



# Agilent Triple Quadrupole LC/MS System

## User Guide



# Notices

## Document Identification

D0037077 Revision A.00  
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Agilent Technologies, Inc.  
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Santa Clara, CA 95051

## Software Revision

This guide is valid for MassHunter 12.1, until superseded.

## Instrument Manufacturing



Manufactured by Agilent  
Technologies Singapore Pte. Ltd.  
No. 1 Yishun Avenue 7, Singapore  
768923

## Operating Temperature

Operating Temperature: 15 °C to 35 °C  
Storage Temperature: -40 °C to 70 °C

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## Safety Notices

### CAUTION

A **CAUTION** notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in damage to the product or loss of important data. Do not proceed beyond a **CAUTION** notice until the indicated conditions are fully understood and met.

### WARNING

A **WARNING** notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in personal injury or death. Do not proceed beyond a **WARNING** notice until the indicated conditions are fully understood and met.

## In This Guide

This guide provides information on the Ultivo, 6475A, and 6495D LC/TQ systems running MassHunter Data Acquisition 12.1 or higher.

## Additional Resources

### User Documentation



Data analysis and library management documentation can be found by scanning the code or navigating to <https://aglt.co/DALibMgmtDocs>.



Instrument documentation, step by step videos, and more can be found by scanning the code or navigating to <https://aglt.co/LCMSUserDocs>.

### Agilent Triple Quadrupole LC/MS Supplies



Make sure that you don't run out of essential columns and supplies. Use this quick reference list to keep your shelves stocked by navigating to <https://aglt.co/LCTQSupplies>.

## Technical Support

To find your local sales and support contact, visit the following page:

<https://www.agilent.com/en/contact-us/page>

For technical support, visit the following page:

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<https://community.agilent.com/>

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## Sustainability Information

### Packaging End-of-Life

The Agilent Triple Quadrupole LC/MS system is packaged using cardboard, polyethylene foam, a polyethylene bag, and a wood pallet. In the US, cardboard is readily recyclable, and while plastic bags are recyclable, the infrastructure is not available in the majority of the market. In the US, Agilent is enrolled in the How2Recycle program (<https://how2recycle.info/>) to facilitate the communication of material recycling instructions. In select countries, Agilent participates in the EU/UK Green DOT Package Recycling Program to support the take-back and responsible management of the packaging materials at their end-of-life. In the remaining EU countries, the cardboard is readily recyclable and the plastic bag, foam and wood pallet are recycled, landfilled, or incinerated depending on the country and its available infrastructure.

### Product End-of-Life

Agilent offers a take-back program for its Triple Quadrupole LC/MS system customers in US, EU, and UK markets. Refer to <https://www.agilent.com/environment/product/index.shtml> for more information.

# Agilent Regulatory Compliance Statement

## CE Compliance



Your Agilent instrument has been designed to comply with the requirements of the applicable directives of the European Union, such as Electromagnetic Compatibility (EMC) Directive, Low Voltage Directive (LVD), Machinery Directive (MD), RoHS Directive, etc.

Agilent has confirmed that each product complies with the relevant Directives by testing samples against the harmonized EN (European Norm) standards published on the Official Journal of the European Union (OJEU).

Proof that a product complies with these directives is indicated by:

- the CE Marking appearing on the rear of the product, and
- the documentation package that accompanies the product containing a copy of the Declaration of Conformity. The Declaration of Conformity is the legal declaration by Agilent that the product complies with the relevant directives listed above, and shows the EN standards to which the product was tested to demonstrate compliance.

## UK Compliance



Your Agilent instrument has been designed to comply with the requirements of the applicable regulations of the United Kingdom, such as The Electromagnetic Compatibility Regulations 2016, The Electrical Equipment (Safety) Regulations 2016, The Supply of Machinery (Safety) Regulations 2008, The Restriction of the Use of Certain Hazardous Substances in Electrical and Electronic Equipment Regulations 2012, etc.


Agilent has confirmed that each product complies with the relevant Regulations by testing samples against the designated standards published on GOV.UK.

Proof that a product complies with these regulations is indicated by:

- the UKCA Marking appearing on the rear of the product, and
- the documentation package that accompanies the product containing a copy of the Declaration of Conformity. The Declaration of Conformity is the legal declaration by Agilent that the product complies with the relevant regulations listed above, and shows the designated standards to which the product was tested to demonstrate compliance.

## Electromagnetic Compatibility

This product conforms to the following regulations on Electromagnetic Compatibility (EMC) and Radio Frequency Interference (RFI):

- CISPR 11/EN 55011: Group 1, Class A
- EC/EN 61326-1
- AUS/NZ 
- Canada ICES-001 (This ISM device complies with Canadian ICES-001. Cet appareil ISM est conforme à la norme NMB-001 du Canada).

**Group 1 ISM equipment** Group 1 contains all Industrial, Scientific, and Medical (ISM) equipment in which there is intentionally generated and/or used conductively coupled radio- frequency energy which is necessary for the internal functioning of the equipment itself.

**Class A equipment** This equipment is suitable for use in all establishments other than domestic and those directly connected to a low voltage power supply network which supplies buildings used for domestic purposes.

This device complies with the requirements of CISPR11, Group 1, Class A as radiation professional equipment. Therefore, there may be potential difficulties in ensuring electromagnetic compatibility in other environments, due to conducted as well as radiated disturbances.

If this equipment does cause harmful interference to radio or television reception, which can be determined by turning the equipment off and on, the user is encouraged to try one or more of the following measures:

- 1 Relocate the radio or antenna.
- 2 Move the device away from the radio or television.
- 3 Plug the device into a different electrical outlet, so that the device and the radio or television are on separate electrical circuits.
- 4 Make sure that all peripheral devices are also certified.
- 5 Make sure that appropriate cables are used to connect the device to peripheral equipment.
- 6 Consult your equipment dealer, Agilent Technologies, or an experienced technician for assistance.

Changes or modifications not expressly approved by Agilent Technologies could void the user's authority to operate the equipment.

## EMC Declaration for South Korea

### 사용자안내문

This equipment has been evaluated for its suitability for use in a commercial environment. When used in a domestic environment, there is a risk of radio interference.

이 기기는 업무용 환경에서 사용할 목적으로 적합성평가를 받은 기기로서 가정용 환경

에서 사용하는 경우 전파간섭의 우려가 있습니다 .

※ 사용자 안내문은 " 업무용 방송통신기자재 " 에만 적용한다 .

## Detachable Power Cord Declaration for Japan

電源コードセットの取扱いについて（日本国内向け）

製品には、同梱された電源コードセットをお使いください。同梱された電源コードセット

は、他の製品では使用できません。

Notice - The power cords for Japanese market

Your product must only use the power cord that was shipped with this product. Do not use this power cord with any other product.

## Sound Emission Certification for Federal Republic of Germany

### Sound pressure

Sound pressure  $L_p < 70 \text{ dB(A)}$  according to DIN EN ISO 7779.

### Schalldruckpegel

Schalldruckpegel  $LP < 70 \text{ dB(A)}$  nach DIN EN ISO 7779.

## Waste Electrical and Electronic Equipment (WEEE) Directive

This product complies with the European WEEE Directive marking requirements. The affixed label indicates that you must not discard this electrical/electronic product in domestic household waste.

**NOTE**

Do not dispose of in domestic household waste.

To return unwanted products, contact your local Agilent office or refer to <https://www.agilent.com/environment/product/index.shtml> for more information.



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## Ultivo Triple Quadrupole LC/MS

### Front view



Figure 1. Front view of Ultivo

## Rear view

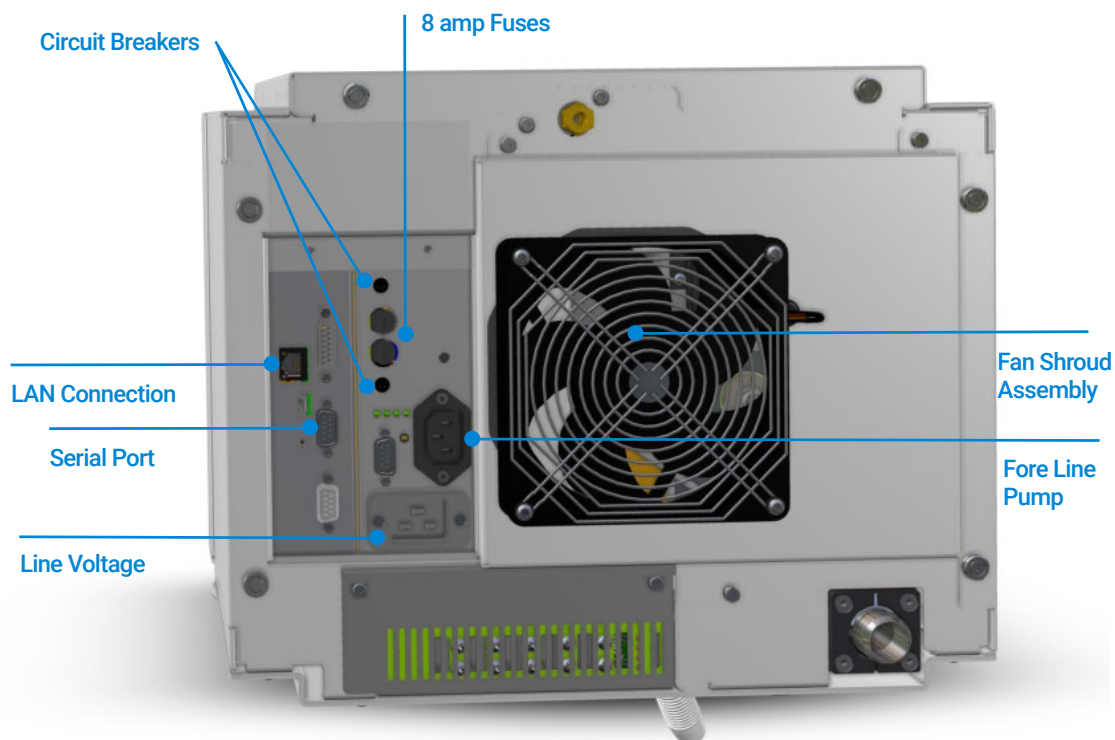
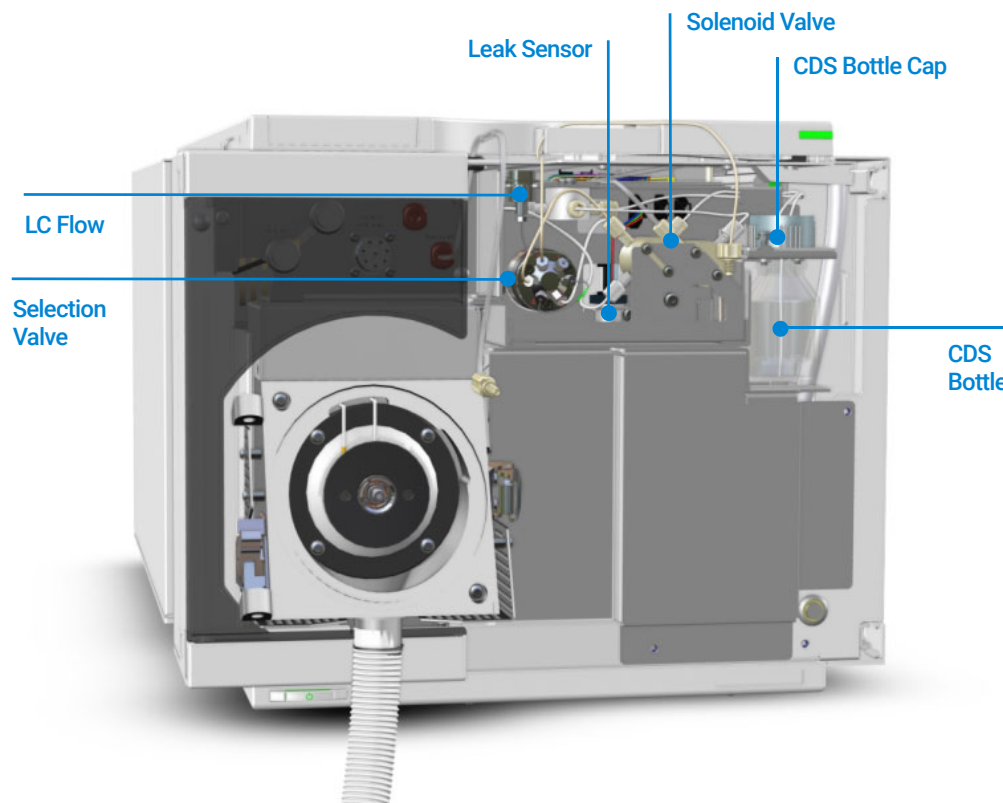


