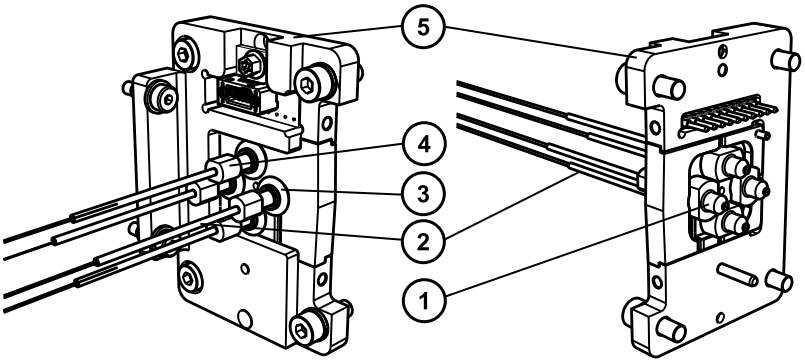
Notice: Do not rotate the impactor pin when wiping it in the lapping film or when wiping the pin clean, because this can damage the pin.

4. Install the impactor pin in the UniSpray source (see Removing and installing the UniSpray impactor pin).

4.29 Replacing the fluidic lines of the ionKey source

If a fluid line becomes damaged, replace it to ensure optimal performance. Each fluid line is pre-fitted with a PEEK connector assembly at the point where it connects to the ionKey source module. You must replace the capillary tubing and the PEEK assembly as a single unit. No parts of the fluid line are reusable once detached.

Figure 4–67:



1. PEEK fluid connector
2. Capillary tubing
3. O-ring
4. Compression fitting
5. Connector plate

To identify the correct tubing assembly for each fluid line, use the following table.

Part number	Order number	Description
430004188	700010399	Inlet tube
430004190	700010400	Infusion tube
430004212	700010401	Waste tube
430004476	700010470	Optional, post-column addition tube

Tip: Part numbers are embossed on the shrink-wrap below the ferrule assembly. You must disconnect the line from the source to see the part number.

4.29.1 Removing a fluidic line

Required Materials

- Chemical-resistant, powder-free gloves
- Flat-blade screwdriver
- T10 TORX driver

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Warning: To avoid electric shock, ensure that the instrument is prepared for working on the source before commencing this procedure.

To remove a fluidic line:

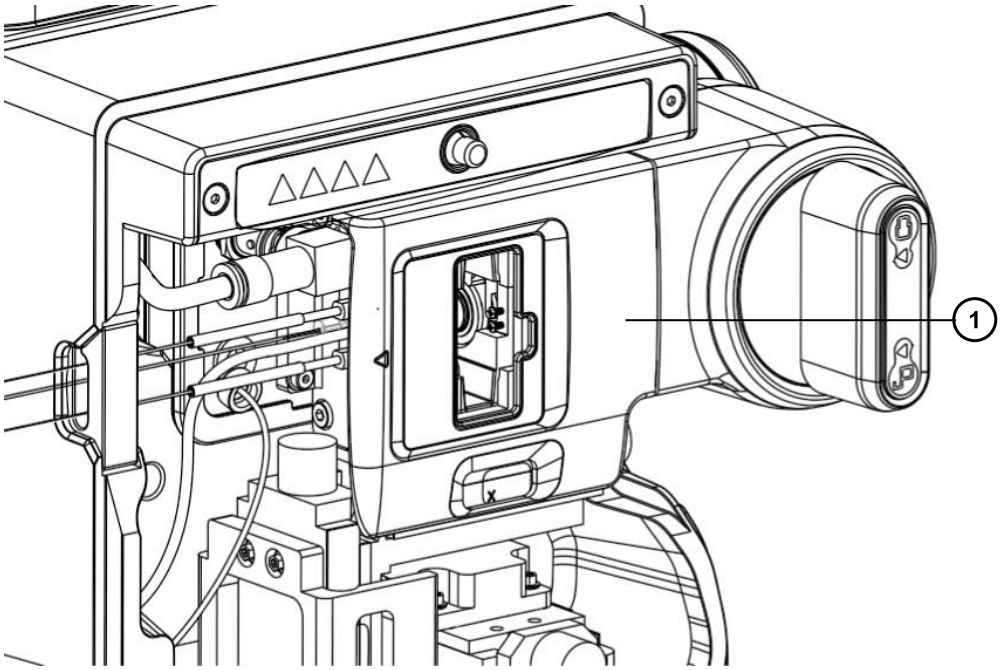
1. Prepare the instrument for working on its source (see Prepare the instrument for working on the source).

   Warning: To avoid burn injuries, take great care while working with the probe and source; these components can be hot.

2. Open the ionKey source front cover and remove the iKey surround.

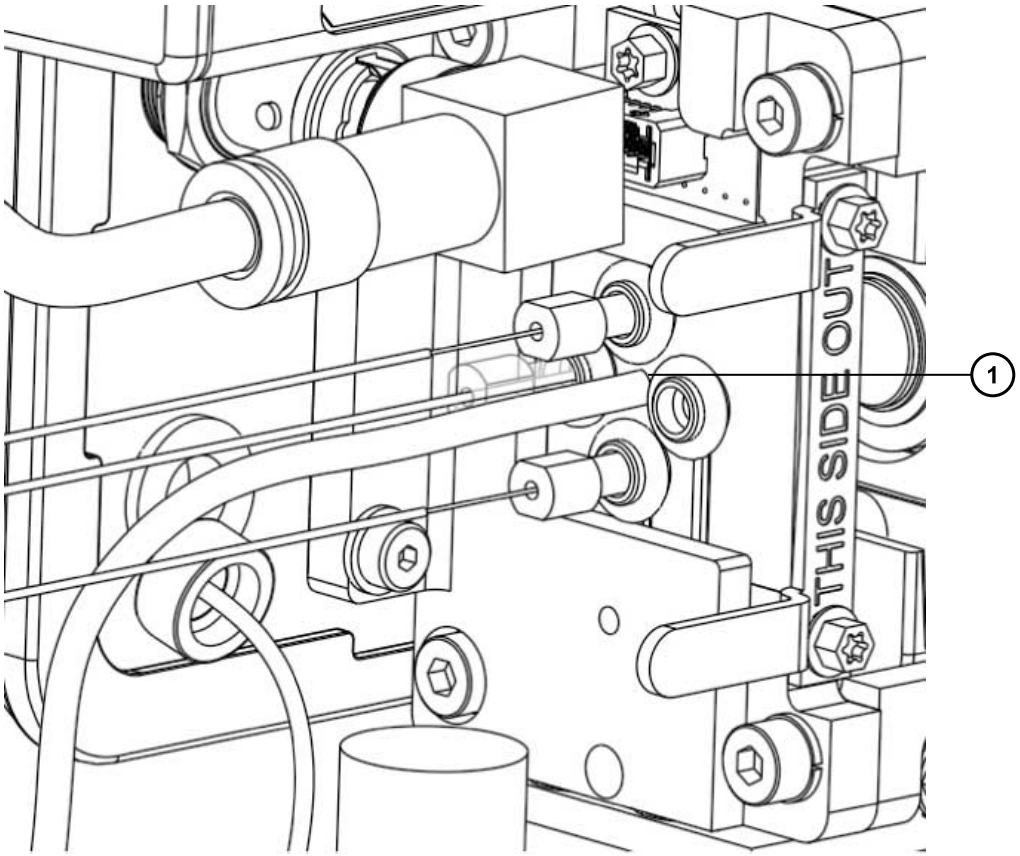
Figure 4–68:



1 iKey surround

3. Unlock and remove any iKey installed in the iKey clamp.
4. Remove the gas line using a flat-blade screwdriver.

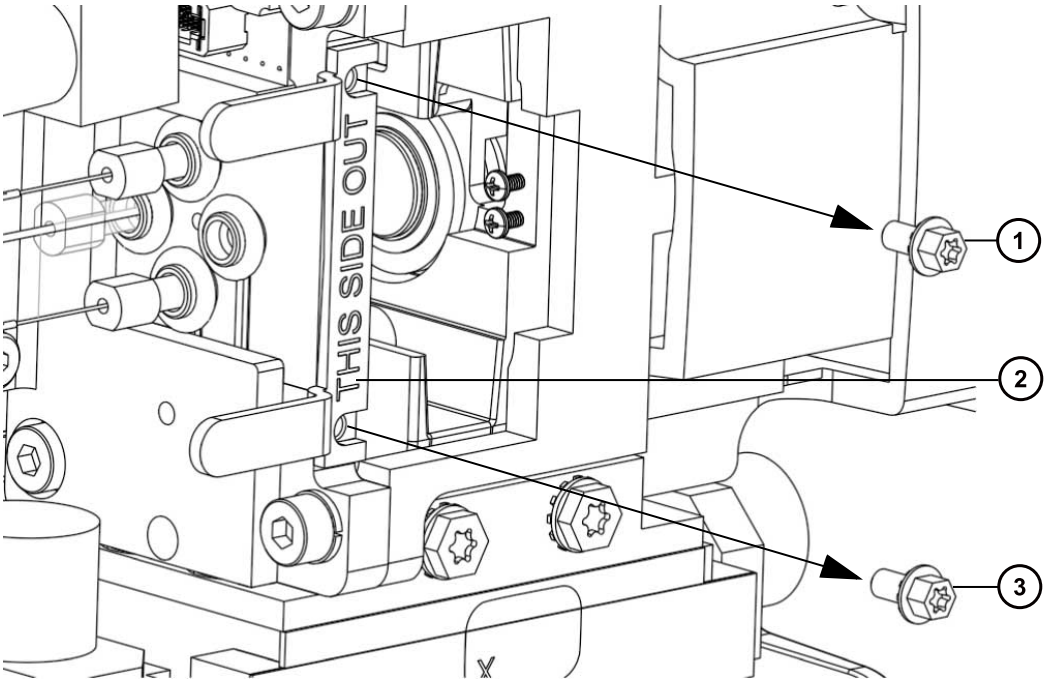
Figure 4–69:



1 Gas line

5. Disconnect the fluidic line being replaced from its source.
6. Remove two T10 Torx screws securing the end plate bracket.