Figure 2. Rear view of Ultivo

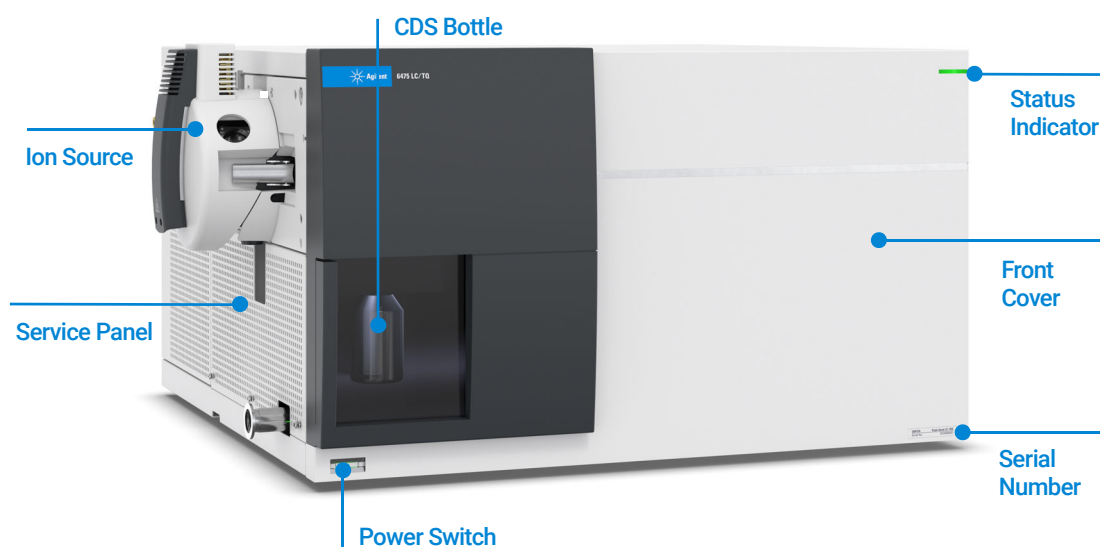
## Calibrant Delivery System



**Figure 3.** Calibrant Delivery System

## 6475A Triple Quadrupole LC/MS

### Front view



**Figure 4.** Front view of 6475A LC/TQ

## Side view

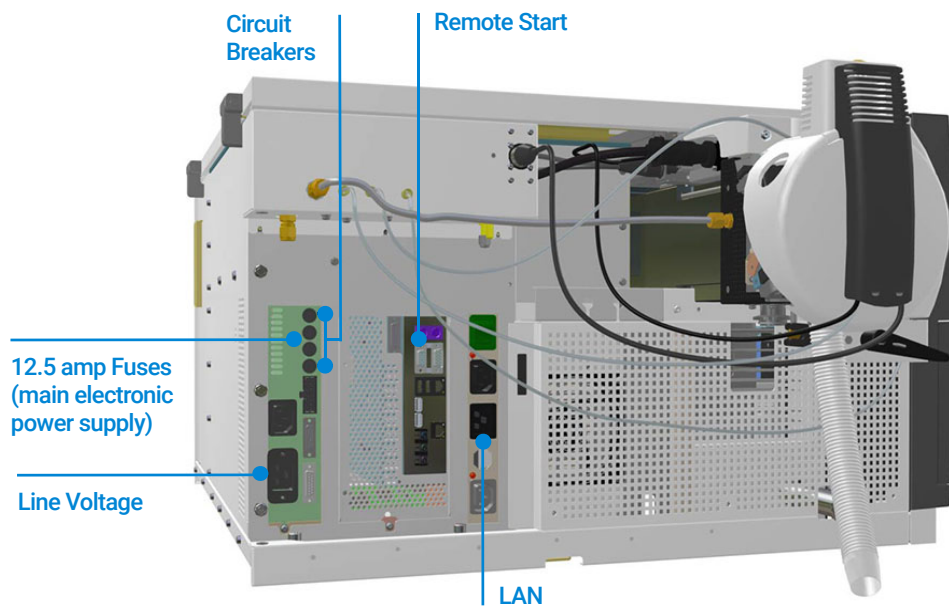
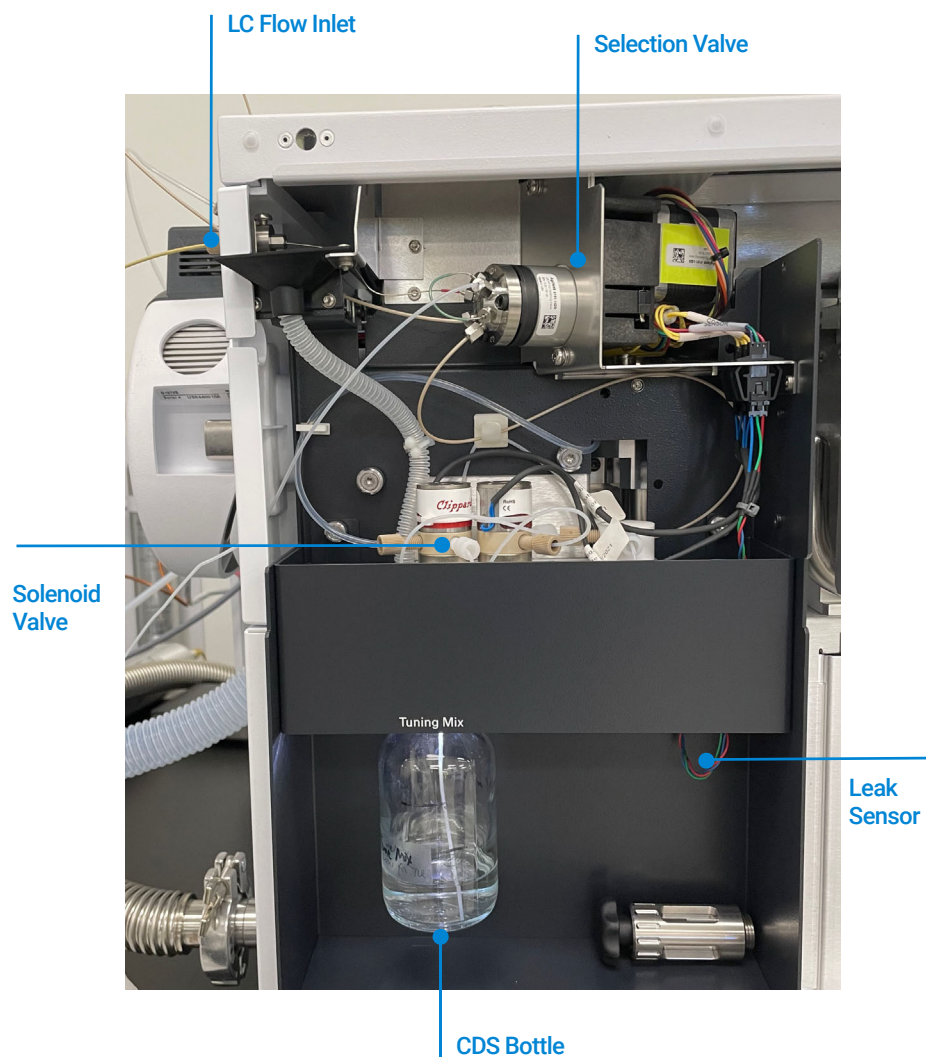


Figure 5. Side view of 6475A LC/TQ

## Calibrant Delivery System

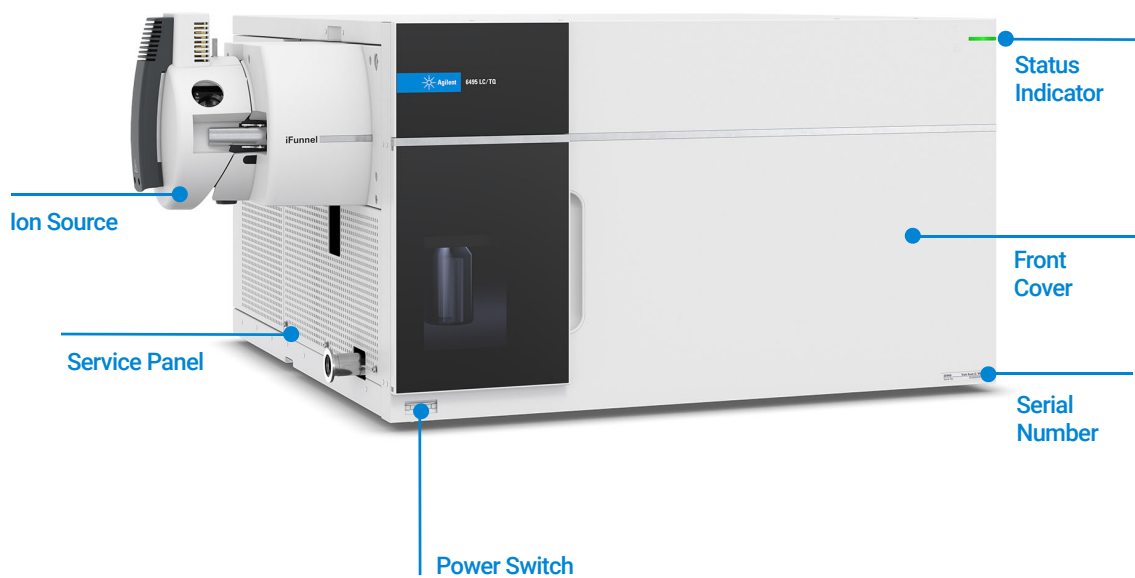


**Figure 6.** Calibrant delivery system



## 6495D Triple Quadrupole LC/MS

### Front view



**Figure 7.** Front view of 6495D LC/TQ

### Side view

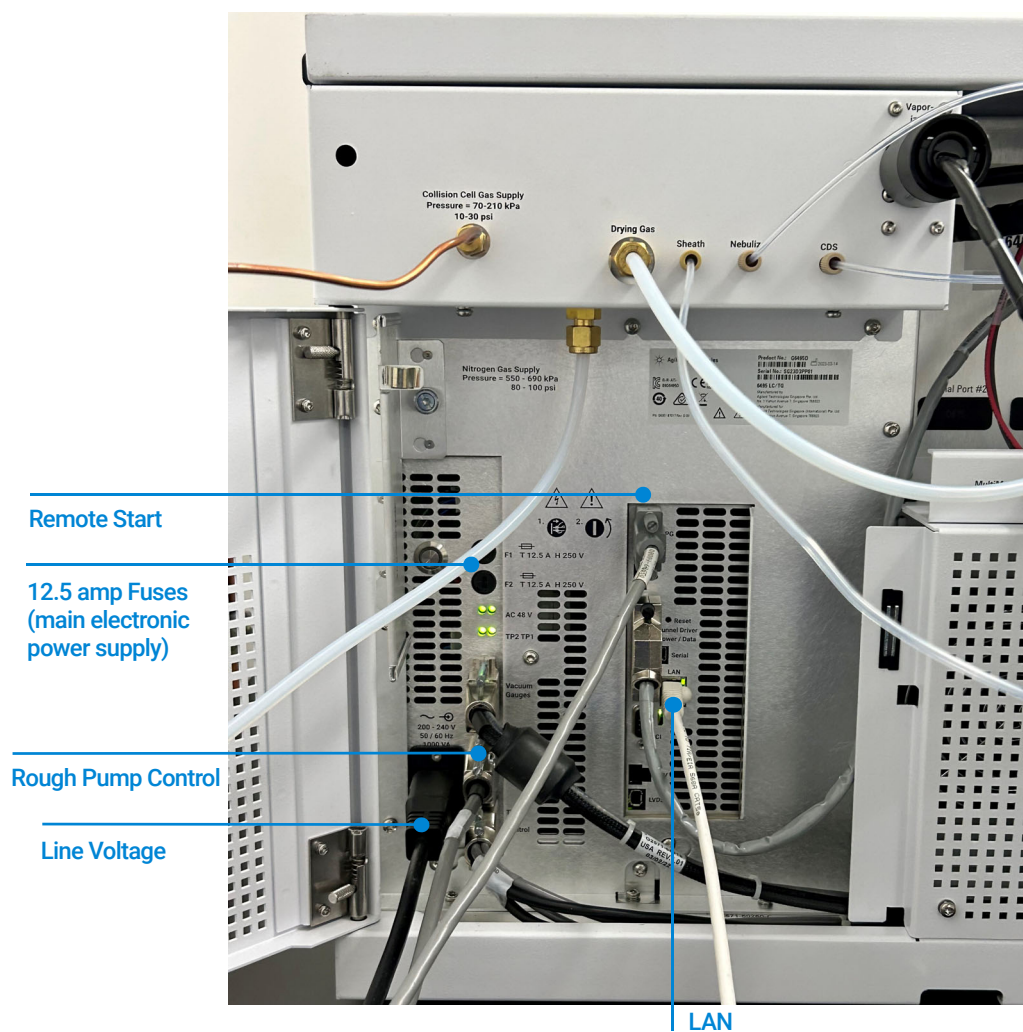


Figure 8. Side view of 6495D LC/TQ

## Calibrant Delivery System

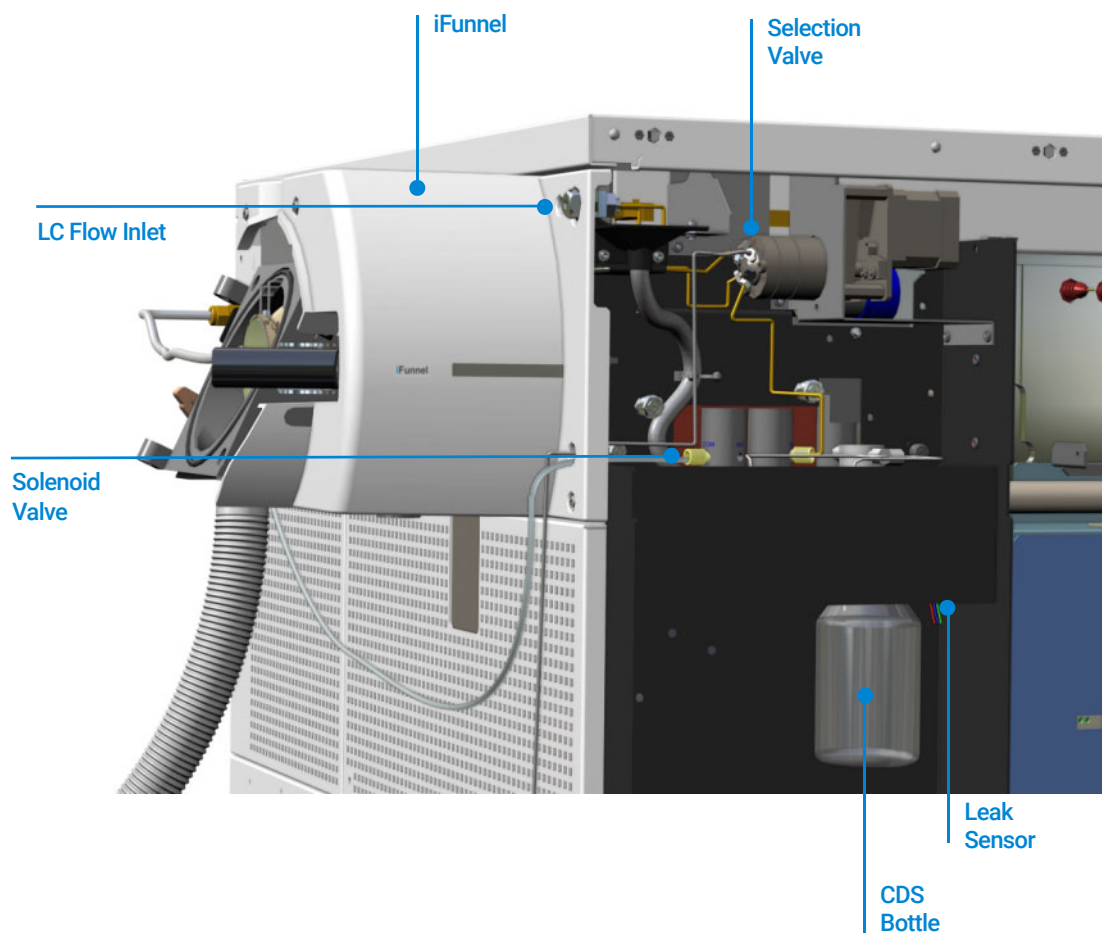


Figure 9. Calibrant delivery system

## Magnets

**CAUTION**

This product contains magnets that may affect the functioning of pacemakers, implanted heart defibrillators, or other active implanted medical devices (AIMD). Follow the AIMD manufacturer guidance when using the product.