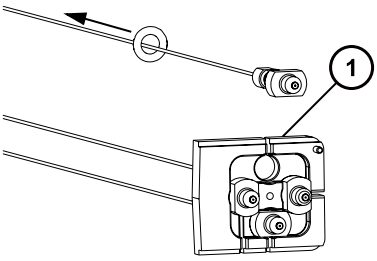
Figure 4–70:



1. T10 Torx screw
2. End plate bracket
3. T10 Torx screw

7. Slide the end plate, along with the capillary tubing, out of the iKey clamp.
8. Gently pull the O-ring from around the tube's fitting and slide the O-ring to the left.
9. Pull enough of the line being replaced to the right and allow the capillary line to slide through its channel to remove it.

Figure 4–71:



1. Channel

10. Remove the O-ring from the tubing.
11. Dispose of the removed tubing in accordance with standard laboratory procedures for contaminated vessels and sharps.

4.29.2 Installing a fluidic line

Required Materials

- Chemical-resistant, powder-free gloves
- Fluid line assembly

Warning: To avoid personal contamination with biohazards or compounds that are toxic, wear clean, chemical-resistant, powder-free gloves when performing this procedure.

Warning: To avoid electric shock, ensure that the instrument is prepared for working on the source before commencing this procedure.

To install a fluidic line:

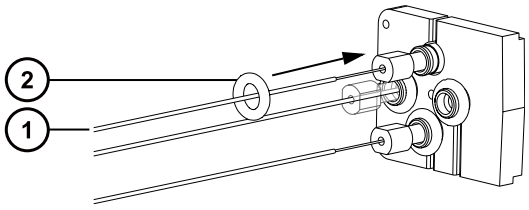
1. Prepare the instrument for working on its source (see Prepare the instrument for working on the source).

   Warning: To avoid burn injuries, take great care while working with the probe and source; these components can be hot.

2. Remove the fitting, lock ring, and ferrule from the ACQUITY UPLC M-Class end of the new fluidic line.
3. Slide the O-ring away from the end plate fitting.
4. Insert the new fluidic line through the appropriate end plate channel and seat the line's fitting into the end plate.

   Figure 4–72:



(1) O-ring

(2) New fluidic line

5. Secure the fitting with the O-ring.
6. Reinstall the end plate, end plate bracket, and gas line.
7. Route the open end of the fluidic line through the fluid line aperture on the left of the source.
8. Reinstall the fitting, ferrule, and lock ring onto the end of the new fluidic line, then connect it to the ACQUITY UPLC M-Class system, or to the onboard IntelliStart Fluidics on the mass spectrometer (see the ionKey and TRIZAIC source plumbing).
9. Reinstall and lock the iKey.
10. Reinstall the iKey surround.

4.30 Cleaning the ionKey source and connectors

Required materials

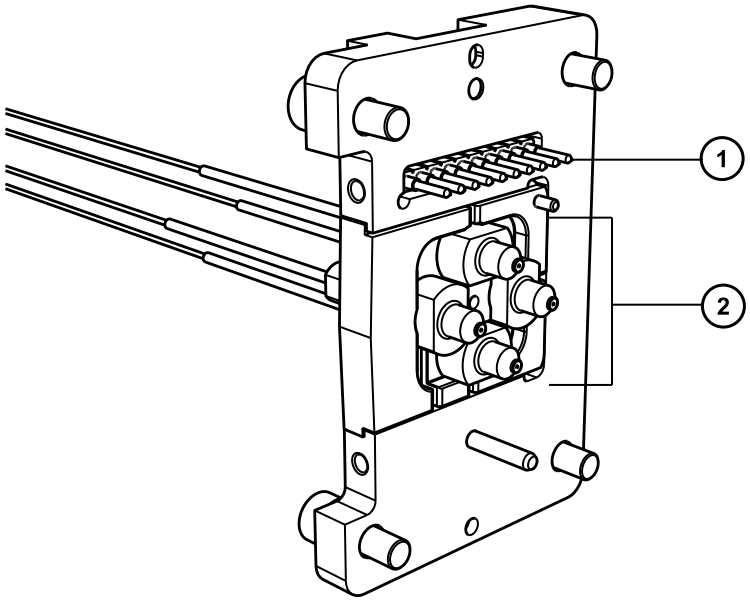
- Chemical-resistant, powder-free gloves
- Lint-free tissue
- Water
- Methanol or isopropyl alcohol
- Compressed air

Notice: To avoid damaging the iKey:

- Handle it with care. The component parts are fragile.
- For recommendations regarding the maximum pressure to subject the device to, see the *iKey Separation Device Care and Use Manual* (part number 720004897EN).
- Do not apply electrospray potential to the emitter without flow.
- Do not drop it.
- Do not immerse it in liquid.
- Do not freeze or overheat it. Keep the iKey within the allowed temperature ranges during operation and in storage.
- Use the iKey sheath to protect the device when it is not in use.
- Do not bend or pull the capillary connection tubing at the ionKey source module coupling.
- Avoid excess voltage, which can erode the emitter over time.
- Do not touch the electrospray emitter, for it can bend.
- Decompress the iKey before you remove it from the source.

During normal operation, the ionKey source does not require cleaning. After repeated use, however, material can accumulate around the fluid-line connectors or electronic connectors in the iKey docking port.

Figure 4–73:



1 Electronic connectors

2 Fluid line connectors

To remove buildup from fluid-line connectors:

Gently swab the fluid-line connectors and outer edges of the docking port with a lint-free tissue saturated with isopropanol or methanol.

4.30.1 To remove buildup from electronic connectors

To remove buildup from fluid-line connectors:

1. Open the source door.
2. From the back, gently direct a stream of air from a clean source across the electronic connectors.

   Note: To prevent contaminating the inside of the source, do not direct air into the source.
3. Close the source door.

4.30.2 To clean the outside surfaces of the ionKey source

To clean the outside surfaces of the ionKey source:

1. Use a lint-free tissue, dampened with water.
2. Clean the other system components according to the supplied documentation.

A Safety advisories

Waters instruments and devices display hazard symbols that alert you to the hidden dangers associated with a product's operation and maintenance. The symbols also appear in product manuals where they accompany statements describing the hazards and advising how to avoid them. This appendix presents the safety symbols and statements that apply to all of Waters' product offerings.

A.1 Warning symbols

Warning symbols alert you to the risk of death, injury, or seriously adverse physiological reactions associated with the misuse of an instrument of device. Heed all warnings when you install, repair, or operate any Waters instrument or device. Waters accepts no liability in cases of injury or property damage resulting from the failure of individuals to comply with any safety precaution when installing, repairing, or operating any of its instruments or devices.

The following symbols warn of risks that can arise when you operate or maintain a Waters instrument or device or component of an instrument or device. When one of these symbols appear in a manual's narrative sections or procedures, an accompanying statement identifies the applicable risk and explains how to avoid it.

Warning: (General risk of danger. When this symbol appears on an instrument, consult the instrument's user documentation for important safety-related information before you use the instrument.)

Warning: (Risk of burn injury from contacting hot surfaces.)

Warning: (Risk of electric shock.)

Warning: (Risk of fire.)

Warning: (Risk of sharp-point puncture injury.)

Warning: (Risk of hand crush injury.)

Warning: (Risk of injury caused by moving machinery.)

Warning: (Risk of exposure to ultraviolet radiation.)

Warning: (Risk of contacting corrosive substances.)

Warning: (Risk of exposure to a toxic substance.)

Warning: (Risk of personal exposure to laser radiation.)

Warning: (Risk of exposure to biological agents that can pose a serious health threat.)

Warning: (Risk of tipping.)

Warning: (Risk of explosion.)

A.1.1 Specific warnings

A.1.1.1 Burst warning

This warning applies to Waters instruments and devices fitted with nonmetallic tubing.

Warning: To avoid injury from bursting, nonmetallic tubing, heed these precautions when working in the vicinity of such tubing when it is pressurized:

- Wear eye protection.
- Extinguish all nearby flames.
- Do not use tubing that is, or has been, stressed or kinked.
- Do not expose nonmetallic tubing to compounds with which it is chemically incompatible: tetrahydrofuran, nitric acid, and sulfuric acid, for example.
- Be aware that some compounds, like methylene chloride and dimethyl sulfoxide, can cause nonmetallic tubing to swell, significantly reducing the pressure at which the tubing can rupture.

A.1.1.2 Mass spectrometer shock hazard

The following warning applies to all Waters mass spectrometers.

Warning: To avoid electric shock, do not remove protective panels from system modules. The components within are not user-serviceable.