### Door magnets

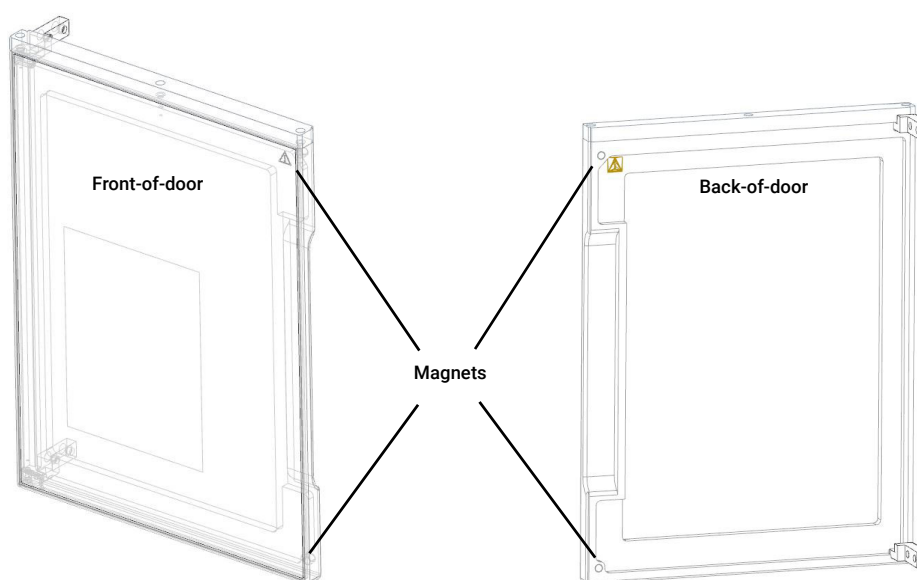


Figure 10. Magnet locations in door

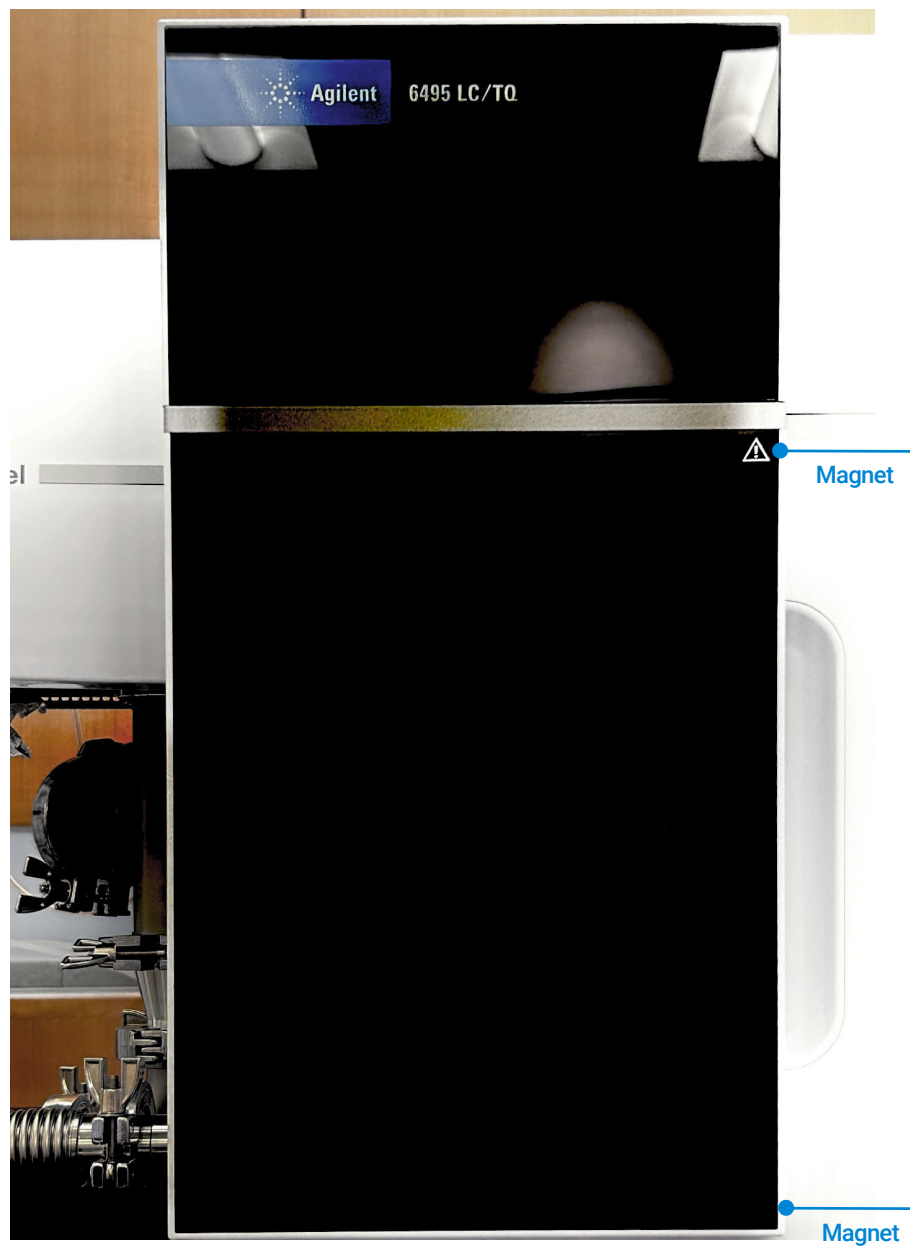
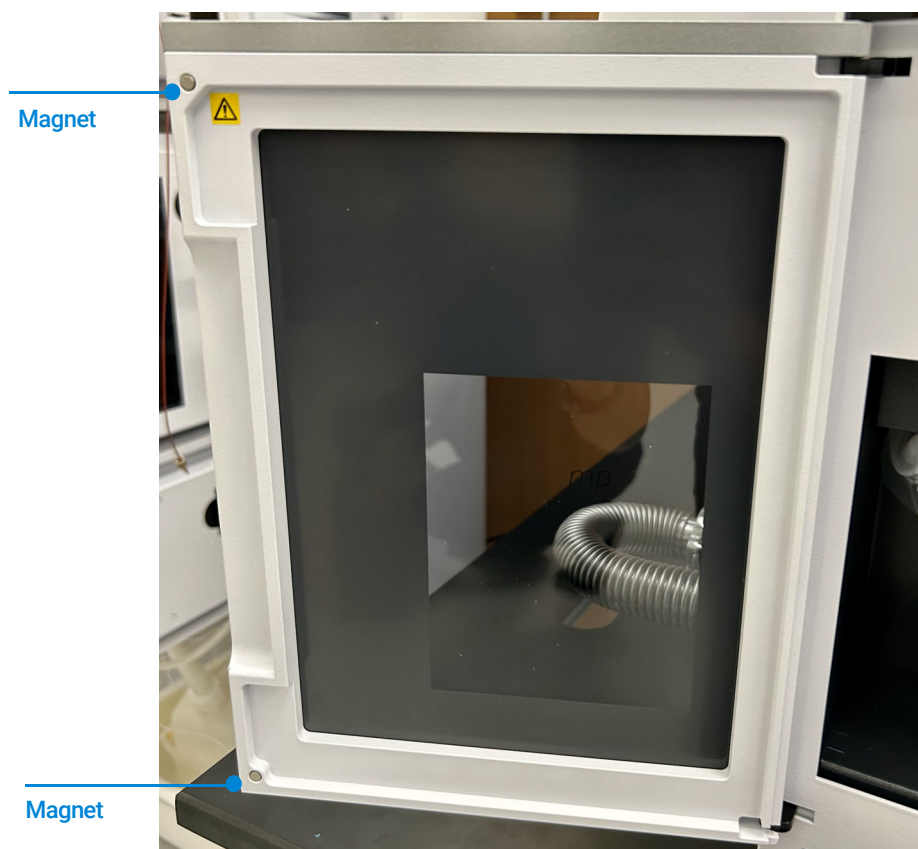


Figure 11. Front of door magnet locations



**Figure 12.** Back of door magnet locations

**Figure 13.**

## Instrument Status Indicator Lights

**Table 1** Status indicator lights on instrument

 <p>Instrument State = BOOTING (FPGA Loaded) Status LED = Blinking Yellow Power Switch LED = Yellow</p>	 <p>Instrument State = ACQUISITION Status LED = Blinking Green Power Switch LED = Green</p>
 <p>Instrument State = BOOTING (LINUX Loaded) Status LED = Yellow Power Switch LED = Green</p>	 <p>Instrument State = FAULT Status LED = Red Power Switch LED = Green</p>
 <p>Instrument State = PUMPING DOWN Status LED = Blinking Yellow Power Switch LED = Green</p>	 <p>Instrument State = VENTING Status LED = Blinking Red Power Switch LED = Yellow</p>
 <p>Instrument State = STANDBY Status LED = Yellow Power Switch LED = Green</p>	 <p>Instrument State = Vented Status LED = Red Power Switch LED = Yellow</p>
 <p>Instrument State = IDLE Status LED = Yellow Power Switch LED = Green</p>	 <p>Instrument State = POWERING DOWN Status LED = Off Power Switch LED = Blinking Yellow</p>
 <p>Instrument State = BACKGROUND SCAN Status LED = Green Power Switch LED = Green</p>	 <p>Instrument State = Off Status LED = Off Power Switch LED = Off</p>

## Instrument Status Indicators in Acquisition

In the MassHunter Data Acquisition program, the Instrument Status window indicates the state of the instrument.

■ Gray

- Offline: The instrument is configured with the system and available to use, but the workstation or client is not currently running. The amount of time for an instrument to reach the Idle state depends on each instrument.
- Disconnected: The connection to the instrument has been closed.

■ Yellow - Unknown: The device is in an unknown run state.

■ Light Orange - Not Ready: The instrument is connected but is not ready to run (due to not reaching the correct temperature or pressure required by the method, for example).

■ Green - Idle: The instrument is on and ready to process samples.

■ Teal - Standby: The instrument is in a standby/sleep state. Put the instrument in Standby mode when it is not in use or when changing the ion source. When the instrument is in Standby mode:

- The source interface is on, the drying gas remains heated, and nebulizer flows are maintained.
- The source and ion optics voltages are turned off, and the mass spectrometer is not sending spectra to the computer.
- For APCI and multimode sources: Vaporizer gas heaters are turned down.
- For the Agilent Jet Stream (AJS ESI) source: The sheath gas temperature, drying gas flow, and drying gas temperature are reduced.
- The spray chamber high voltages are turned off.
- The mass spectrometer stops generating spectra.

■ Magenta - Pre-run/Injecting: The instrument is on and is preparing to start acquisition.

■ Blue - Running, Post Run: The instrument is currently collecting data.

■ Orange - Tuning: The instrument is in the process of adjusting MS parameters.

■ Red - Instrument Error: The instrument has an error and cannot process samples.



## Ion Sources

### Electrospray Ionization (ESI) source

Electrospray relies in part on chemistry to generate analyte ions in solution before the analyte reaches the mass spectrometer. The LC eluent is sprayed (nebulized) into a chamber at atmospheric pressure in the presence of a strong electrostatic field and heated drying gas.

The electrostatic field causes further dissociation of the analyte molecules. The heated drying gas causes the solvent in the droplets to evaporate. As the droplets shrink, the charge concentration in the droplets increases. Eventually, the repulsive force between ions with like charges exceeds the cohesive forces and ions are ejected (desorbed) into the gas phase. These ions are attracted to and pass through a capillary sampling orifice into the mass analyzer.



**Figure 14.** ESI cover, ion source, and spray shield

## Agilent Jet Stream (AJS ESI) source

The Agilent Jet Stream (AJS ESI) source uses:

- the same ionization technique as the ESI source.
- thermal gradient focusing technology, which is a process in which super-heated nitrogen ( $N_2$ ) is used to improve ion generation and desolvation.
- improves sensitivity 5x or more for many small-molecule compounds that undergo electrospray ionization.



**Figure 15.** AJS ESI cover, ion source, and spray shield

## Atmospheric Pressure Chemical Ionization (APCI) source

In Atmospheric Pressure Chemical Ionization (APCI), the LC mobile phase is sprayed through a heated vaporizer (typically 250 °C to 400 °C) at atmospheric pressure. The heat vaporizes the liquid. The resulting gas-phase solvent molecules are ionized by electrons discharged from a corona needle.

The solvent ions then transfer charge to the analyte molecules through chemical reactions (chemical ionization). The analyte ions pass through a capillary sampling orifice into the mass analyzer. APCI is applicable to a wide range of polar and nonpolar molecules.

APCI rarely results in multiple charging, so APCI is typically used for molecules smaller than 1,500 u.

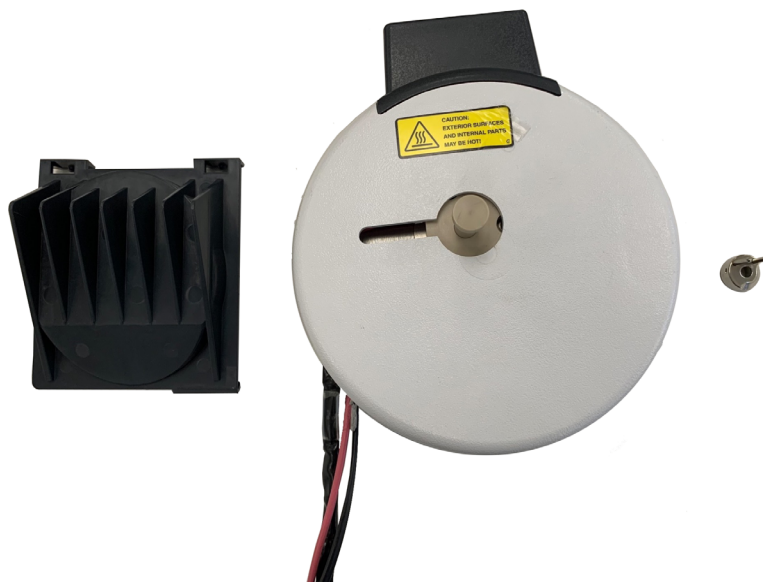
Because high temperatures are also involved, APCI is not appropriate for analysis of large biomolecules. APCI is used with normal-phase chromatography more often than electrospray is because the analytes are usually nonpolar.



Figure 16. APCI cover, ion source, and spray shield

## Multimode Ionization (MMI) source

The Multimode source for LC/MS can simultaneously do ESI and APCI ionization. The Multimode source can operate in ESI mode only, in APCI mode only, or in mixed ESI/APCI mode. This technology significantly improves the speed, accuracy, and productivity of high-throughput screening in drug discovery and other research applications.

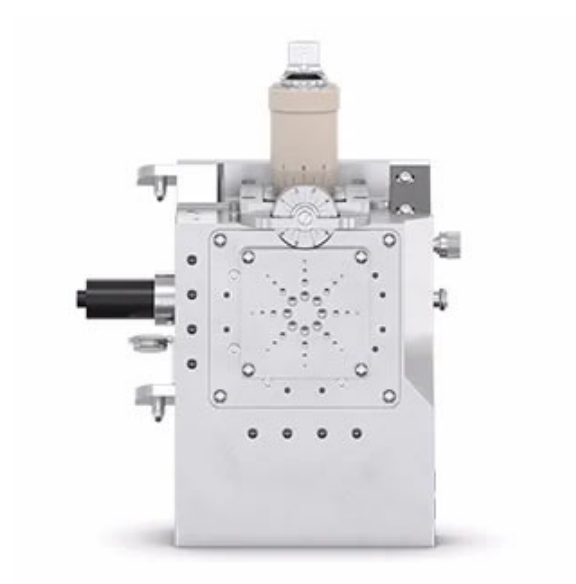


**Figure 17.** MMI cover, ion source, and spray shield

Simultaneous ESI and APCI capability and high LC flow rate compatibility (up to 2 mL/min) means more compounds can be detected in less time with the Agilent Multimode source.

## Nanospray ESI source

The Agilent nanospray ESI source is a flexible solution for laboratories running low-flow LC/MS applications. The nanospray source allows both commercially available and custom nanoflow columns to be used with Agilent LC/MS systems.



**Figure 18.** Nanospray ESI source

## 3

## Tuning

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## About Tuning

When the MS is used as a detector for a liquid chromatograph, a mass spectrum is associated with each data point in the chromatogram. To obtain high quality, accurate mass spectra, the MS must be optimized to:

- Maximize sensitivity
- Maintain acceptable resolution
- Ensure accurate mass assignments.

Tuning is the process of adjusting MS parameters to achieve these goals.

Tuning is primarily concerned with finding the correct settings for the parameters that control the transmission, filtering, and detection of ions. It is accomplished by introducing a calibrant into the LC/MS and generating ions. Using these ions, the tune parameters are then adjusted to achieve sensitivity, resolution, and mass assignment goals. With a few exceptions, the parameters that control ion formation are not adjusted. They are set to fixed values known to be good for generating ions from the calibrant solution.

There are three different types of tunes that can be performed on your instrument, autotune, checktune, and diagnostic tune. All tunes, except for the diagnostic tune, can be scheduled to maximize instrument uptime.

## Autotune and checktune

A checktune is used to determine if the tuning mix ion masses are properly assigned and if the response or sensitivity of these ions is within expectations. In other words, a checktune verifies peak width and mass axis to make sure they are correct before starting a data acquisition. See **“Calibrating the LC/TQ (Checktune)”** on page 44.

An autotune only needs to run after preventative maintenance or if there is a problem with checktune. Everything is automatic since the tuning mix is delivered by the calibrant delivery system, which is switched on automatically during the tune. See **“Calibrating the LC/TQ (Autotune)”** on page 48.

Use **Table 2** to select the correct tuning mix for the source installed.

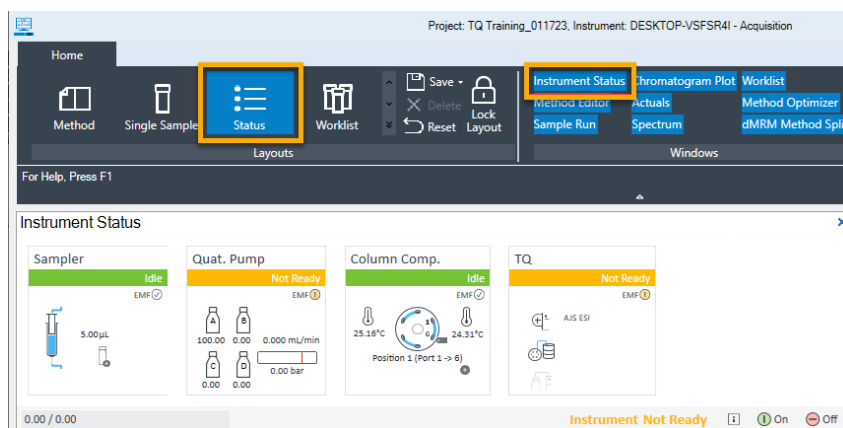
**Table 2** Tuning mixes

Source	Tuning mix	Part Number
ESI	ESI-L Low Concentration Tuning Mix	G1969-85000
AJS ESI	ESI-L Low Concentration Tuning Mix	G1969-85000
MMI	MMI-L Low Concentration Tuning Mix	G1969-85020
APCI	APCI-L Low Concentration Tuning Mix	G1969-85010

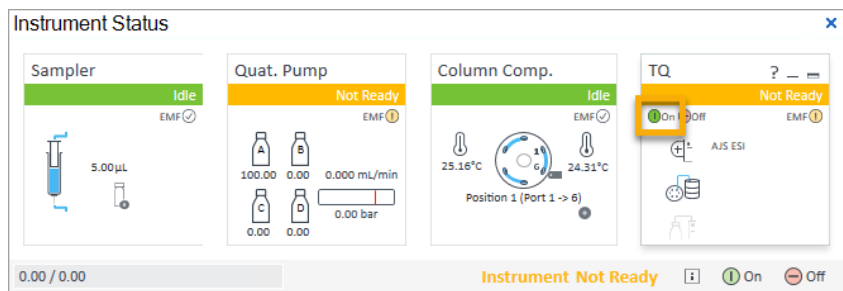


## Starting the Instrument

- 1 Follow the procedures in **“Starting Up and Shutting Down the Instrument”** on page 61 to begin operation of the instrument.
- 2 Display the Instrument Status window if it is not visible in the Mass Hunter Data Acquisition program, in one of the following ways:
  - Open the Status layout.
  - On the ribbon, click **Instrument Status** in the **Windows** section.