The following warning applies to certain mass spectrometers when they are in Operate mode.

Warning: To avoid harmless, static-like electric shock, ensure the mass spectrometer is in Standby mode before you touch any of its external surfaces that are marked with this high voltage warning symbol.

A.1.1.3 Mass spectrometer flammable solvents warning

This warning applies to mass spectrometers performing an analysis that requires the use of flammable solvents.

Warning: To prevent ignition of flammable solvent vapors in the enclosed space of a mass spectrometer's ion source, ensure that nitrogen flows continuously through the source. The nitrogen supply pressure must not fall below 690 kPa (6.9 bar, 100 psi) during an analysis requiring the use of flammable solvents. Also a gas-fail device must be installed, to interrupt the flow of LC solvent should the nitrogen supply fail.

A.1.1.4 Biohazard warning

The following warning applies to Waters instruments and devices that can process material containing biohazards, which are substances that contain biological agents capable of producing harmful effects in humans.

Warning: To avoid infection with potentially infectious, human-sourced products, inactivated microorganisms, and other biological materials, assume that all biological fluids that you handle are infectious.
Specific precautions appear in the latest edition of the US National Institutes of Health (NIH) publication, *Biosafety in Microbiological and Biomedical Laboratories* (BMBL). Observe Good Laboratory Practice (GLP) at all times, particularly when working with hazardous materials, and consult the biohazard safety representative for your organization regarding the proper use and handling of infectious substances.

A.1.1.5 Biohazard and chemical hazard warning

This warning applies to Waters instruments and devices that can process biohazards, corrosive materials, or toxic materials.

Warning: To avoid personal contamination with biohazards, toxic materials, or corrosive materials, you must understand the hazards associated with their handling.
Guidelines prescribing the proper use and handling of such materials appear in the latest edition of the National Research Council's publication, *Prudent Practices in the Laboratory: Handling and Management of Chemical Hazards*.
Observe Good Laboratory Practice (GLP) at all times, particularly when working with hazardous materials, and consult the safety representative for your organization regarding its protocols for handling such materials.

A.2 Notices

Notice advisories appear where an instrument or device can be subject to use or misuse that can damage it or compromise a sample's integrity. The exclamation point symbol and its associated statement alert you to such risk.

Notice: To avoid damaging the instrument's case, do not clean it with abrasives or solvents.

A.3 Bottles Prohibited symbol

The Bottles Prohibited symbol alerts you to the risk of equipment damage caused by solvent spills.

Prohibited: To avoid equipment damage caused by spilled solvent, do not place reservoir bottles directly atop an instrument or device or on its front ledge. Instead, place the bottles in the bottle tray, which serves as secondary containment in the event of spills.

A.4 Required protection

The Use Eye Protection and Wear Protective Gloves symbols alert you to the requirement for personal protective equipment. Select appropriate protective equipment according to your organization's standard operating procedures.

Requirement: Use eye protection when performing this procedure.

Requirement: Wear clean, chemical-resistant, powder-free gloves when performing this procedure.

A.5 Warnings that apply to all Waters instruments and devices

When operating this device, follow standard quality-control procedures and the equipment guidelines in this section.

Warning: Changes or modifications to this unit not expressly approved by the party responsible for compliance could void the user's authority to operate the equipment.

Avertissement : Toute modification sur cette unité n'ayant pas été expressément approuvée par l'autorité responsable de la conformité à la réglementation peut annuler le droit de l'utilisateur à exploiter l'équipement.

Warnung: Jedwede Änderungen oder Modifikationen an dem Gerät ohne die ausdrückliche Genehmigung der für die ordnungsgemäße Funktionstüchtigkeit verantwortlichen Personen kann zum Entzug der Bedienungsbefugnis des Systems führen.

Avvertenza: qualsiasi modifica o alterazione apportata a questa unità e non espressamente autorizzata dai responsabili per la conformità fa decadere il diritto all'utilizzo dell'apparecchiatura da parte dell'utente.

Advertencia: cualquier cambio o modificación efectuado en esta unidad que no haya sido expresamente aprobado por la parte responsable del cumplimiento puede anular la autorización del usuario para utilizar el equipo.

警告： 未經有關法規認證部門允許對本設備進行的改變或修改,可能會使使用者喪失操作該設備的權利。

警告： 未经有关法规认证部门明确允许对本设备进行的改变或改装，可能会使使用者丧失操作该设备的合法性。

경고: 규정 준수를 책임지는 당사자의 명백한 승인 없이 이 장치를 개조 또는 변경할 경우, 이 장치를 운용할 수 있는 사용자 권한의 효력을 상실할 수 있습니다.

警告: 規制機関から明確な承認を受けずに本装置の変更や改造を行うと、本装置のユーザーとしての承認が無効になる可能性があります。

Warning: Use caution when working with any polymer tubing under pressure:

- Always wear eye protection when near pressurized polymer tubing.
- Extinguish all nearby flames.
- Do not use tubing that has been severely stressed or kinked.
- Do not use nonmetallic tubing with tetrahydrofuran (THF) or concentrated nitric or sulfuric acids.
- Be aware that methylene chloride and dimethyl sulfoxide cause nonmetallic tubing to swell, which greatly reduces the rupture pressure of the tubing.

Avertissement : Manipulez les tubes en polymère sous pression avec precaution:

- Portez systématiquement des lunettes de protection lorsque vous vous trouvez à proximité de tubes en polymère pressurisés.
- Eteignez toute flamme se trouvant à proximité de l’instrument.
- Evitez d'utiliser des tubes sévèrement déformés ou endommagés.
- Evitez d'utiliser des tubes non métalliques avec du tétrahydrofurane (THF) ou de l'acide sulfurique ou nitrique concentré.
- Sachez que le chlorure de méthylène et le diméthylesulfoxyde entraînent le gonflement des tuyaux non métalliques, ce qui réduit considérablement leur pression de rupture.

Warnung: Bei der Arbeit mit Polymerschläuchen unter Druck ist besondere Vorsicht angebracht:

- In der Nähe von unter Druck stehenden Polymerschläuchen stets Schutzbrille tragen.
- Alle offenen Flammen in der Nähe löschen.
- Keine Schläuche verwenden, die stark geknickt oder überbeansprucht sind.
- Nichtmetallische Schläuche nicht für Tetrahydrofuran (THF) oder konzentrierte Salpeter- oder Schwefelsäure verwenden.
- Durch Methylenchlorid und Dimethylsulfoxid können nichtmetallische Schläuche quellen; dadurch wird der Berstdruck des Schlauches erheblich reduziert.

Avvertenza: fare attenzione quando si utilizzano tubi in materiale polimerico sotto pressione:

- Indossare sempre occhiali da lavoro protettivi nei pressi di tubi di polimero pressurizzati.
- Spegnere tutte le fiamme vive nell'ambiente circostante.
- Non utilizzare tubi eccessivamente logorati o piegati.
- Non utilizzare tubi non metallici con tetraidrofurano (THF) o acido solforico o nitrico concentrati.
- Tenere presente che il cloruro di metilene e il dimetilsolfossido provocano rigonfiamenti nei tubi non metallici, riducendo notevolmente la pressione di rottura dei tubi stessi.

Advertencia: se recomienda precaución cuando se trabaje con tubos de polímero sometidos a presión:

- El usuario deberá protegerse siempre los ojos cuando trabaje cerca de tubos de polímero sometidos a presión.
- Si hubiera alguna llama las proximidades.
- No se debe trabajar con tubos que se hayan doblado o sometido a altas presiones.
- Es necesario utilizar tubos de metal cuando se trabaje con tetrahidrofurano (THF) o ácidos nítrico o sulfúrico concentrados.
- Hay que tener en cuenta que el cloruro de metileno y el sulfóxido de dimetilo dilatan los tubos no metálicos, lo que reduce la presión de ruptura de los tubos.

警告： 當在有壓力的情況下使用聚合物管線時，小心注意以下幾點。

- 當接近有壓力的聚合物管線時一定要戴防護眼鏡。
- 熄滅附近所有的火焰。
- 不要使用已經被壓癟或嚴重彎曲管線。
- 不要在非金屬管線中使用四氫呋喃或濃硝酸或濃硫酸。
- 要了解使用二氯甲烷及二甲基亞楓會導致非金屬管線膨脹，大大降低管線的耐壓能力。

警告： 当有压力的情况下使用管线时，小心注意以下几点：

- 当接近有压力的聚合物管线时一定要戴防护眼镜。
- 熄灭附近所有的火焰。
- 不要使用已经被压瘪或严重弯曲的管线。
- 不要在非金属管线中使用四氢呋喃或浓硝酸或浓硫酸。
- 要了解使用二氯甲烷及二甲基亚枫会导致非金属管线膨胀，大大降低管线的耐压能力。

경고: 가압 폴리머 튜브로 작업할 경우에는 주의하십시오.

- 가압 폴리머 튜브 근처에서는 항상 보호 안경을 착용하십시오.
- 근처의 화기를 모두 끄십시오.
- 심하게 변형되거나 꼬인 튜브는 사용하지 마십시오.
- 비금속(Nonmetallic) 튜브를 테트라히드로푸란(Tetrahydrofuran: THF) 또는 농축 질산 또는 황산과 함께 사용하지 마십시오.
- 염화 메틸렌(Methylene chloride) 및 디메틸술폭시드(Dimethyl sulfoxide)는 비금속 튜브를 부풀려 튜브의 파열 압력을 크게 감소시킬 수 있으므로 유의하십시오.