- 3 Hover over the TQ device pane and click **On**.




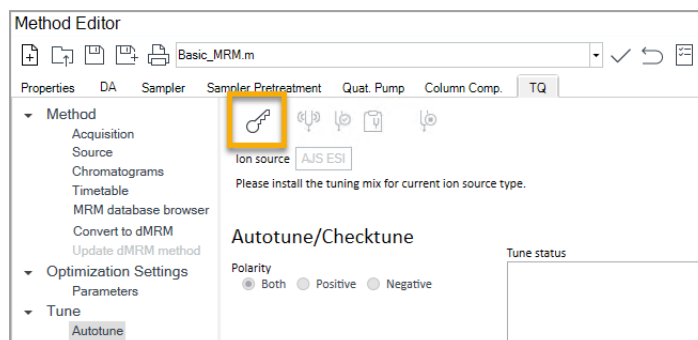
- 4 Monitor baseline and adjust plot if necessary. See **“Monitoring baseline and adjusting plot”** on page 66.

## Calibrating the LC/TQ (Checktune)




### 6475A and Ultivo

A checktune can be run with the following ion sources: ESI, AJS ESI, MMI, and APCI.

- 1 In the Method Editor window, click the **TQ** tab.
- 2 Click **Tune > Autotune** in the left pane.
- 3 Click  **Request tune control**.



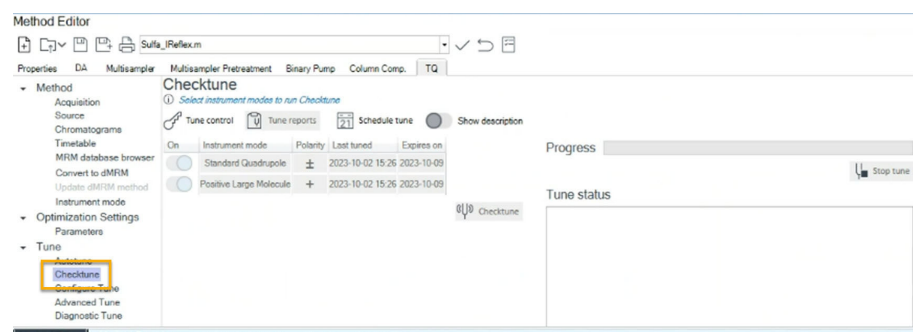
This button locks control of the TQ instrument. When tune has control of the TQ instrument, a single sample run or a worklist cannot be started and the method editor is locked.

- 4 Select a polarity.
  - If **Both** is selected, the system will automatically run in the positive mode followed by the negative mode.
- 5 Click  **Checktune instrument**.
  - When clicked, tune setpoints are applied. If an action is not selected within the timeout period, the system will go back to the method setpoints.
  - To stop the tune during operation, click .
- 6 When the tune completes, review the report(s).
- 7 Click  **Release tune control** to release control of the TQ instrument.

## 6495D

A checktune can be run with the following ion sources: ESI, AJS ESI, MMI, and APCI.

- 1 In the Method Editor window, click the **TQ** tab.
- 2 Click **Tune > Checktune** in the left pane.



This button locks control of the TQ instrument. When tune has control of the TQ instrument, a single sample run or a worklist cannot be started and the method editor is locked.

- 3 Click **Tune control**.
- 4 Select an appropriate Instrument mode slider.

On	Instrument mode	Polarity	Last tuned	Expires on
<input checked="" type="radio"/>	Standard Quadrupole	+	2023-10-02 15:26	2023-10-09
<input type="radio"/>	Positive Large Molecule	+	2023-10-02 15:26	2023-10-09

## NOTE


The polarity is chosen for this instrument using the functionality "**Configure Tune (6495D only)**" on page 46.

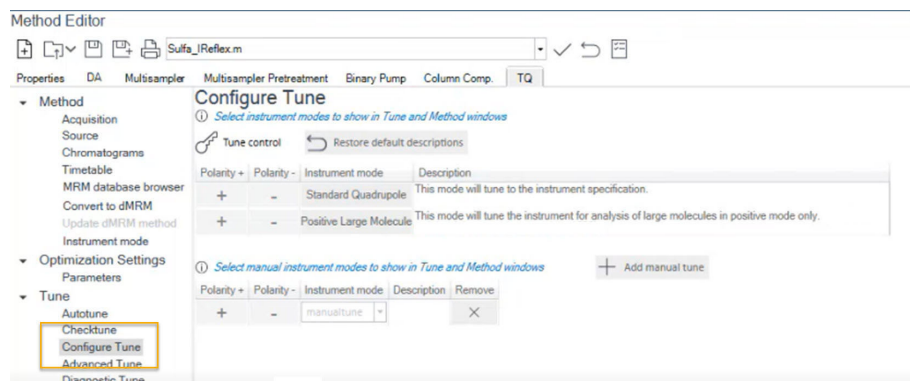
- 5 Click **Checktune**. When clicked, tune setpoints are applied. If an action is not selected within the timeout period, the system will go back to the method setpoints.
  - a To stop the tune during operation, click .
- 6 When the tune completes, review the report(s).
- 7 Click **Tune control** to release control of the TQ instrument.

## Configure Tune (6495D only)


Configure Tune is used to select standard instrument modes and polarity to show in Tune and the method editor and add a description for each instrument mode. Note: Standard Quadrupole Instrument mode must be enabled in at least one polarity.

Manual Instrument Modes, created via Advanced Tune, may be selected through Add Manual Tune and can be configured for polarity, and have a description for each manual Instrument Mode. Up to ten manual Instrument Modes may be configured. Manual Instrument modes cannot have a checktune or autotune run against them.

- 1 In the Method Editor window, click the **TQ** tab.
- 2 Click **Tune > Configure Tune** in the left pane.
- 3 Click  **Tune control**.



This button locks control of the TQ instrument and must be selected to select configuration settings.

- 4 All standard instrument modes are listed in the tune table. Adjust the Polarity+ and Polarity- options as needed by clicking **+** or **-**.
- 5 Click the Description cell to edit the description as needed.
- 6 Click  **Tune control** to release control of the TQ instrument and apply the new configuration to the Instrument modes.

### Tuning

#### Configure Tune (6495D only)


#### NOTE

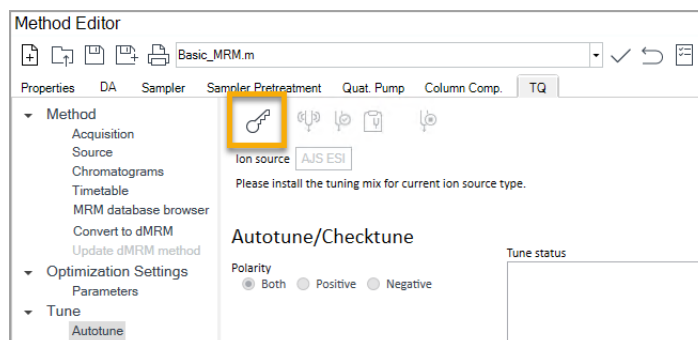
To use manual instrument modes, permissions must be configured for the user profile. This application can only be accessed with specified user permissions. Access to the Manual Tune privilege must be enabled in OLCP to access BOTH Configure Tune and Advanced Tune. See the OpenLab Control Panel Help for more information on setting permissions.

## Calibrating the LC/TQ (Autotune)

### 6475A and Ultivo




An autotune can be run with the following ion sources: ESI, AJS ESI, MMI, and APCI.

- 1 In the Method Editor window, click the **TQ** tab.
- 2 Click **Tune > Autotune** in the left pane.
- 3 Click  **Request tune control**.




This button locks control of the LC/TQ instrument. When tune has control of the LC/TQ instrument, a single sample run or a worklist cannot be started.

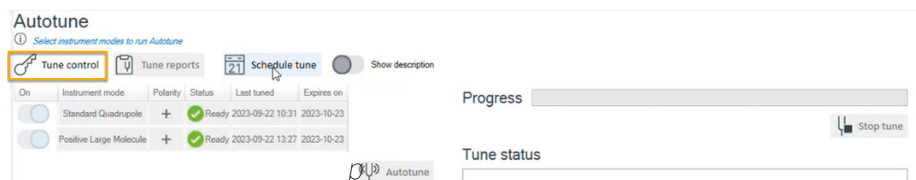
When clicked, tune setpoints are applied. If an action is not selected within the timeout period, the system will go back to the method setpoints.

- 4 Select a polarity.
  - If only **Positive** or **Negative** polarity is selected, subsequent acquisition methods are only available with that polarity.
  - If **Both** is selected, the system will automatically run in the positive mode followed by the negative mode.
- 5 Click  **Autotune the instrument**.
  - a To stop the tune during operation, click .
- 6 When the tune completes, review the report(s).
- 7 Click  **Release tune control** to release control of the LC/TQ instrument.

## 6495D

An autotune can be run with the following ion sources: ESI, AJS ESI, MMI, and APCI.

- 1 In the Method Editor window, click the **TQ** tab.
- 2 Click **Tune > Autotune** in the left pane.
- 3 Click  **Tune control**.



This button locks control of the LC/TQ instrument. When tune has control of the LC/TQ instrument, a single sample run or a worklist cannot be started.




When clicked, tune setpoints are applied. If an action is not selected within the timeout period, the system will go back to the method setpoints.

- 4 Select an appropriate Instrument mode slider.

On	Instrument mode	Polarity	Last tuned	Expires on
<input checked="" type="radio"/>	Standard Quadrupole	+	2023-10-02 15:26	2023-10-09
<input checked="" type="radio"/>	Positive Large Molecule	+	2023-10-02 15:26	2023-10-09

### NOTE


The polarity is chosen for this instrument using the functionality "**Configure Tune (6495D only)**" on page 46.

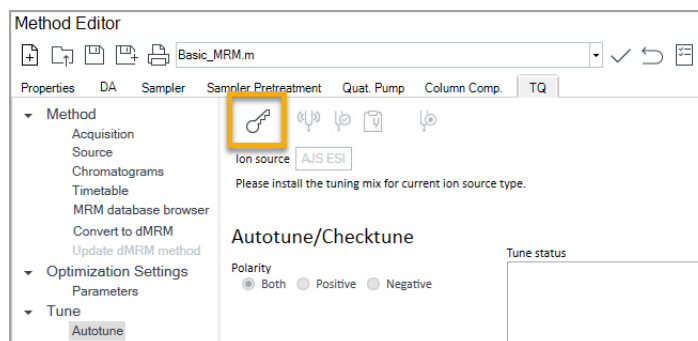
- 5 Click  **Autotune**. When clicked, tune setpoints are applied. If an action is not selected within the timeout period, the system will go back to the method setpoints.
  - a To stop the tune during operation, click .
- 6 When the tune completes, review the report(s).
- 7 Click  **Tune control** to release control of the TQ instrument.

## Generating a Detailed Tune Report



### 6475A and Ultivo

A detailed tune report can be generated after autotune or checktune has run. Only the latest tune report will generate a detailed report; e.g. if the last tune run was a checktune, then only a detailed checktune report will be generated.

- 1 In the Method Editor window, click the **TQ** tab.
- 2 Click **Tune > Autotune** in the left pane.
- 3 Click  **Request tune control**.





This button locks control of the TQ instrument. When tune has control of the LC/TQ instrument, a single sample run or a worklist cannot be started.

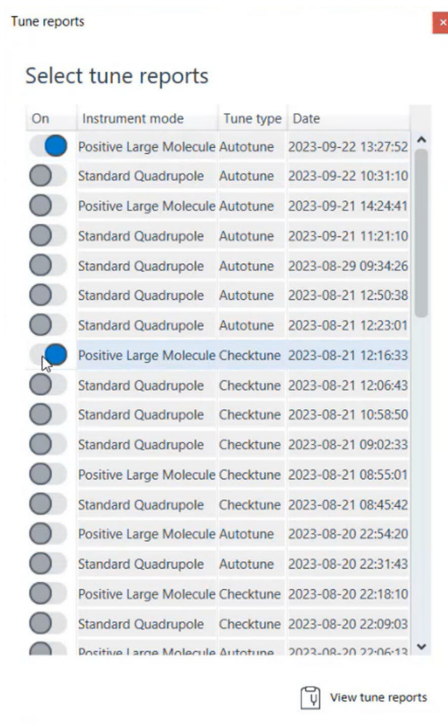
- 4 Click  **Generate Detailed Tune Report**. If this button is not available, then run either a checktune or an autotune.
- 5 Click  **Release tune control** in the toolbar to release control of the TQ instrument.



## 6495D

A detailed tune report can be generated after autotune or checktune has run.

- 1 In the Method Editor window, click the **TQ** tab.
- 2 Select **Tune > Autotune** or **Tune > Checktune** in the left pane.
- 3 Click  **Tune control** in the toolbar to lock control of the instrument..
- 4 Click  **Tune reports**. The tune reports window opens.
  - If no reports are available, then run either a checktune or an autotune.
- 5 Use the toggles to select reports for viewing.

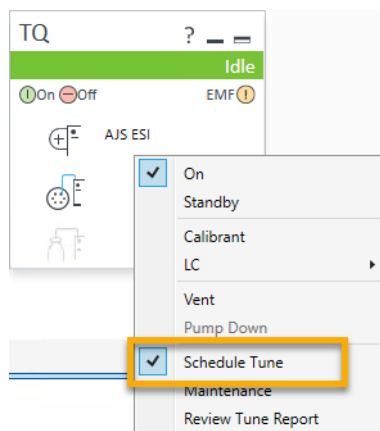


- 6 Click  **View tune reports** generate PDFs for viewing in a PDF viewer.

## Scheduling a Checktune


Automatically set the instrument to periodically produce checktune reports at specified intervals.

- 1 In the Instrument Status window, right-click the TQ device.
- 2 Click **Schedule Tune**.



The **Schedule Tune** dialog box opens.

**NOTE**

For the 6495D, access to Schedule Tune is also available within **Method Editor > Tune > Autotune** or **Checktune** and clicking  **Schedule Tune**.

## Tuning

### Scheduling a Checktune

- 3 Select **Checktune** in the left pane.

The right pane shows the information for scheduling a checktune.

#### NOTE

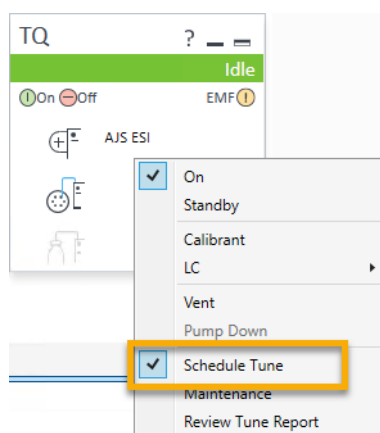
The polarity is chosen for this instrument using the functionality “**Configure Tune (6495D only)**” on page 46.

- 4 Click the **Scheduling** slider to switch **Scheduling** on.
- 5 Select either **Weekly** or **Monthly**.
- 6 Select other options to indicate how often to schedule the checktune.
- 7 Click **Save**.

## Scheduling an Autotune


To specify to run an autotune automatically:

- 1 In the Instrument Status window, right-click the TQ device.
- 2 Click **Schedule Tune**.

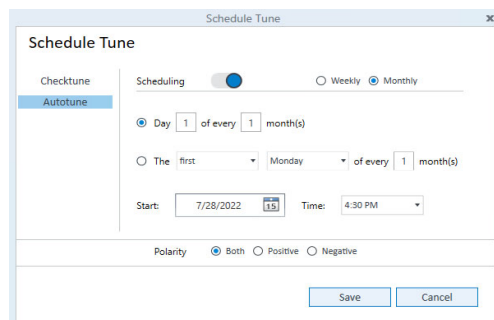


The Schedule Tune dialog box opens.

### NOTE

For the 6495D, access to Schedule Tune is also available within **Method Editor > Tune > Autotune** or **Checktune** and clicking  **Schedule Tune**.

- 3 Select **Autotune** in the left pane. The right pane shows the information for scheduling an autotune.



**NOTE**

The polarity is chosen for this instrument using the functionality "**Configure Tune (6495D only)**" on page 46.

- 4 Click the Scheduling slider to switch Scheduling on.
- 5 Select either **Weekly** or **Monthly**.
- 6 Select other options to indicate how often to schedule the autotune.
- 7 Click **Save**.

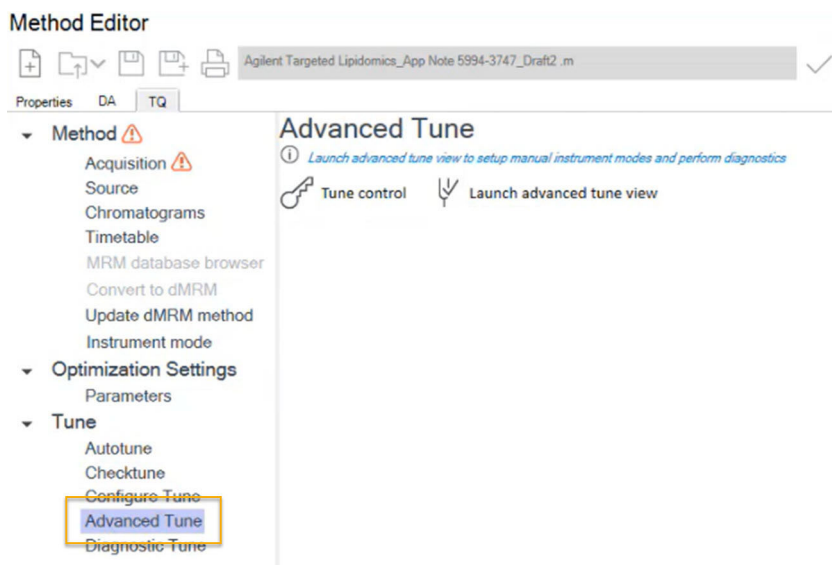
## Advanced Tune (6495D only)



In the Advanced Tune section, launch the advanced tune view to perform a manual tune.

### NOTE

This application can only be accessed with specified user permissions. Access to the Manual Tune privilege must be enabled in OLCP to access BOTH Configure Tune and Advanced Tune. See the OpenLab Control Panel Help for more information on setting permissions.

- 1 In the Method Editor window, click the **TQ** tab.
- 2 Click **Tune > Advanced tune** in the left pane.



- 3 Click  **Tune control** in the toolbar to lock control of the instrument.
- 4 Click  **Launch advanced tune view** to open the Manual Tune View window. The Advanced Tune program opens separate from MassHunter.

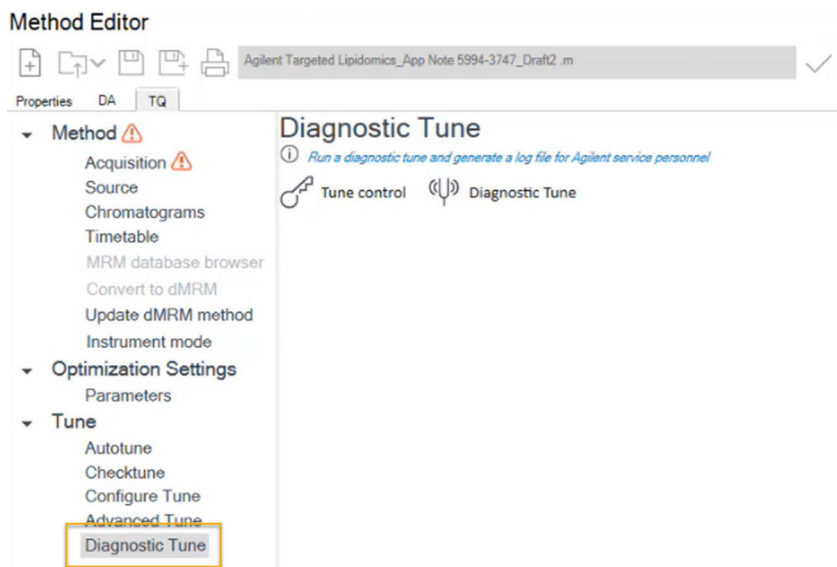
## Diagnostic Tune (6495D only)



In the Diagnostic Tune section, execute a Diagnostic Tune to produce a log file called TCDBackup.zip, which can be sent to Agilent service personnel. It is created and retrieved from the OpenLab Control Panel in the Logs section under **Administration > Diagnostics**.

### NOTE

A diagnostic tune should only be performed when the autotune has failed. Ensure sufficient tune solution in CDS bottle before starting. During normal operation, a diagnostic tune will last approximately 3 hours.

- 1 In the Method Editor window, click the **TQ** tab.
- 2 Click **Tune > Diagnostic tune** in the left pane.



- 3 Click  **Tune control** in the toolbar to lock control of the instrument.
- 4 Click  **Diagnostic Tune** to open the Manual Tune View window. The Advanced Tune program opens separate from MassHunter.

## 4

## Basic Operation

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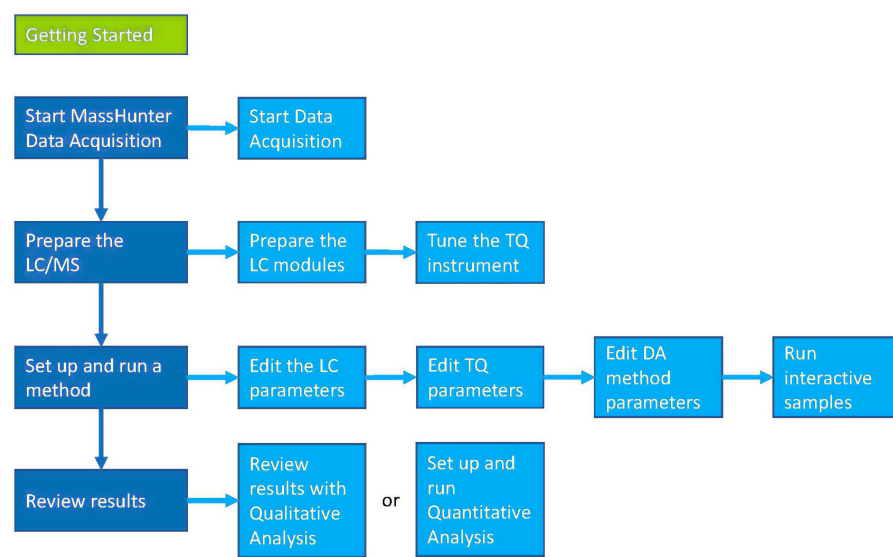
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## Overview

The roadmap below shows the steps to set up and run a batch of samples from start to finish. Follow the instructions in this section to get started and review guiding information for each step.



## Starting Up and Shutting Down the Instrument

### Starting in Standby mode

- 1 Check that nitrogen gas for the drying gas and for the collision cell are turned on.
- 2 Turn on the power for the computer and monitor.
- 3 Check that the instrument and rough pump are plugged into a power outlet.
- 4 Press the front power switch on the instrument.

The vacuum system automatically starts to pump down the instrument, and the electronics are turned on. The system card boots up and the firmware starts.

### Turning off the instrument

Before turning off the instrument, complete any data acquisition steps and save your data.

#### CAUTION

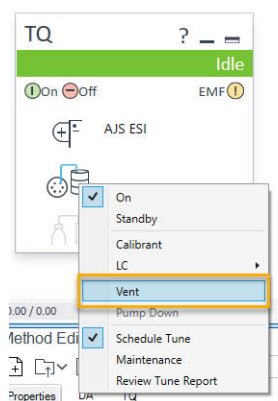
**To prevent instrument damage, always vent the system before pressing the power button.**

#### WARNING

**Do not touch the spray shield and related spray chamber components. They are likely to be hot.**

- 1 Turn off the solvent flow.  
If there is any analyte in any of the components in the sample delivery system, flush the delivery system with pure solvent before continuing.
- 2 Check that the ballast valve on the rough pump is closed (if applicable).

- 3 In MassHunter Data Acquisition, right-click the TQ icon in the Instrument Status window and select **Vent** to vent the system. Click **Yes** to continue.



When venting the system, the following occurs:

- The spray chamber high voltages, the drying gas heater, the quad heaters, the collision cell gas, the nebulization flow, the detector, and other lens voltages are turned off.
  - The drying gas flow is set to Standby.
  - If the APCI source is installed, the vaporizer heater is also turned off.
  - If the installed source is an Agilent Jet Stream source, the sheath gas heater is also turned off.
  - The rough pump turns off when the turbo speed is below a certain threshold.
- 4 Wait until the instrument completely vents.
  - 5 Close the MassHunter Data Acquisition program and shut down the computer.
  - 6 Press the power switch located in the lower left front corner of the instrument.
  - 7 Unplug the main power cable behind the service panel.
    - This action prevents the turbo pump components from overheating.

## Starting the MassHunter Data Acquisition Software

The instructions below include the following assumptions:

- The hardware and software are installed.
- The instrument is configured. For information on configuring your instrument, refer to the MassHunter Control Panel online help.
- The LC modules and the Triple Quad LC/MS are turned on, but the LC pump is not running.

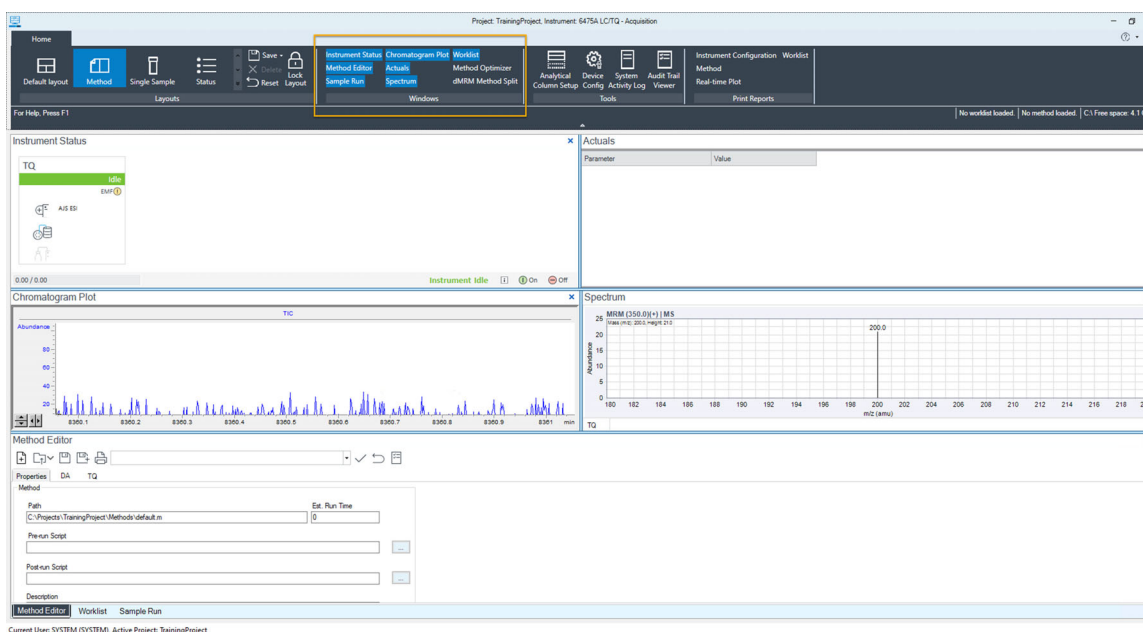
After installation, all the Agilent MassHunter Workstation Software icons appear on the desktop.

To start the MassHunter Data Acquisition program,

- 1 Double-click the **Control Panel** icon on the desktop, or select **Windows Start > Agilent Technologies > Control Panel**.
- 2 In Control Panel, select an instrument and click **Launch** to open the project in Acquisition. For more information, refer to the MassHunter Control Panel online help or the Introduction Workbook.

## MassHunter Data Acquisition windows

When the MassHunter Data Acquisition program opens, the main window appears. These windows provide the tools to set up acquisition methods, run samples interactively or automatically, monitor instrument status, monitor runs, and tune the instrument.



### Showing and hiding the windows

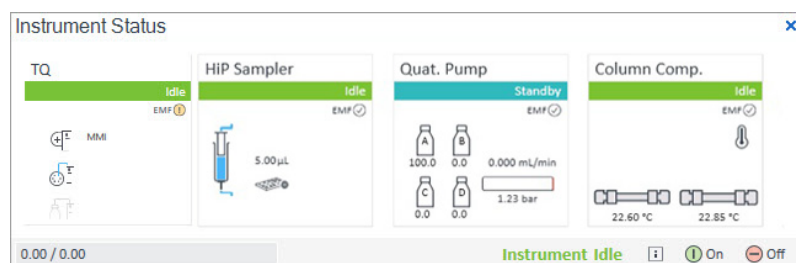
To show or hide a window, click the window name in the Windows group of the ribbon. Or, hide a window by clicking the **X** icon in the upper right corner of the window. At least one window must be shown.

Click in a window and press **F1** to obtain help on the active window. Drag a window border to resize the window. Double-clicking the title of the window, the window “floats” outside of the main window. Double-click the title bar again to “dock” the window.

## Instrument Status window

This window displays the status of each device configured with the instrument: **Error**, **Not ready**, **Pre-run**, **Post-run**, **Running**, **Injecting**, **Idle**, **Offline**, or **Standby**. You also set non-method control and configuration parameters for the LC devices and the MS instrument.

This window displays the current status of each device both as text and by its color-coding. See [“Instrument Status Indicators in Acquisition”](#) on page 34.



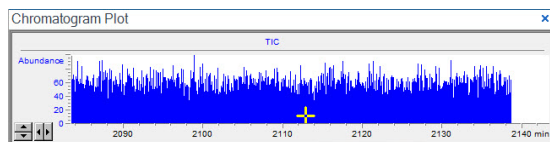
## Actuals window

This window displays the current value of selected instrument parameters. See [“Set up to view real-time parameter values \(actuals\).”](#) on page 71 for more information.

Parameter	Value
TQ: Not Ready Text	
TQ: Run State	Idle
TQ: High Vac	7.63E-6 Torr
TQ: Gas Temperature	325 °C
TQ: Rough Vac	1.00E+1 Torr
TQ: Turbo1 Speed	100.0 %
TQ: Firmware Version	8.1.4
TQ: Pump1 Current	3.000 A
TQ: Instrument State	BackgroundAcq

## Chromatogram Plot window

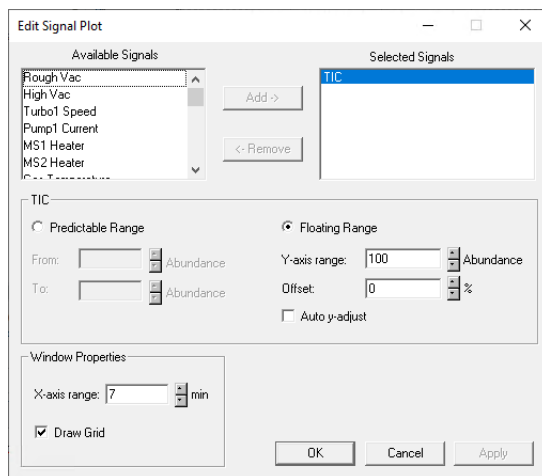
This window displays the chromatogram plots in real time. These plots can be user-defined signals and/or instrument parameters.