警告: 圧力のかかったポリマーチューブを扱うときは、注意してください。

- 加圧されたポリマーチューブの付近では、必ず保護メガネを着用してください。
- 近くにある火を消してください。
- 著しく変形した、または折れ曲がったチューブは使用しないでください。
- 非金属チューブには、テトラヒドロフラン(THF)や高濃度の硝酸または硫酸などを流さないでください。
- 塩化メチレンやジメチルスルホキシドは、非金属チューブの膨張を引き起こす場合があり、その場合、チューブは極めて低い圧力で破裂します。

This warning applies to Waters instruments fitted with nonmetallic tubing. This warning applies to instruments operated with flammable solvents.

Warning: The user shall be made aware that if the equipment is used in a manner not specified by the manufacturer, the protection provided by the equipment may be impaired.

Avertissement : L'utilisateur doit être informé que si le matériel est utilisé d'une façon non spécifiée par le fabricant, la protection assurée par le matériel risque d'être défectueuses.

Warnung: Der Benutzer wird darauf aufmerksam gemacht, dass bei unsachgemäßer Verwendung des Gerätes die eingebauten Sicherheitseinrichtungen unter Umständen nicht ordnungsgemäß funktionieren.

Avvertenza: si rende noto all'utente che l'eventuale utilizzo dell'apparecchiatura secondo modalità non previste dal produttore può compromettere la protezione offerta dall'apparecchiatura.

Advertencia: el usuario deberá saber que si el equipo se utiliza de forma distinta a la especificada por el fabricante, las medidas de protección del equipo podrían ser insuficientes.

警告： 使用者必須非常清楚如果設備不是按照製造廠商指定的方式使用，那麼該設備所提供的保護將被消弱。

警告： 使用者必须非常清楚如果设备不是按照制造厂商指定的方式使用，那么该设备所提供的保护将被削弱。

경고: 제조업체가 명시하지 않은 방식으로 장비를 사용할 경우 장비가 제공하는 보호 수단이 제대로 작동하지 않을 수 있다는 점을 사용자에게 반드시 인식시켜야 합니다.

警告: ユーザーは、製造元により指定されていない方法で機器を使用すると、機器が提供している保証が無効になる可能性があることに注意して下さい。

A.6 Warnings that address the replacing of fuses

The following warnings pertain to instruments and devices equipped with user-replaceable fuses. Information describing fuse types and ratings sometimes, but not always, appears on the instrument or device.

Finding fuse types and ratings when that information appears on the instrument or device:

Warning: To protect against fire, replace fuses with those of the type and rating printed on panels adjacent to instrument fuse covers.

Avertissement : pour éviter tout risque d'incendie, remplacez toujours les fusibles par d'autres du type et de la puissance indiqués sur le panneau à proximité du couvercle de la boite à fusible de l'instrument.

Warnung: Zum Schutz gegen Feuer die Sicherungen nur mit Sicherungen ersetzen, deren Typ und Nennwert auf den Tafeln neben den Sicherungsabdeckungen des Geräts gedruckt sind.

Avvertenza: per garantire protezione contro gli incendi, sostituire i fusibili con altri dello stesso tipo aventi le caratteristiche indicate sui pannelli adiacenti alla copertura fusibili dello strumento.

Advertencia: Para evitar incendios, sustituir los fusibles por aquellos del tipo y características impresos en los paneles adyacentes a las cubiertas de los fusibles del instrumento.

警告： 為了避免火災，更換保險絲時，請使用與儀器保險絲蓋旁面板上所印刷之相同類型與規格的保險絲。

警告： 为了避免火灾，应更换与仪器保险丝盖旁边面板上印刷的类型和规格相同的保险丝。

경고: 화재의 위험을 막으려면 기기 퓨즈 커버에 가까운 패널에 인쇄된 것과 동일한 타입 및 정격의 제품으로 퓨즈를 교체하십시오.

警告: 火災予防のために、ヒューズ交換では機器ヒューズカバー脇のパネルに記載されているタイプおよび定格のヒューズをご使用ください。

Finding fuse types and ratings when that information does not appear on the instrument or device:

Warning: To protect against fire, replace fuses with those of the type and rating indicated in the “Replacing fuses” section of the Maintenance Procedures chapter.

Avertissement : pour éviter tout risque d'incendie, remplacez toujours les fusibles par d'autres du type et de la puissance indiqués dans la rubrique "Remplacement des fusibles" du chapitre traitant des procédures de maintenance.

Warnung: Zum Schutz gegen Feuer die Sicherungen nur mit Sicherungen ersetzen, deren Typ und Nennwert im Abschnitt "Sicherungen ersetzen" des Kapitels "Wartungsverfahren" angegeben sind.

Avvertenza: per garantire protezione contro gli incendi, sostituire i fusibili con altri dello stesso tipo aventi le caratteristiche indicate nel paragrafo "Sostituzione dei fusibili" del capitolo "Procedure di manutenzione".

Advertencia: Para evitar incendios, sustituir los fusibles por aquellos del tipo y características indicados en la sección "Sustituir fusibles".

警告： 為了避免火災，更換保險絲時，應使用「維護步驟」章節中「更換保險絲」所指定之相同類型與規格的保險絲。

警告： 为了避免火灾，应更换“维护步骤”一章的“更换保险丝”一节中介绍的相同类型和规格的保险丝。

경고: 화재의 위험을 막으려면 유지관리 절차 단원의 "퓨즈 교체" 절에 설명된 것과 동일한 타입 및 정격의 제품으로 퓨즈를 교체하십시오.

警告: 火災予防のために、ヒューズ交換ではメンテナンス項目の「ヒューズの交換」に記載されているタイプおよび定格のヒューズをご使用ください。

A.7 Electrical symbols

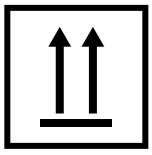
The following electrical symbols and their associated statements can appear in instrument manuals and on an instrument’s front or rear panels.

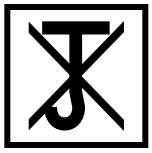
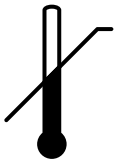
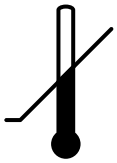
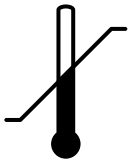
Symbol	Description
	Electrical power on

Symbol	Description
	Electrical power off
	Standby
	Direct current
	Alternating current
	Alternating current (3 phase)
	Safety ground
	Frame, or chassis, terminal
	Fuse
	Functional ground
	Input
	Output

A.8 Handling symbols

The following handling symbols and their associated statements can appear on labels affixed to the packaging in which instruments, devices, and component parts are shipped.

Symbol	Description
	Keep upright!
	Keep dry!
	Fragile!

Symbol	Description
	Use no hooks!
	Upper limit of temperature
	Lower limit of temperature
	Temperature limitation

B External connections

Warning: To avoid skeletal or muscle injury associated with lifting heavy objects, use appropriate machinery and the supplied harness to lift the mass spectrometer.

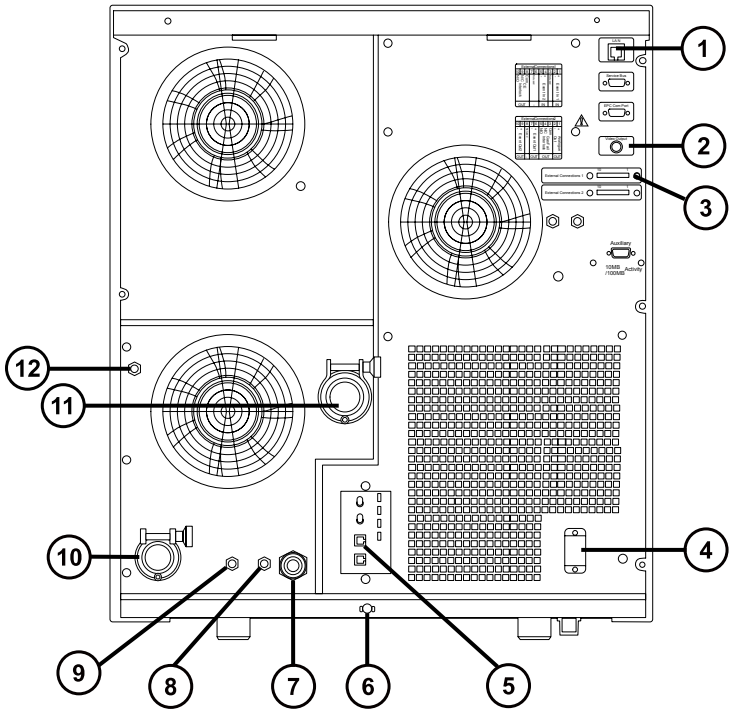
Notice: To avoid damaging the mass spectrometer, observe the following precautions:

- Contact Waters Technical Service before moving the instrument.
- If you must transport the instrument, or remove it from service, contact Waters Technical Service for recommended cleaning, flushing, and packaging procedures.

B.1 External wiring and vacuum connections

Rear panel connections appear in the figure below. Note that the connectors and controls not identified are for use by Waters engineers only.

Figure B–1: Mass spectrometer rear panel connectors:



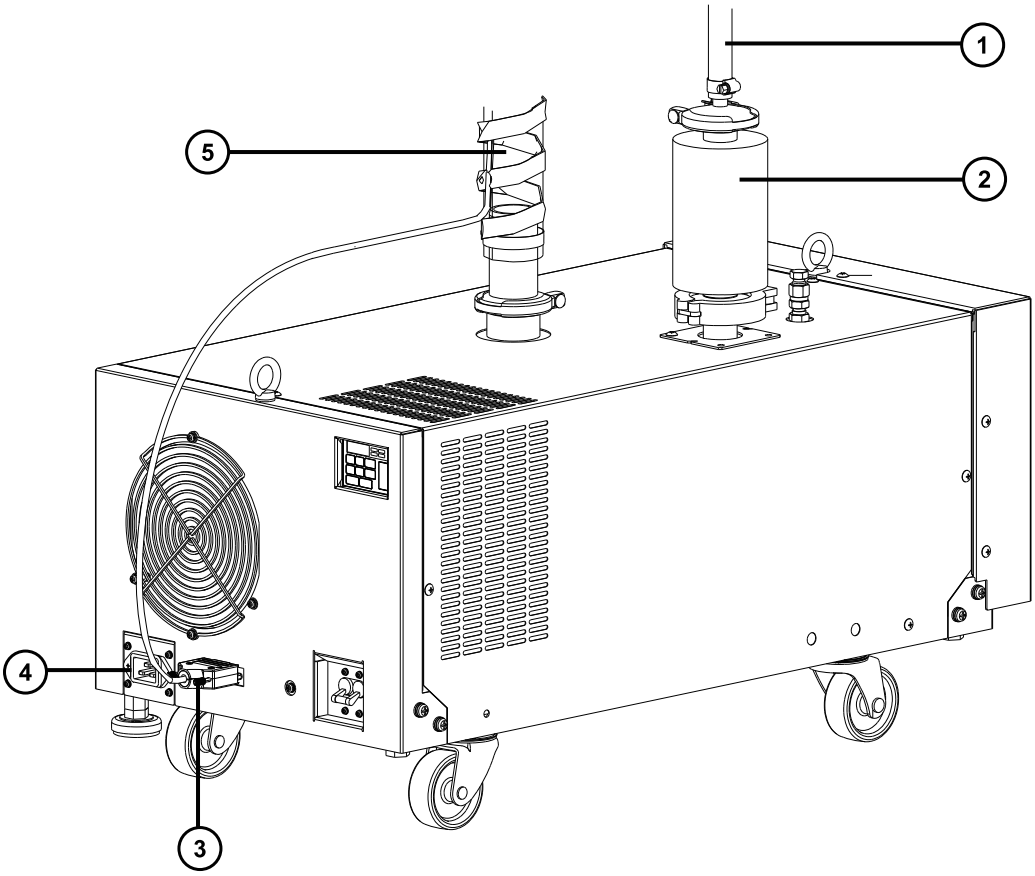
1. Shielded Ethernet
2. Video camera connection (for use with the optional NanoFlow ESI or IonKey source)
3. Event inputs and outputs
4. Power
5. Roughing pump connectors
6. Roughing pump grounding connnection
7. Nitrogen exhaust
8. Nitrogen inlet
9. Pilot valve port
10. Turbo vacuum
11. Source vacuum
12. Collision cell gas inlet

B.2 Connecting the EBARA oil-free roughing pump

To ensure proper ventilation, install the pump in a location that allows these clearance distances for each side:

- 100 mm or more at the front, rear, and top of the pump.
- 50 mm or more at each side of the pump.

Figure B–2: EBARA oil-free roughing pump



1. Exhaust tubing
2. Exhaust silencer
3. Control signal connector
4. Power connector
5. Vacuum hose

Required materials

- Chemical-resistant, powder-free gloves
- 7-mm nut driver
- Sharp knife

The following items are included in the installation kit:

- NW25 center rings
- NW25 clamps
- NW40 center rings
- NW40 clamps
- NW40 elbow
- NW40 tee piece
- NW40 to NW16 reducer
- NW40 to NW25 reducer
- 12.7-mm clear PVC exhaust tubing
- PVC hose clamps
- Vacuum hose

To connect the oil-free roughing pump:

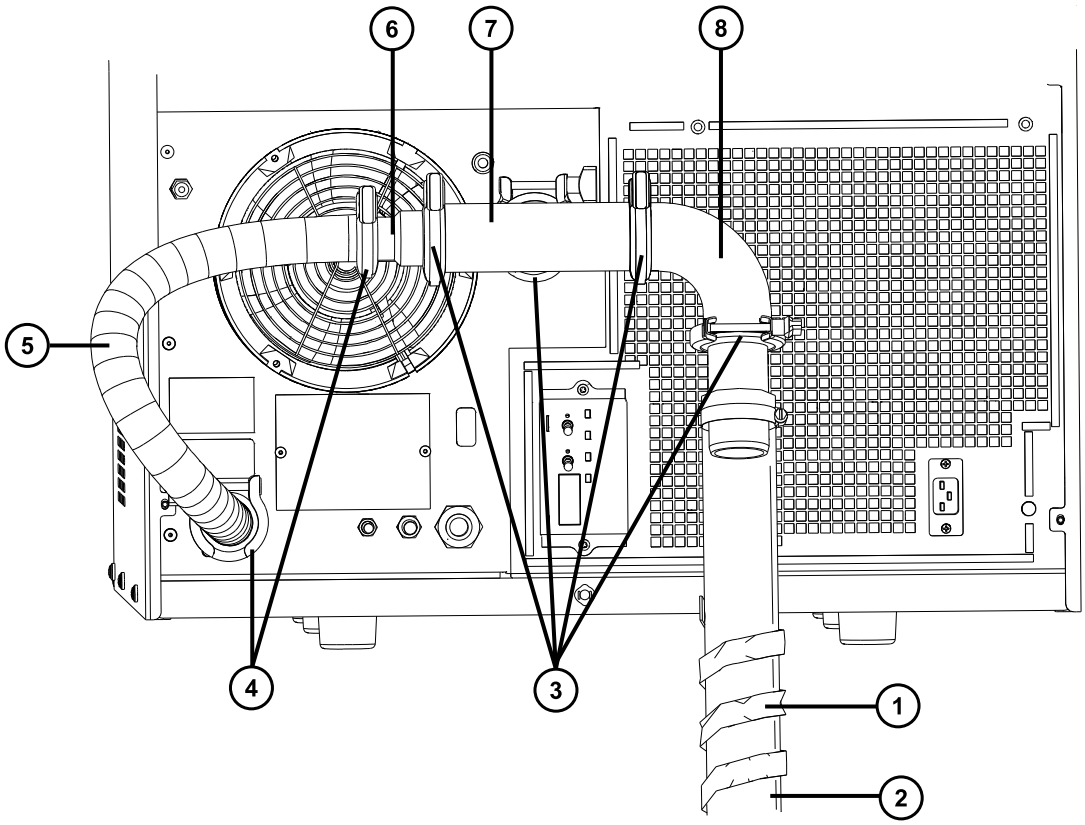
Warning: To avoid personal contamination with biohazards or compounds that are toxic, wear clean, chemical-resistant, powder-free gloves when performing this procedure.

Warning: To avoid injury, do not lift the pump. To move the pump, use its wheels.

1. Connect the roughing pump's vacuum hoses according to the figures below.

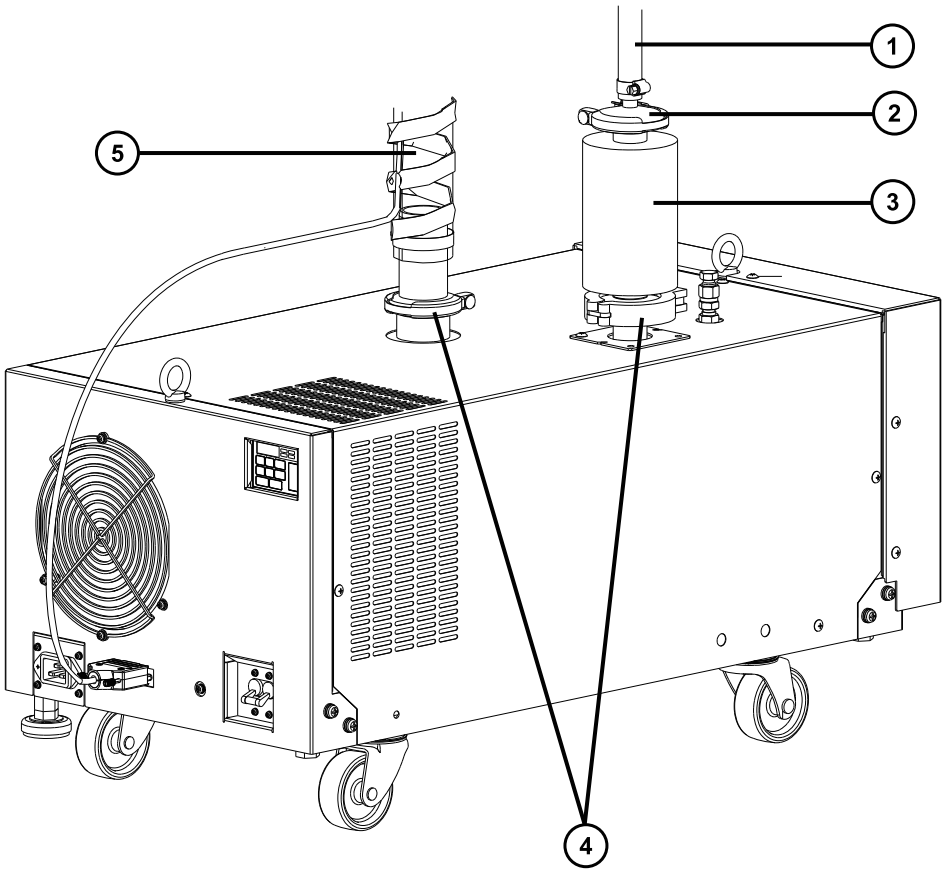
   Important: To avoid gas leaks, use the sharp knife to cut the PVC exhaust tubing squarely (that is, perpendicular to its horizontal axis).