### Monitoring baseline and adjusting plot

The **Edit Signal Plot** dialog allows the selection of various instrument parameters and signals for display in the Chromatogram Plot window. The signals and their display characteristics can be adjusted as described in this section. The customizations made to the plot remain, even when the Acquisition software is closed and reopened.

- 1 In the Chromatogram Plot window, right-click the Chromatogram Plot window, and select **Change**. The **Edit Signal Plot** dialog box opens.



- 2 Select the signal to monitor and set the X and Y range for the plot.



## Basic Operation

### Spectrum window

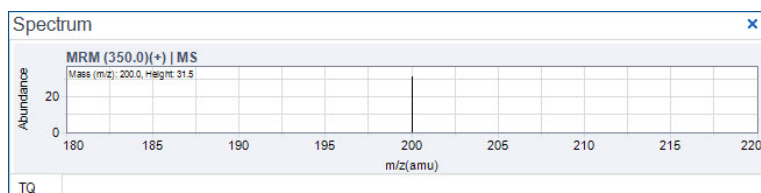
#### NOTE

To add other MS signals, such as EICs, setpoints, and actuals, select these on the **TQ** tab in the Method Editor window.

- Click **OK** to close the **Edit Signal Plot** dialog box.

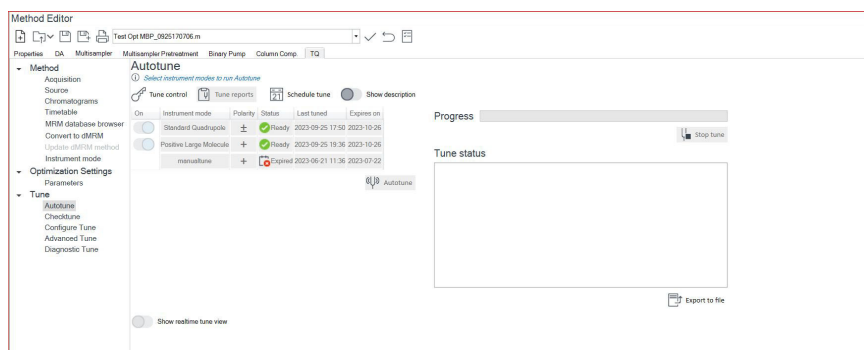
## Spectrum window

This window displays the spectral plot in real time. Additional tabs are displayed for other modules.



## Method Editor window

In this window, enter acquisition parameters for the method. Tune values are displayed on the Autotune tab.



## Sample Run window

In this window, enter sample information to run individual samples interactively, and start a single sample run. Specify an **Override DA Method** and select either **Both Acquisition and DA** (to run Data Analysis as part of the method) or **Acquisition Only** for the **Part of Method to run**.

Parameter Name	Parameter Value
Sample ID	
Override DA Method	
Part of Method to run	Acquisition Only
Equilib Time (min)	0

## Worklist window

In this window, enter sample information for multiple samples. When running the worklist, the samples are automatically run in the order listed. Select whether to run **Acquisition Only** or **Both Acquisition and DA** for the **Part of method to run** option in the Worklist Run Parameters dialog box.

	Status	Sample Name	Sample Position	Method	Data File	Sample Type	Level Name	Inj Vol (ul)	Comment	Sample Group	Info.
1	✓ Pending	Sample1	PA-A1	default.m	WorklistData-0001.d	Sample		As Method			
2	✓ Pending	Sample2	PA-A2	default.m	WorklistData-0002.d	Sample		As Method			
3	✓ Pending	Sample3	PA-B1	default.m	WorklistData-0003.d	Sample		As Method			
4	✓ Pending	Sample4	PA-B2	default.m	WorklistData-0004.d	Sample		As Method			

## Method Optimizer window

Method Optimizer operates in both Workstation and Networked Workstation configurations. The Method Optimizer can automate product ion selection, collision energies, fragmentor voltages, and source parameters. For more information, refer online help or the Introduction Workbook.

Method Optimizer

What type of optimization do you wish to perform?

Select one of the optimization modes

**Guided**  
Automated  
Compound-by-compound

**Guided Method Optimization:**  
The user is guided through a series of steps to optimize a method. A systematic pause for user input and data review is required between each major phase of the optimization.

- Creates the most suitable MRM transitions from a list of chemical formulas or precursor ions
- Optimizes and fine-tunes MRM specific parameters
- Optimizes and fine-tunes Ion Source and front-end ion optics parameters
- Optionally updates compound and method database

Review results Next

## dMRM Method Split window

The dMRM Method Split window operates in both Workstation and Networked Workstation configurations. This window facilitates splitting methods with many dMRM transitions into separate methods with fewer dMRM transitions.

dMRM Method Split

Please choose a method to split

... ☐ Number of methods 2 ☐ Maximum concurrent MRMs 200 ☐ Minimum dwell time (ms) 2 Split

## Preparing the LC Modules

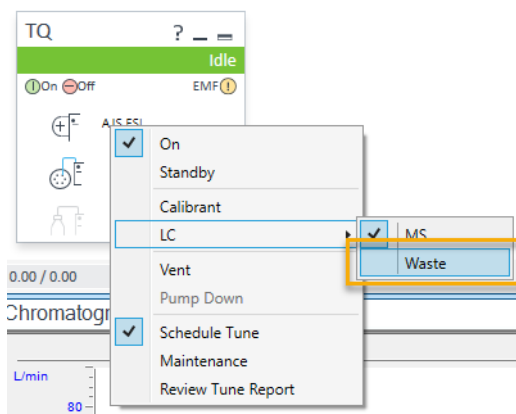
While conditioning or equilibrating the column, it is possible to tune the Triple Quad LC/MS.

### Switch LC stream to Waste

When not acquiring data, switch the direction of the LC stream away from the MS ion source and to waste.

When the LC is connected to a VWD or DAD, monitor the fluctuations of the VWD or DAD real-time chromatogram before a run.

- a Right-click the **TQ** device in the Instrument Status window.
- b Select **LC > Waste**.

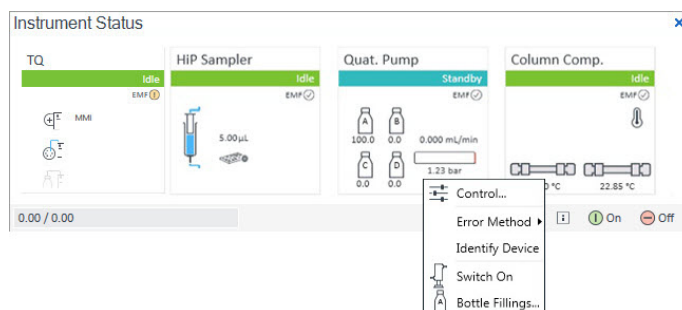


- 4 Purge the LC pump.
  - Follow the specific user guide directions for purging the installed pump model.
- 5 Set up to condition or equilibrate the column.
  - a In the Method Editor window, click **Apply** in the toolbar to download the LC parameters to the LC.

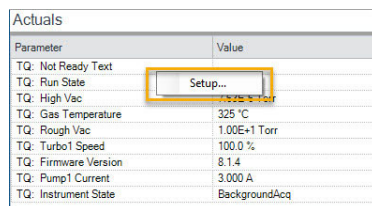
## Basic Operation

### Switch LC stream to Waste

- b Right-click an LC module in the Instrument Status window and select one of the commands to change any non-method control parameters, if needed.

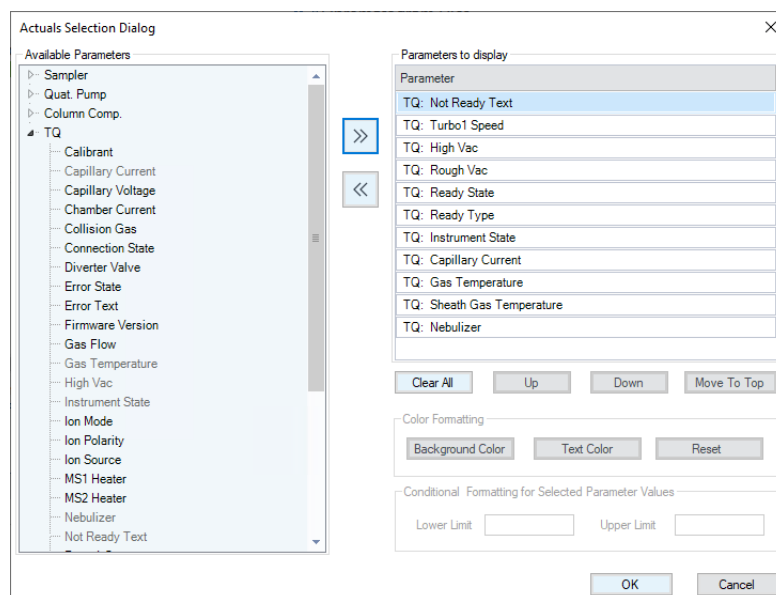


- c Monitor the baseline and adjust the plot to make sure the column is equilibrated and the baseline stable. (See [step 6](#) and [step 7](#) in this procedure.)
- 6 Set up to view real-time parameter values (actuals).  
The Actuals window can be customized to display instrument conditions for viewing.
    - a Click **Actuals** in the ribbon to display the Actuals window.
    - b Right-click the **Actuals** window and select **Setup**.



- c Select parameters to appear in the Actuals window.

In the **Available Parameters** list, expand a device to see a list of the instrument parameters for that device. Only configured devices will be shown in the list.



- d Select the parameters of interest, and click **Add**. Repeat this step for all the parameters to view.
- e Select any parameter in the **Parameters to display** list to remove from display, and click **Remove**.
- f Customize the background color and the text color for any parameters in the **Parameters to display** list.
- g Set a conditional formatting range for the parameters that are numbers.

#### NOTE

If the value of the parameter is not within the limits entered, then the background of the parameter is set to red.

- h Click **OK** when finished selecting parameters.

#### NOTE

The parameters selected appear in the Actuals window. The customizations made will remain, even if the Mass Hunter Data Acquisition software is closed and reopened.

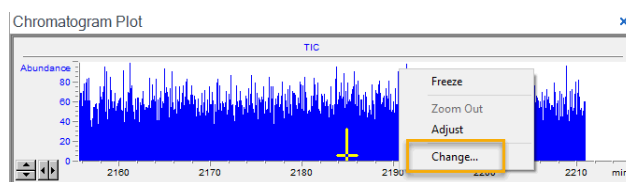
## Basic Operation

### Switch LC stream to Waste

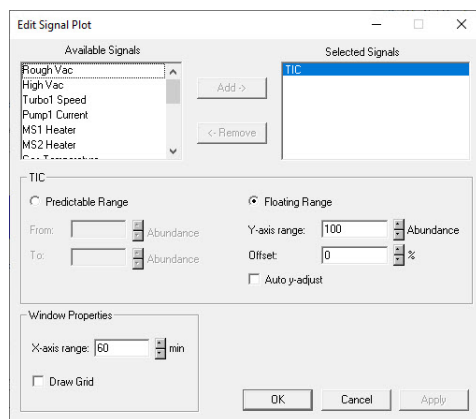
#### 7 Set up real-time plot displays.

As the column is conditioning, set up the displays to monitor the effluent.

- a In the Chromatogram Plots window, right-click the chromatogram plot, and select **Change**.



- b In the **Edit Signal Plot** dialog box, select the type of display signal, and click **OK**.



## Preparing the Triple Quad LC/MS

### Performing a checktune or autotune

See [Chapter 3](#), “Tuning”.

### Switching LC stream to MS

After you condition the column and tune the instrument, switch the LC stream from **Waste** to **MS**. See [“Switch LC stream to Waste”](#) on page 70 for how to do this.

### Monitoring MS baseline and spectral displays

If you did not monitor the LC baseline with a VWD or DAD, make sure that the instrument baseline is stable and no spectra of interfering intensity appear in the display.

If you did monitor the LC baseline with a VWD or DAD, change back to the default instrument displays.

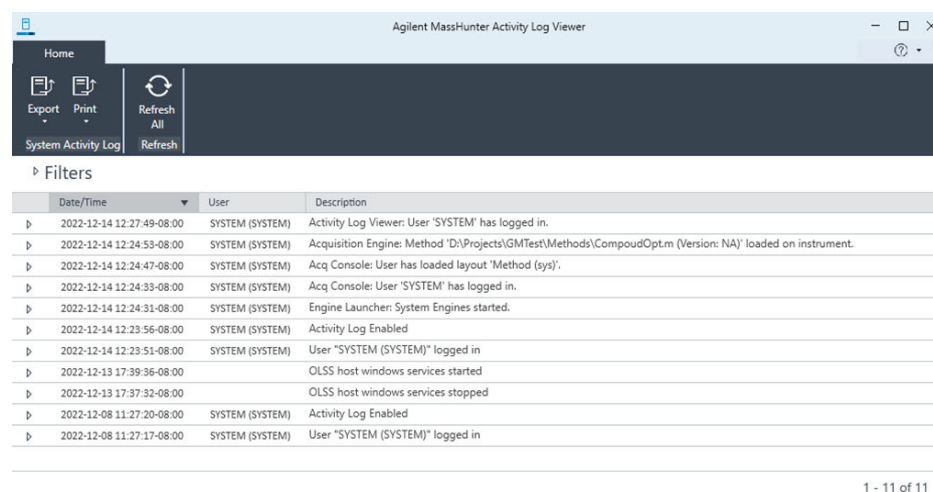
- 1 Right-click the chromatogram plot, and click **Change**.
- 2 Select the MS signal, and click **OK**.




## Viewing the System Activity Log for events and errors

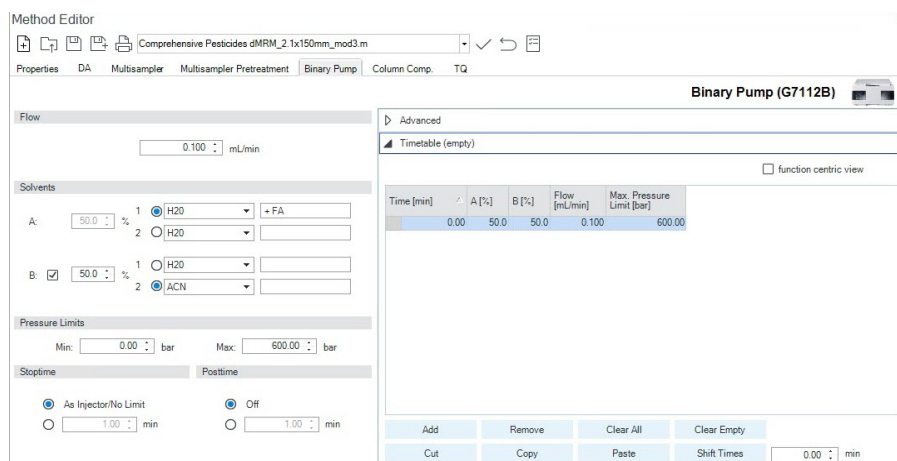
The System Activity Log provides information regarding errors to assist with troubleshooting.

To view the log, click **System Activity Log** from the Tools section in the ribbon of the Mass Hunter Data Acquisition program, and view the logged events.



## Setting Up an Acquisition Method

- 1 Set up the method in the Method Editor window:
  - a Enter or select the values and settings for each of the tabs below.
  - b *Optional.* To download the settings to the instrument, click ✓ **Apply**.
  - c To save the method, click  **Save As**.
  - d Name the method and click **OK**.
- 2 Enter values for all of the LC modules configured for the instrument.



Method Editor

Comprehensive Pesticides dMRM\_2.1x150mm\_mod3.m

Properties DA Multisampler Multisampler Pretreatment **Binary Pump** Column Comp. TQ

**Binary Pump (G7112B)**

Flow: 0.100 mL/min

Solvents

A: 50.0 % 1: H2O 2: H2O

B: 50.0 % 1: H2O 2: ACN

Pressure Limits

Min: 0.00 bar Max: 600.00 bar

Stop time Post time

As Injector/No Limit Off

1.00 min 1.00 min

Advanced

Timetable (empty)

function centric view

Time [min]	A [%]	B [%]	Flow [mL/min]	Max. Pressure Limit [bar]
0.00	50.0	50.0	0.100	600.00

Add Remove Clear All Clear Empty

Cut Copy Paste Shift Times 0.00 min

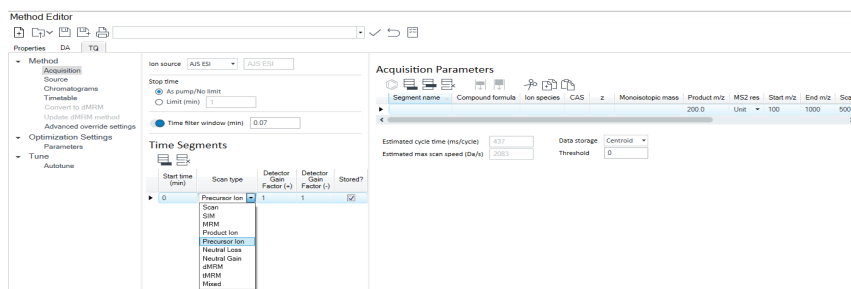
- 3 Enter the TQ parameter values.
  - a On the Acquisition tab, select the Scan type from the list in the **Time Segments** table. The Acquisition Parameters table is cleared when you change the **Scan type**. The parameters available on the right change depending on the **Scan type** for the selected **Time Segment**.

If you are changing the **Scan type** from **MRM** to **Dynamic MRM** or to **Triggered MRM**, you can copy and paste the transitions from the original **Scan segments** table to the Clipboard and then to the new **Scan segments** table. See the online help for more information.

## Basic Operation

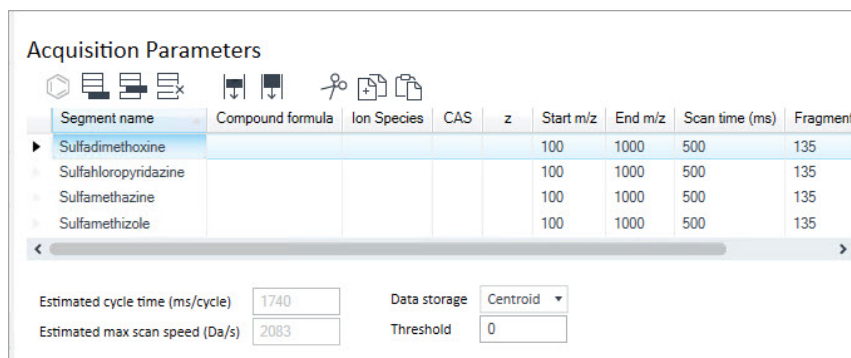
### Setting Up an Acquisition Method

- b Enter any Acquisition values that you want to change. Multiple **Scan segments** are allowed.



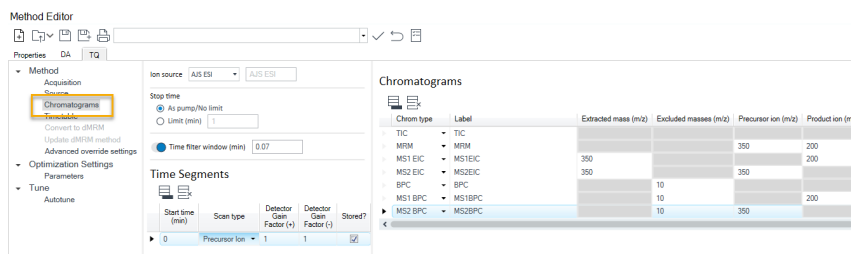
- c Set up to change instrument parameters with segments and scans:

- a To add a segment, click **Add Row** or **Insert Row**.
- b Enter the parameters for each Scan segment.



- 4 *Optional*. Set up signals for the Chromatogram plot:

- a Click **Chromatograms**.
- b Select the Chrom Type, and type other plot values.



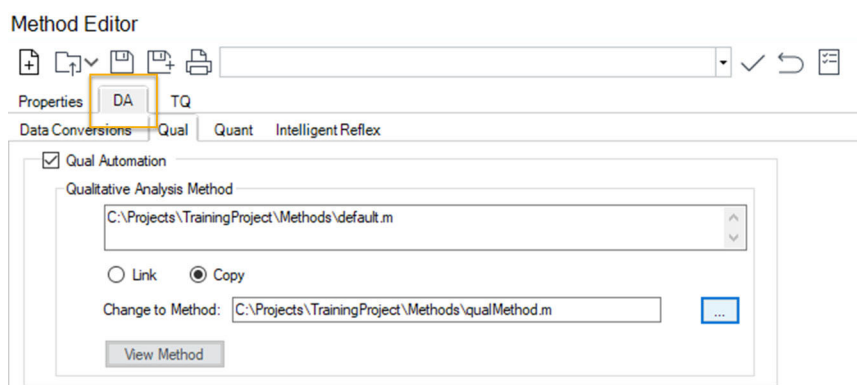
## Basic Operation

### Setting Up an Acquisition Method

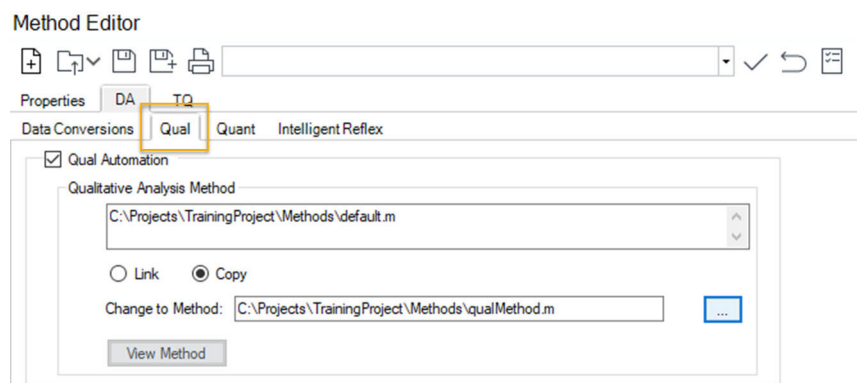
- 5 Set up the data analysis (DA) parameters.

A method can contain Qualitative Analysis parameters, Quantitative Analysis parameters, or a combination. The **Qual Automation** check box is marked on the Qual tab and the **Quant Automation** check box is marked on the Quant tab.

- a Select the **DA** tab.




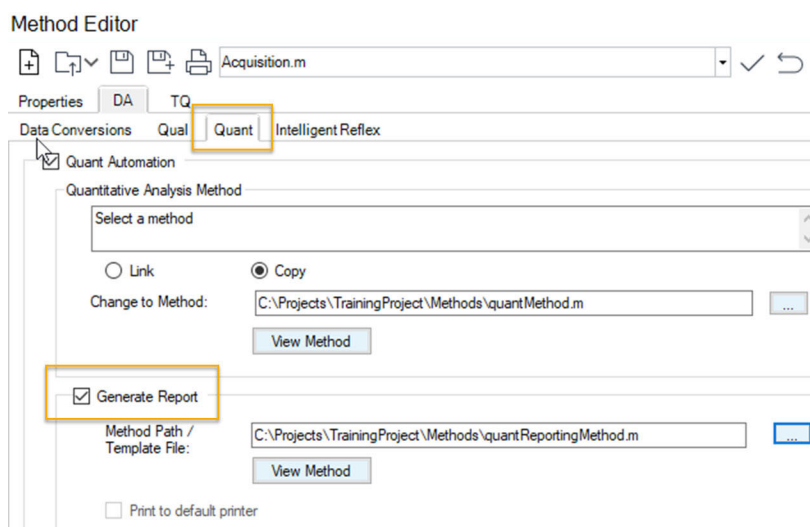
- b *Optional.* For information on the **Data Conversions** tab, refer to the online help.
- c *Optional.* On the **Qual** tab, mark the **Qual Automation** check box. The name of the current Qualitative Analysis method is shown in the box. To change the Qualitative Analysis method that is connected, click **browse** to select a different method. When the Acquisition method is saved, the selected Qualitative Analysis method is copied or linked to the Acquisition method.





## Basic Operation

### Setting Up an Acquisition Method

- d *Optional.* On the **Quant** tab, mark the **Quant Automation** check box. The name of the current Quantitative Analysis method is shown in the list. To change the Quantitative Analysis method that is connected, click  **Browse** to select a different method. When the Acquisition method is saved, the selected Quantitative Analysis method is copied or linked to the Acquisition method.
- e *Optional.* Mark the **Generate Report** check box on the Quant tab. Then, select the **Method Path/Template File** to use. To print the report, mark the **Print to default printer** check box. Mark the **Publish** check box to create a CSV file, a TXT file, or a PDF file.



- f *Optional.* For information on the **Intelligent Reflex** tab, refer to the online help.
- 6 *Optional.* On the **Properties** tab, set up the properties for this method.
- 7 Save the method.
  - a Click  **Save** or  **Save As**.
  - b If the Audit Trail Settings in Control Panel are set to prompt for a reason when the method is saved, enter the **Reason for creating a new version of this method**. Refer to the MassHunter Control Panel online help for more information. Click **OK**.
  - c If necessary, name the method and click **OK**.

## Setting Up and Running a Single Sample

- 1 Click the **Sample Run** window.
- 2 Enter the **Sample Name**, the **Data File Name** and **Path**, and other values.
- 3 *Optional.* Enter the **Additional Information**. If needed, change the value of the parameters in the **Additional Information** list.

Sample Run

Sample

Name:  Position:

Injection Volume:   $\mu$ L

Comment:

Data File

☒ Auto Increment

Name:  View Data

Path:

Additional Information

Parameter Name	Parameter Value
Sample ID	
Override DA Method	
Part of Method to run	Acquisition Only
Equilib Time (min)	0

Method Editor | **Sample Run** | Worklist

Run a Data Analysis method from this window by selecting **Both Acquisition and DA** or **Acquisition Only** for the **Part of Method to run**.

### NOTE


If using Both Acquisition and DA **Part of Method to run**, the **Override DA method** is required.

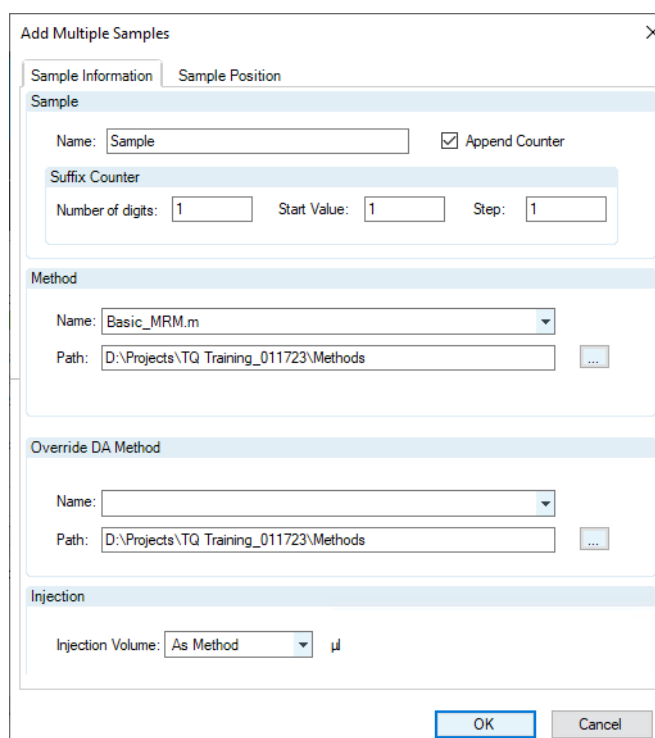
Additional Information

Parameter Name	Parameter Value
Sample ID	
Override DA Method	
Part of Method to run	Both Acquisition and DA
Equilib Time (min)	0

- 4 To start the single sample run, click ► **Run** in the Sample Run window toolbar.

## Setting Up and Running a Worklist

- 1 Click **Worklist** to show the Worklist window.
- 2 Click **Add Multiple Samples** . The **Add Multiple Samples** dialog box opens.  
Note: Samples can also be added one-by-one (user only needs to run a few samples, or several replicates of the same sample).
- 3 Enter all the information on the **Sample Information** tab.



**Add Multiple Samples**

Sample Information | Sample Position

**Sample**

Name:  ☒ Append Counter

**Suffix Counter**

Number of digits:  Start Value:  Step:

**Method**

Name:  Path:  ...

**Override DA Method**

Name:  Path:  ...

**Injection**

Injection Volume:  µl

OK Cancel

## Basic Operation

### Setting Up and Running a Worklist

- 4 On the **Sample Position** tab, specify the sample vial locations (make sure that the specific sample tray type has been configured by right-clicking the autosampler device image).

**Add Multiple Samples**

Sample Information | **Sample Position**

☐ Current Configuration

Select Well-plate or Vial Tray

Select Tray

- Well-plate Tray
  - Plate 1
  - Plate 2
  - Plate 3
  - Plate 4
  - Plate 5
  - Plate 6
  - Plate 7
  - Plate 8

Plate/Tray Type: \*96Agilent\*

Selection Origin:
   
☒ Top left ☐ Top right
   
☐ Bottom left ☐ Bottom right


Block Increment:
   
☒ Row major
   
☐ Column major
   
☐ Serpentine

Number of samples: 0      Number of replicates: 1

Well-plate/Tray

	1	2	3	4	5	6	7	8	9	10	11	12
A												
B												
C												
D												
E												
F												
G												
H												

OK Cancel

- 5 Specify the locations, and click **OK**.
- 6 To set up the worklist run, click **Worklist Run Parameters** .



## Basic Operation

### Setting Up and Running a Worklist

- 7 On the **Run Parameters** tab, type the paths for the method.

Worklist Run Parameters ✕

Run Parameters | Intelligent Reflex | Additional Parameters | Barcode

Operator Information

Operator name

Run Information

Part of Method to run  ☒ Synchronous DA

Run Type  ☒ Stop worklist on DA error

Data File Settings

▶ Root Folder

▶ Sub-Folders

▶ File Naming

▶ Tree View for File Path and Name

Method Paths

Method  ...

Override DA  ...

Scripts

☐ Pre-worklist  ...

☐ Post-worklist  ...

☐ Acquisition clean-up  ...

☐ Post-analysis  ...

Disk space Information (GB)

Available Disk space  Free Disk space threshold

Run Settings

☒ Overlapped injection Wait Time for Ready  (min)

## Basic Operation

### Setting Up and Running a Worklist

- 8 In the **Data File Settings** section, click the caret to display fields to enter or select the folders for the data files. Select the **File Naming** options.

Data File Settings

Root Folder

Root Data Folder: C:\Projects\TrainingProject\Data

Sub-Folders

Sub-folder 1: <Empty> Sub-folder 2: <Empty> Sub-folder 3: <Empty>

File Naming


Part 1: User Text Part 2: Counter[0001] Part 3: <Empty>

WorklistData

☒ Use separator for file name parts

Tree View for File Path and Name

C:\Projects\TrainingProject\Data\WorklistData-0001.d

- 9 For information on the **Intelligent Reflex** tab, refer to the online help.
- 10 *Optional.* On the **Additional Parameters** tab, enter a comment, and click **OK**.
- 11 To start the worklist, click  **Run Worklist**.

#### NOTE

To use an acquisition method that has a different data analysis (DA) method than the method entered in the worklist, show the column called **Override DA Method** in the worklist by using the **Show/Hide/Order Columns** dialog box. In this column, browse for and select the method containing the DA parameters you want to use for the sample. The DA part of this method is used instead of the DA part of the current method.

Or, select this method in the **Add Multiple Samples** dialog box.

## Reviewing Results with Qualitative Analysis

Use the Qualitative Analysis program to do these tasks and more:

- Review results for acquisition method development
- Select the most appropriate precursor and product ions for MRM analyses
- Find compounds
- Identify compounds
- Molecular feature extraction

Refer to the online help for the Qualitative Analysis software to learn more.

## Analyzing Data with Quantitative Analysis

Another primary tool for analyzing and reporting instrument results is the Quantitative Analysis program.

Do the exercises in the *Quantitative Analysis Familiarization Guide* to learn how to quantitate the acquired data files:

- Set up a batch and a method to automatically quantitate a set of samples
- Review results by learning how to view and use the Batch-at-a-Glance results screen
- Identify and use outliers to change the method and requantitate the data using a better calibration curve fit or other more appropriate settings

Refer to the online help for the Quantitative Analysis program to learn how to do more operations to analyze your data.