Figure B–3: Roughing pump tubing connections to rear of the Xevo TQ-XS mass spectrometer



1. Roughing pump electrical cable attached to vacuum hose
2. Vacuum hose to roughing pump
3. NW40 clamps
4. NW25 clamps
5. Flexible vacuum tubing
6. NW40/NW25 reducer
7. NW40 tee piece
8. NW40 elbow

Figure B–4: Roughing pump tubing connections to the EBARA pump

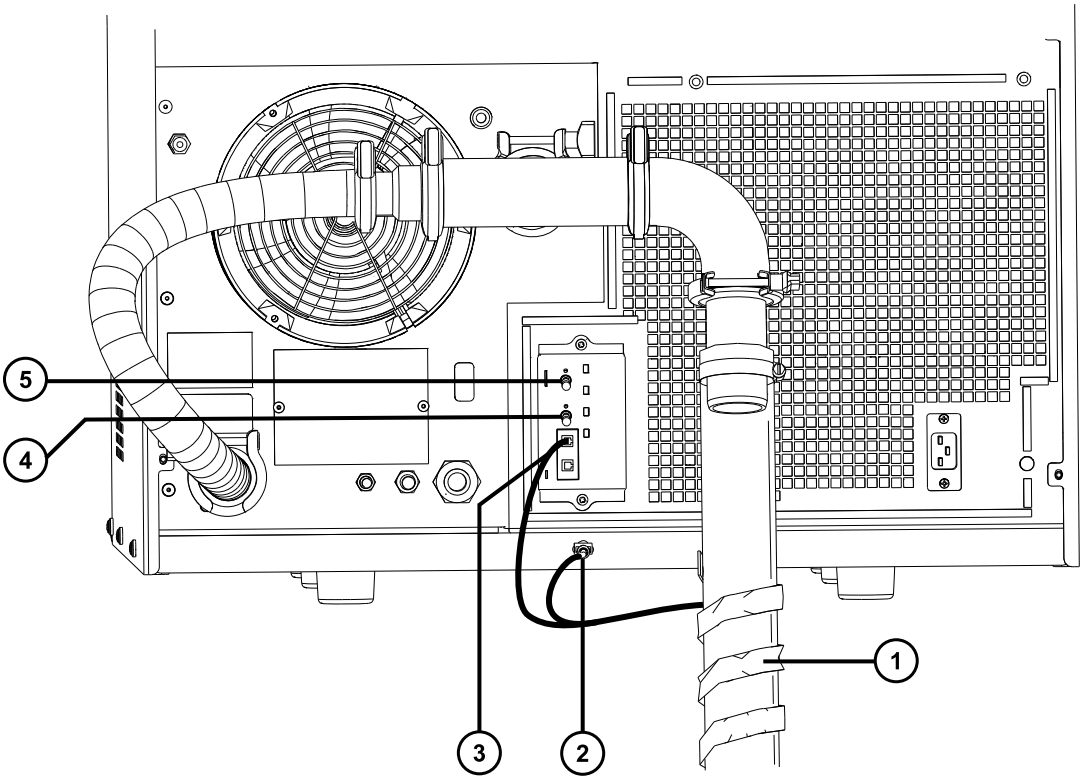


1. Exhaust tubing
2. NW40/NW16 reducer
3. Exhaust silencer
4. NW40 clamps
5. Vacuum hose from rear of the Xevo TQ-XS

2. Make the electrical connections to the roughing pump (see Making connections to the Ebara oil-free roughing pump).

B.3 Making the electrical connections to the Ebara oil-free roughing pump

Figure B–5: Roughing pump electrical connections:



1. Tape attaching electrical cables to the vacuum hose
2. Grounding connector
3. Backing pump control connector
4. Electronics ON/OFF switch (for use by Waters engineers only)
5. Pump override switch (for use by Waters engineers only)

To make the electrical connections for the oil-free roughing pump:

1. Connect the roughing pump power cord to the main power source.
2. Connect the relay cable from the roughing pump's control signal connector to the upper backing pump control connector on the mass spectrometer’s rear panel.

Tip: Use only the upper backing pump control connector. Leave the lower connector marked Delayed backing pump control, disconnected.

3. Connect the grounding cable to the grounding connection.

B.4 Connecting to the nitrogen gas supply

Required materials

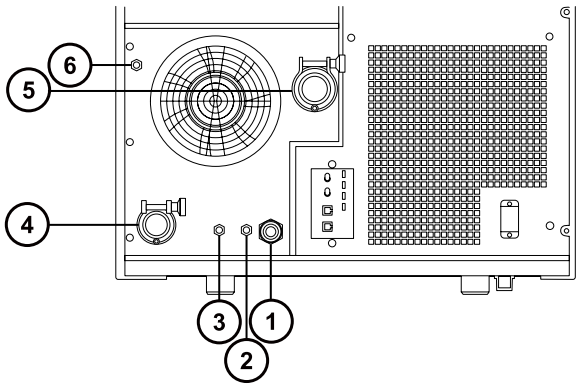
- Chemical-resistant, powder-free gloves
- 6-mm PTFE tubing (included in the Xevo G2-S Tof Installation Kit)
- Nitrogen regulator (not supplied)

To connect the nitrogen gas supply:

1. Connect one free end of the 6-mm PTFE tubing to the nitrogen inlet port on the rear of the instrument.

   Requirement: Do not cut the 6-mm (¼-in) PTFE tubing to size; use the entire, supplied 5-m (16-ft) length.

Figure B–6: Nitrogen and collision cell gas inlet, and vacuum connectors:



1. Nitrogen exhaust
2. Nitrogen inlet port
3. Pilot valve port
4. Turbo vacuum

5 Source vacuum

6 Collision cell gas inlet

2. Attach a nitrogen regulator to the nitrogen supply.

   Requirement: The nitrogen must be dry and oil-free, with a purity of at least 95%.

3. Connect the free end of the 6-mm PTFE tubing to the nitrogen regulator.
4. Set the nitrogen regulator to 690 kPa (6.9bar, 100 psi).
5. Ensure that there are no gas leaks at any of the nitrogen gas supply fittings.

B.5 Connecting to the collision cell gas supply

Required materials

- Chemical-resistant, powder-free gloves
- 7/16-inch open-end wrench
- 1/8-inch Swagelok nut and ferrule
- 1/8-inch stainless steel tube (supplied with the mass spectrometer)
- Argon regulator (not supplied)

To connect the collision cell gas supply:

1. Use the 1/8-inch Swagelok nut and ferrule to connect the 1/8-inch stainless steel tube to the collision cell gas inlet on the rear of the mass spectrometer (see the figure in Connecting to the nitrogen gas supply).
2. Use the 7/16-inch wrench to tighten the 1/8-inch Swagelok nut.
3. Attach the argon regulator to the argon supply.

   Requirement: The argon must be dry and of high purity (99.997%).

4. Connect the free end of the tube to the collision gas supply.
5. Set the argon regulator to 50 kPa (0.5 bar, 7 psi).

B.6 Connecting the nitrogen exhaust line

Required materials

- Chemical-resistant, powder-free gloves
- Utility knife

- Nitrogen exhaust trap bottle
- 4-mm PTFE tubing and 12-mm PTFE tubing (included in the Xevo TQ-XS installation kit)

To connect the nitrogen exhaust line:

Warning: To prevent the nitrogen exhaust from carrying biologically hazardous, toxic, or corrosive LC solvents, you must use a nitrogen exhaust trap bottle and a laboratory exhaust system. The laboratory exhaust system must provide a minimum vacuum of 0.20 kPa (2 mbar, 0.03 psi) below atmospheric pressure (negative pressure).

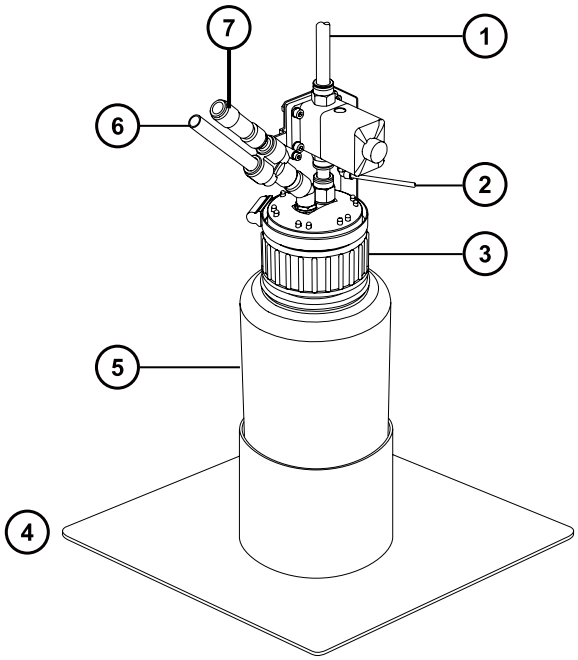
Warning: To avoid the buildup of hazardous gases, do not place the nitrogen exhaust trap bottle in an enclosed cabinet.

Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

Notice: To prevent serious damage to the instrument, two separate exhaust systems are required: one for nitrogen, the other for the roughing pumps. Vent the exhausts to atmosphere through separate lines. Oil mist can seriously damage the instrument if the nitrogen exhaust line connects with the roughing pump exhaust line. Your warranty does not cover damage caused by routing exhaust lines incorrectly.

1. Locate the nitrogen exhaust trap bottle in an accessible area below the instrument.

Figure B–7: Nitrogen exhaust trap bottle:



1. To laboratory exhaust port
2. From instrument pilot valve port
3. Cap
4. Bottle support
5. Nitrogen exhaust trap bottle
6. From instrument exhaust connection
7. One-way valve

> **Notice:** To avoid gas leaks, use the sharp knife to cut the PVC exhaust tubing squarely (that is, perpendicular to its horizontal axis).

2. Cut a length of 4-mm tubing long enough to connect the instrument to the nitrogen exhaust trap bottle.
3. Connect one end of the tubing to the pilot valve port on the instrument's rear panel.
4. Connect the free end of the tubing to the pilot valve port on the nitrogen exhaust trap bottle.
5. Cut a length of 12-mm tubing long enough to connect the instrument to the nitrogen exhaust trap bottle.
6. Connect one end of the tubing to the exhaust port on the instrument's rear panel.
7. Connect the free end of the tubing to the inlet port on the nitrogen exhaust trap bottle.

> **Notice:** To avoid gas leaks, use the sharp knife to cut the PVC exhaust tubing squarely (that is, perpendicular to its horizontal axis).

8. Cut a second length of 12-mm tubing long enough to connect the nitrogen exhaust trap bottle to the exhaust vent.
9. Insert one end of the tubing into the outlet port on the nitrogen exhaust trap bottle.
10. Route the free end of the tubing to the exhaust vent.

B.7 Connecting liquid waste lines

To ensure waste materials are safely drained to the waste container, connect both the bottle tray and mass spectrometer's drain cup to the waste container.

Required materials

- Chemical-resistant, powder-free gloves
- Waste container

To connect the liquid waste line:

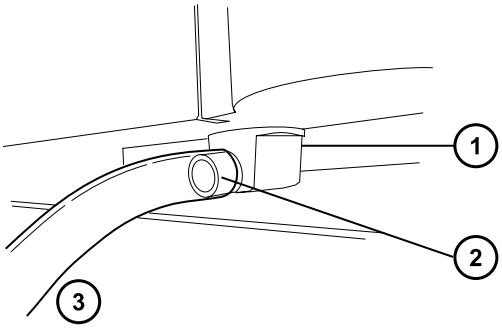
Warning: To avoid personal contamination with biohazards, toxic materials, and corrosive materials, wear chemical-resistant gloves when performing this procedure.

1. Place a suitable waste container below the mass spectrometer.

   Notice: To avoid distorting the drip tray or causing the drain cup to leak, restrain the drain cup when attaching or removing the waste line.

2. Slide a drain line over the barbed fitting of the drain (located at the bottom, left-hand side of the mass spectrometer, and on the base of the bottle tray).

   Figure B–8:



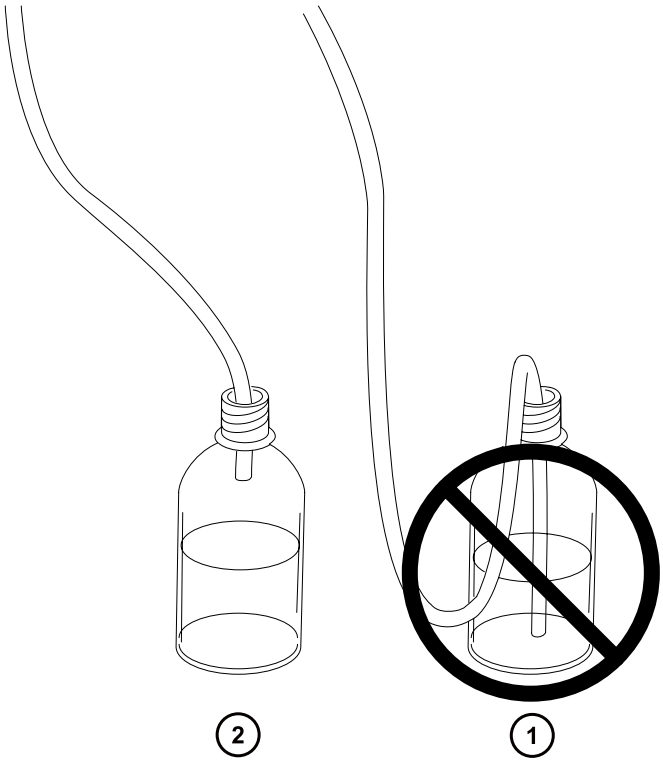
1. Drain cup
2. Barbed fitting
3. Drain line

Warning: To prevent leakage of biologically hazardous, toxic, or corrosive materials,

- do not crimp or bend drain lines. A crimp or bend can impede flow to the waste container.
- empty the waste container before the lower end of the drain tubes are covered by waste solvent.

3. Route the waste lines to the waste container. If necessary, shorten the waste tubes so that their ends are above the surface of the waste solvent.

Figure B–9: Positioning of drain tube:



1 Incorrect

2 Correct

B.8 Connecting the workstation (systems with no ACQUITY LC)

Before connecting the workstation to the instrument, set up the workstation according to its accompanying instructions. Locate the workstation within three meters (ten feet) of the mass spectrometer.

Requirement: Use shielded network cables with the mass spectrometer to ensure compliance with FCC limits.

B.8.1 Connecting to the workstation

To connect the workstation:

1. Connect the monitor to the workstation PC.
2. Connect one end of the shielded, crossover, network cable to the port labeled instrument LAN on the workstation rear panel.
3. Connect the free end of the shielded, crossover, network cable to the Ethernet port in the top, right-hand corner of the mass spectrometer's rear panel.

B.9 Connecting Ethernet cables (systems with ACQUITY LC)

Requirement: Use shielded network cables with the mass spectrometer to ensure compliance with FCC limits.

To make Ethernet connections:

1. Connect one end of one shielded Ethernet cable to the ACQUITY instrument's network switch, and then connect the free end to the Ethernet card on the preconfigured ACQUITY workstation.

   Tip: On preconfigured systems, the Ethernet card is identified as the Instrument LAN card.
2. Connect one end of the other shielded Ethernet cable to the Ethernet port in the top, right-hand corner of the mass spectrometer's rear panel, and then connect the free end to the ACQUITY instrument's network switch.

B.10 Input/output signal connectors

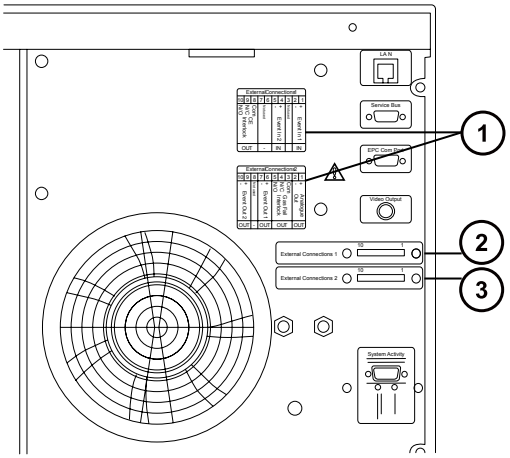
Warning: To avoid electric shock, all electrical connections to the rear panel must be separated from hazardous voltages by double or reinforced insulation. Circuits of this type are classified as safety extra low voltage (SELV). Examples of circuits that are typically SELV include contact closure inputs and outputs for auto-samplers, and UV, RI, and fluorescence detector signal outputs for LC/MS systems. The electrical connections on the rear panel of this mass spectrometer are all SELV.

Note: To avoid damaging the instrument,

- do not apply a voltage to the Analog (out) connectors; these are active connections driven by the instrument.
- do not apply voltages higher than those shown in the tables.

Two removable connectors (designated External Connections 1 and External Connections 2) on the mass spectrometer's rear panel hold the screw terminals for input/output signals. The connectors are keyed so that they can receive a signal cable inserted only one way.

Figure B–10: Input and output connector locations:



1 External connections identification tables

2 External connections 1

3 External connections 2

Figure B–11: Input/output signal connector configuration:

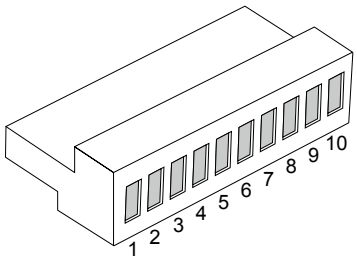


Table B–1: External connections 1:

Pin	Function	Rating
1	Event In 1+, digital signal, optimum +3.3V max +5V	+5 V
2	Event In 1-, digital ground, 0V	0 V
3	Not used	
4	Event In 2+, digital signal, optimum +3.3V max +5V	+5 V
5	Event In 2-, digital ground, 0V	0 V
6	Not used	
7	Not used	
8	CE Interlock Out, common	+30 V d.c., 100 mA
9	CE Interlock Out, normally closed (N/C)	+30 V d.c., 100 mA
10	CE Interlock Out, normally open (N/O)	+30 V d.c., 100 mA

Table B–2: External connections 2:

Pin	Function	Rating
1	Analog Out +, instrument-driven electrical output	None
2	Analog Out -, ground	None
3	Gas Fail Interlock, common	+30 V d.c., 100 mA
4	Gas Fail Interlock, normally closed (N/C)	+30 V d.c., 100 mA
5	Gas Fail Interlock normally open (N/O)	+30 V d.c., 100 mA
6	Event Out 1 +	+30 V d.c., 100 mA
7	Event Out 1 -	+30 V d.c., 100 mA
8	Not used	
9	Event Out 2 +	+30 V d.c., 100 mA
10	Event Out 2 -	+30 V d.c., 100 mA

B.11 Connecting to the electricity source

The mass spectrometer requires a separate, grounded electricity source. The ground connection in the electrical outlet must be common and connected near the system.

To connect to the electricity source:

Recommendation: Use a line conditioner or an uninterruptible power supply (UPS) for optimum long-term input voltage stability.

Warning: To avoid electric shock, use the SVT-type power cord in the United States and HAR-type (or better) cord in Europe. The main power cord must be replaced only with one of adequate rating. For information regarding what cord to use in other countries, contact your local Waters distributor.

1. Connect the female end of the power cord to the receptacle on the rear panel of the mass spectrometer.
2. Connect the male end of the mass spectrometer power cord to a suitable 200 to 240 V AC wall outlet.

C Materials of Construction and Compatible Solvents

To confirm the integrity of the source exhaust system, you must address any safety issues raised in this Appendix.

C.1 Preventing contamination

For information on preventing contamination, refer to *Controlling Contamination in UltraPerformance LC/MS and HPLC/MS Systems* (part number 715001307). You can find this document on www.waters.com; click **Services and Support** > **Support**.

C.2 Items exposed to solvent

The items that appear in the following table can be exposed to solvent. You must evaluate the safety issues if the solvents used in your application differ from the solvents typically used with these items. See Solvents used to prepare mobile phases for details about the most common ingredients used to prepare mobile phases.

Table C–1: Items exposed to solvent:

Item	Material
Autotune reservoirs	High-density polyethylene
Corona discharge pin mounting contact	PEEK
Gas exhaust port	Stainless steel
Ion block assembly	Stainless steel and PEEK
Ion block screws	Gold-plated stainless steel
Ion block support	PEEK
Isolation valve	Stainless steel and PEEK
O-rings	Viton or PTFE-encapsulated Viton
Probe adjuster bellows	Viton
Probe shaft	PEEK
Pumping block	Aluminium and Xylan

Table C–1: Items exposed to solvent: (continued)

Item	Material
Solvent waste/leak management	Tygon tubing 2375, polyurethane
Source enclosure	Aluminium
Source enclosure view port	Silica float glass
Trap bottle	Polypropylene
Trap bottle push-in fittings	Nitrile butadiene rubber, stainless steel, polybutylene terephthalate, and polyoxymethylene
APPI lamp drive assembly	
APPI lamp drive mounting shaft	Stainless steel
APPI lamp drive repeller electrode	Stainless steel
APPI lamp drive insulator	PEEK
APPI lamp window	Magnesium fluoride

C.3 Solvents used to prepare mobile phases

These solvents are the most common ingredients used to prepare mobile phases for reverse-phase LC/MS (API):

- Water
- Methanol
- Acetonitrile
- Formic acid (≤0.1%)
- Acetic acid (≤0.1%)
- Ammonium acetate (<50 mM)
- Ammonium formate (<50 mM)
- Trifluoroacetic acid (TFA) (<0.2%)
- Ammonium hydroxide (<1%)
- Ammonium bicarbonate (<50 mM)

These solvents are not expected to cause any problems with the materials identified in Items exposed to solvent.

Strong solvents used to prepare mobile phases for normal-phase LC/MS (for example, hexane or tetrahydrofuran (THF)) will adversely affect the performance of the materials shown in the table Items exposed to solvent and must not be used. You must evaluate the safety issues if these

solvents are used as additives to the mobile phases at reduced concentration, or as sample diluents.

D IntelliStart Fluidics System Plumbing

D.1 Preventing contamination

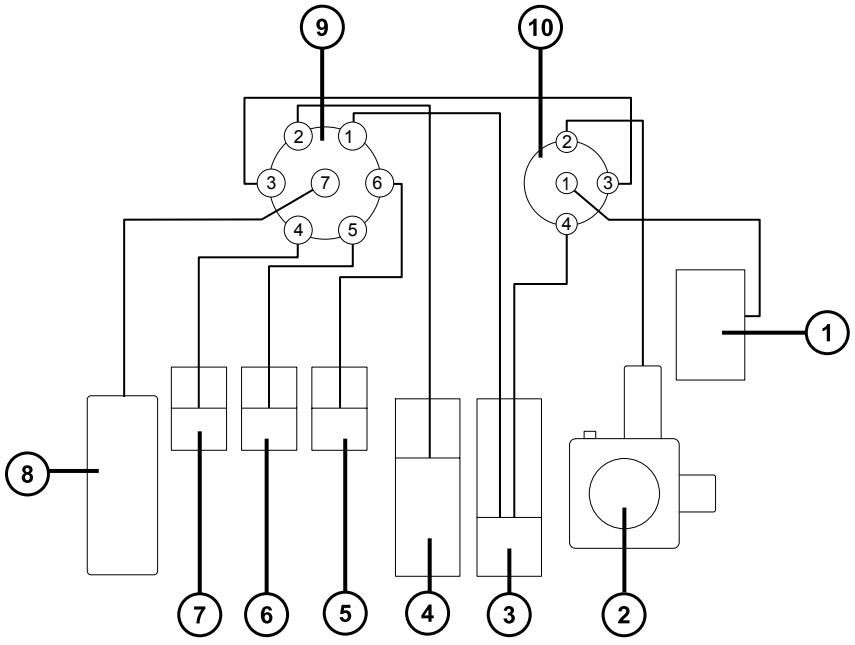
For information on preventing contamination, refer to *Controlling Contamination in UltraPerformance LC/MS and HPLC/MS Systems* (part number 715001307). You can find this document on www.waters.com; click **Services and Support** > **Support**.

D.2 Plumbing schematic

For further information, refer to the diagram on the inside of the fluidics valve access door (see Waters ACQUITY Xevo TQ-XS UPLC/MS system).

Requirement: Ensure that the end of the tubing is fully submerged in the solvent in the wash reservoir.

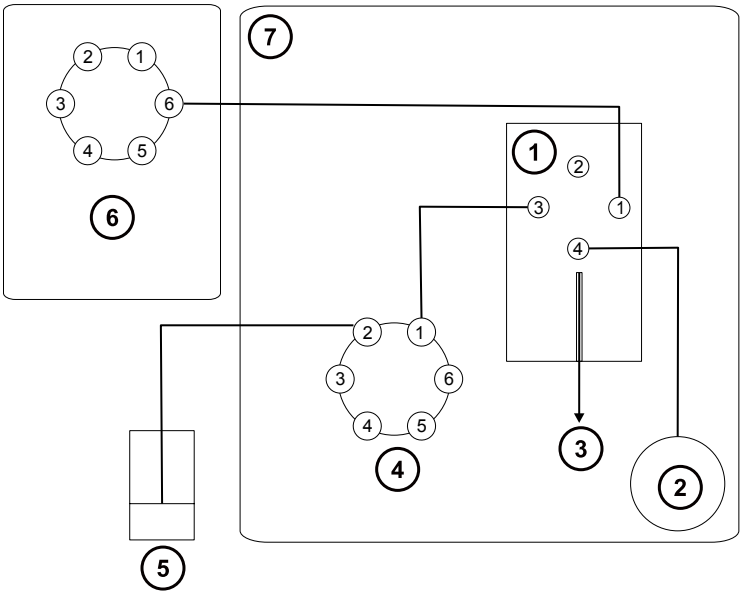
Figure D–1:



1. ACQUITY system
2. Source
3. Waste
4. Wash
5. Vial C
6. Vial B
7. Vial A
8. Analyte pump
9. Selector valve
10. Diverter valve

D.3 ionKey and TRIZAIC source plumbing

Figure D–2: ionKey and TRIZAIC source plumbing



1. TRIZAIC tile or iKey
2. Syringe
3. Emitter
4. HTM trap valve (TRIZAIC only)
5. Waste
6. nanoACQUITY UPLC SM, AQUITY UPLC M-class µSM, or trap device
7. ionKey or TRIZAIC source

D.4 Tubing specifications

The following table gives the internal diameter (ID), external diameter (ED), color, length, and quantity for the IntelliStart Fluidics tubing.

Table D–1: Replacement tubing specifications:

Connection	ID (inches)	ED (inches)	Color	Length (mm)	Quantity
Selector valve to diverter valve	0.005	1/16	Red	200	1
Vial	0.020	1/16	Orange	600	3
Wash	0.020	1/16	Orange	1000	1
Pump	0.040	1/16	Natural	500	1
Waste	0.040	1/16	Natural	1000	2