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## 5

## Maintenance

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## Maintenance Overview

Your instrument needs to be serviced and maintained to avoid contamination, which prevents signal suppression, reduces background noise, minimizes adduct formation, and enables the instrument to operate at its peak performance. In order to achieve the most accurate results, routine and periodic maintenance is crucial.

The difference between routine and periodic maintenance is that routine maintenance is done regularly to keep the equipment in good working condition, while periodic maintenance is done at specific intervals to prevent breakdowns or failures.

MassHunter Acquisition software keeps track of the number of injections and the number of days since a maintenance activity was performed for your TQ instrument using the Early Maintenance Feedback (EMF) dashboard. EMF allows you to plan for scheduled maintenance when it is convenient and increase the instrument uptime. If a limit is exceeded for an EMF item that is enabled, then the EMF icon changes to yellow, and the tooltip displays the cause in the device pane. Set the limits for each EMF item in the Maintenance dialog box following instructions detailed in online help.

This Maintenance chapter is broken down into maintenance procedures listed by routine, then periodic maintenance tasks with their recommended schedule of performance, with the EMF procedures cross referenced in the final section. Consult the online help or contact your Agilent consultant for further information.



## Routine Tasks

### Cleaning the spray chamber - daily

Perform this maintenance daily or at the end of each shift or anytime you suspect carryover contamination from one sample or analysis to another.

**NOTE**

Use the weekly cleaning procedure if symptoms of contamination persist or if the spray shield or capillary cap show significant discoloration that cannot be removed by the regular, daily cleaning.

Tools needed:

- Clean, powder-free nitrile gloves
- Clean lint-free cloth
- LC/MS-grade isopropanol
- LC/MS-grade water
- Clean wash bottle

To perform daily cleaning of the spray chamber,

- 1 Put on clean powder-free nitrile gloves.
- 2 Lower the drying gas temperature to the minimum level.
- 3 For APCI/multimode, lower the vaporizer heater temperature to the minimum level.

**WARNING**

**Make sure the source is cooled before you clean the spray shield.**

- 4 In a clean wash bottle, prepare a 50:50 mix of LC/MS-grade isopropanol and LC/MS-grade water.
- 5 Open the spray chamber.
- 6 Dampen a clean lint-free cloth with a mixture of LC/MS-grade isopropanol and LC/MS-grade water.
- 7 Wipe the spray shield and the area around the spray shield.
- 8 Close the spray chamber.

## Checking and filling the calibrant bottle - weekly

### Schedule

Perform this procedure monthly or weekly if you tune the instrument frequently, or if the calibrant has expired.

### Equipment List

- APCI calibrant
- APCI-L tuning mix
- ESI-L tuning mix
- MMI-L tuning mix
- Reference mix
- Clean powder-free nitrile gloves

### Steps for checking calibrant levels

- 1 Check to make sure that enough tuning mix is present to immerse the end of the intake tube.
- 2 If the tuning mix level is within a few millimeters of the end of the intake tube, refill the calibrant bottle.

### Steps for refilling the calibrant bottle

- 1 Rinse the calibrant bottle once with water, then twice with ACN before refilling.

### CAUTION

Dispose of rinsing agents appropriately.

- 2 Label the calibrant bottle with the tuning mix expiration date.
- 3 Refill the calibrant bottle with the appropriate tuning mix.
- 4 Put the intake tube into the calibrant bottle as you lift the calibrant bottle into position.

### CAUTION

Do not touch the intake tube unless you are wearing clean gloves.

- 5 Attach the calibrant bottle onto the fixed bottle cap. Turn the calibrant bottle counterclockwise to tighten.

**CAUTION**

The bottle only needs to be snug. Do not over-tighten the bottle. A leaky bottle cap can prevent the bottle from pressurizing and can lead to the evaporation of the contents.

**CAUTION**

The tuning mixes are not interchangeable. Failure to change the tuning mix when the source or inlet assembly is changed can result in miscalibration of the instrument and errors in mass assignments.

## Cleaning the spray chamber - weekly

Perform this maintenance weekly or whenever symptoms indicate that contamination exists in the spray chamber and normal daily cleaning does not correct the problem.

Tools needed:

- Clean powder-free nitrile gloves
- Clean lint-free cloth
- LC/MS-grade isopropanol
- LC/MS-grade water
- Clean wash bottle
- 4000 grit abrasive paper

To perform weekly cleaning of the spray chamber,

- 1 Put on clean powder-free nitrile gloves.
- 2 Disconnect the nebulizer sample line and sample nebulizer gas tubing from the nebulizer.
- 3 Disconnect all cables and tubings from the instrument.
- 4 Open the latch of spray chamber.
- 5 Open the spray chamber.
- 6 Put the source under a fume hood.

**Maintenance****Cleaning the spray chamber - weekly**

- 7 Dampen a clean lint-free cloth with a mixture of LC/MS-grade isopropanol and LC/MS-grade water. For Multimode, be careful not to touch the thermocouple probe.
- 8 Wipe the interior of the spray chamber with a clean lint-free cloth.
- 9 Make sure you wear clean gloves. Use a tech wipe to hold the parts as you remove them. They will be warm.
- 10 Clean the spray shield, capillary cap, end plates, and contact ring under fume hood. Carefully remove the canted coil spring from the capillary cap before cleaning.
- 11 Use 4000 grit abrasive paper to clean contaminants from the parts.
- 12 Put the spray shield, capillary cap, end plates, and contact ring in the beaker.
- 13 Add a 50:50 mix of LC/MS-grade isopropanol and LC/MS-grade water in a beaker.
- 14 Put the beaker in sonication for 5 minutes.
- 15 Drain the solvent and remove the parts from the beaker.
- 16 Dry the parts by using nitrogen gas.
- 17 Carefully insert the canted coil back into the capillary cap.
- 18 Reinstall the contact ring, end plate, capillary cap, and spray shield.
- 19 Reinstall the spray chamber on the instrument.
- 20 Close the spray chamber.
- 21 Close the latch of spray chamber.
- 22 Connect all cables and tubings to the instrument.

**CAUTION**

**Do not bend or blunt the tip of the needle, as it will decrease system performance. Sharpening the needle is not needed.**

- 23 Pull and twist the 4000 grit abrasive paper along the needle and off the tip of the needle.

**CAUTION**

**Do not hit the tip of the corona needle. The tip can bend, which can decrease system performance.**

- 24 Starting at the base of the needle, wipe the needle with a clean lint-free cloth. The cloth can be dry or dampened with LC/MS-grade isopropanol.

**CAUTION**

**Do not hit the tip of the corona needle. The tip can bend, which can decrease system performance.**

**25** Connect the nebulizer sample line and sample nebulizer gas tubing to the nebulizer.

## Flushing the nebulizer - weekly

Passing the vapors of solvents like IPA, methanol, acetonitrile, or water through the LC/MS system is called steam cleaning and is used to clean possible contamination in the LC/MS system. The usual conditions are:

- LC pump flow to 0.5 ml/min
- Nebulizer pressure to 60 psi
- Drying gas to 13 L/min
- Drying gas temp to 350 °C

Make sure the MS stream selection valve is set to go to the MS. Steam Cleaning overnight has been shown to be one of the most important factors in improving the signal-to-noise level by reducing the contaminations.

To clean an MS, there are two options:

- Plain water/MeOH at high temp – 50:50 proportion
- IPA/MeOH/Water at high temperature

The IPA/MeOH/Water combo can be anything. IPA, maybe 50 (IPA):25:25. IPA cleans both aqueous and organic.

### Schedule

Check the nebulizer weekly. If needed, flush traces of samples and buffers out of the tubing, valves, and nebulizer.

### Equipment List

- LC/MS-grade methanol
- LC/MS-grade water

### Steps

- 1 Install a mix of 30 to 70% methanol in water into a LC solvent bottle.
- 2 Remove the column from the LC column compartment.
- 3 Remove nebulizer from spray chamber and support the nebulizer so that it sprays into an appropriate waste container (beaker, bottle, etc.).
- 4 Control the LC flow through the acquisition software to pull from the solvent bottles.
- 5 Set flow rate to not more than 1 ml per minute.

**Maintenance**

## Flushing the nebulizer - weekly

- 6 Flush for 3 to 5 minutes. For heavy build up, additional flushing may be required.

## Periodic Tasks

### Checking the rough pump oil level

#### Schedule

Once every three months/once per quarter (recommended).

#### Equipment List

- Clean chemical-resistant gloves
- Safety glasses
- Funnel
- 10-mm hex key
- Paper towel or shop rag
- Small plastic tub
- AFV 60 Gold Oil

#### Steps

- 1 The oil level should be between the marks for Max and Min.
- 2 Check that the pump oil is clear and the color is lighter than amber.
- 3 If the pump oil is dark or full of suspended particles, replace it.



## Draining and replacing the MS40+ pump oil and replacing the filter

### Schedule

Replace the pump oil every six months. Replace it sooner if the oil appears dark or cloudy.

### Equipment List

- Clean chemical-resistant gloves
- Safety glasses
- Funnel
- Pair of pliers
- Filter
- Filter cap O-ring
- Small cap O-ring
- MS40 exhaust filter cap removal tool
- 10-mm hex key
- Paper towel or shop rag
- Small plastic tub
- AFV 60 Gold Oil

### Steps for draining the MS40+ pump oil

- 1 Put on clean, chemical-resistant gloves.
- 2 Place the instrument into 'Standby,' then 'Vent'.
- 3 Allow the rough pump to turn off automatically, waiting for approximately 15 minutes.
- 4 Unplug all power cords.
- 5 Remove the inlet and outlet pipes before opening the oil drain cap.
- 6 Place a tank for waste oil, for example, a small plastic tub under the oil drain plug.
- 7 Unscrew the oil fill cap, rotating it counterclockwise using a 10-mm hex key. Remove it from the instrument and place it in a secure location.

- 8 Unscrew slowly the oil drain cap by rotating it counterclockwise using the 10-mm hex key. Let the oil flow out. In the meantime, clean the inside of the drain plug.
- 9 After the oil has been drained, close the drain plug tight.
- 10 Take the tank of waste oil away and clean thoroughly, using rags of cotton or other suitable material to dry.

**Steps for replacing the MS40+ pump oil**

- 1 Unscrew the oil fill cap, rotating it counterclockwise using a 10-mm hex key.
- 2 Remove it from the instrument and place it in a secure location.
- 3 Add AVF 60 Gold oil until reaching the maximum level on the sight glass.
- 4 Close the oil fill cap tight using the 10-mm hex key.
- 5 Replace the oil mist filter.

**Steps for replacing the MS40+ oil mist filter**

- 1 Disconnect the exhaust tube.
- 2 Unscrew the filter cap using the MS40 exhaust filter cap removal tool.
- 3 Remove the O-ring from the filter cap.
- 4 Remove the old filter from the instrument.
- 5 Remove the O-ring from the filter.
- 6 Install the new, small O-ring on the new filter, then install the filter into the pump in the proper orientation. Make sure the distance of the filter is greater than 2 cm from outside the cap threads.
- 7 When properly installed, the filter cap is flush to the pump. The back end of the filter is seated inside the filter mount. It may be necessary to wiggle or adjust the filter to seat it in the correct position.
- 8 Install the new, large O-ring and filter cap.
- 9 Connect the exhaust tube.
- 10 Plug in the rough pump and all power cords from the LC/MS instrument.
- 11 Press the front power switch to initiate pump down, returning the instrument to normal operation.

## Draining and replacing the MS120+ pump oil

### Schedule

Drain the pump when any of these conditions occur:

- 8000 hours scheduled, or yearly
- when oil is dirty
- when the oil reaches the minimum level

### Equipment List

- Clean chemical-resistant gloves
- Safety glasses
- Funnel
- 10-mm hex key
- Paper towel or shop rag
- Small plastic tub
- AFV 60 Gold Oil

### Steps for draining the MS120 pump oil

- 1 Put on clean, chemical-resistant gloves.
- 2 Ensure that the wheels of the pump are locked and braked securely before proceeding.
- 3 Turn off the pump and wait for the oil to cool for approximately 40 minutes or more.
- 4 Remove the cover by unscrewing the screws holding it in place. Place the cover and screws in a secure location.
- 5 Place a drain pan or small plastic tub, approximately 3 liters in size, under the pump tank.
- 6 Unscrew the oil filling plug and place it in a secure location.
- 7 Remove the oil discharge plug, clean the inside, and place it in a secure location.
- 8 Screw the oil drain pipe onto the discharge.
- 9 Allow the oil to drain through the pipe into the drain pan. To ensure complete drainage, raise the back wheels of the pump by 40 mm.

**Maintenance****Draining and replacing the MS120+ pump oil**

- 10** When the oil is completely drained, remove the oil drain pipe.
- 11** Reinstall the oil filling plug and discharge plug.
- 12** If the drained oil is polluted or contains water, add the minimum level of oil and run the pump at the maximum level for at least five minutes.
- 13** Drain the oil from the pump again.
- 14** Repeat the oil-filling procedures.

**Steps for replacing the MS120 pump oil**

- 1** Unscrew the oil filling plug and place it in a secure location.
- 2** Add the minimum level of oil and run the pump at the maximum level for at least five minutes.
- 3** Check the oil level to make sure it is at the maximum level. Add oil if necessary.

## Replacing the MS120+ pump filter

### Schedule

Replace the pump filter at 8000 hours scheduled, or yearly.

### Equipment List

- Clean chemical-resistant gloves
- Safety glasses
- Funnel
- 10-mm hex key
- Paper towel or shop rag
- Small plastic tub
- AFV 60 Gold Oil

### Steps

- 1 Put on clean, chemical-resistant gloves.
- 2 Remove the cover by unscrewing the screws holding it in place. Place the cover and screws in a secure location.
- 3 Remove the oil fill plug and place in a secure location.
- 4 Attach the oil discharge pipe to the oil filling hole with the charge fitting.
- 5 Use the funnel to add AFV 60 Gold oil to the instrument to between the MIN and MAX lines, or up to half of the sight glass. Make sure not to exceed the maximum fill line.
- 6 Remove the funnel and the discharge pipe from the instrument.
- 7 Reinstall the oil fill plug.
- 8 Run the pump at maximum vacuum level for at least 2 minutes. If the room temperature is lower than 18 °C, run the pump at maximum pressure with the inlet port closed and no load for approximately 15 minutes.
- 9 Stop the pump, check the oil level, then add more oil if needed using the prior steps.
- 10 When oil level is satisfactory, reinstall the cover using a screwdriver.

## Replace Oil Mist/Exhaust Filter - MS120+

### Schedule

Replace the exhaust filter when any of these conditions occur:

- 8000 hours scheduled, or yearly
- considerable pump temperature increase
- in extreme cases, spontaneous ignition of oil lubricant.

### Equipment List

- Clean chemical-resistant gloves
- Safety glasses
- X3702-68201 MS 120 Exhaust Filter Cartridge

- 1 Put on clean, chemical-resistant gloves.
- 2 Remove the cover by unscrewing the screws holding it in place. Place the cover and screws in a secure location.
- 3 Remove the tank cover by unscrewing the screws holding it in place. Place the tank cover, screws and gasket in a secure location.
- 4 Remove and replace the exhaust filter and its O Ring.
- 5 Reassemble the gasket and tank cover using a screwdriver.
- 6 Reinstall the cover using a screwdriver.

## Replacing the nitrogen gas filters

### Schedule

Yearly, or when flagged by EMF.

### Equipment List

- 2 1/2-inch OD Mounting Clip for Big Universal Trafps (2/pk) - Part number UMC-5-2
- RMSN-4 1/4-inch Nitrogen

### Steps

#### NOTE

Before installing the trap, make sure the system is free of leaks and the system is generally in good working order.

- Maximum operating pressure is 250 PSIG.
- Maximum operating temperature is 100 °C.
- Maximum flow rate is 8 liters per minute.

#### CAUTION

**If you are using stainless steel tubing, please order the purifier with stainless steel fittings RMSH-2-SS or RMSH-4-SS. Using brass fittings with stainless steel tubing increases the risk of cross-threading.**

- 1 Shut down your LC/MC or reduce the GC heated zone temperatures.
- 2 Set the gas source supply pressure to 10–15 psi and maintain flow in the gas source line before disconnecting it from the inlet of the old trap.
- 3 Remove the protective nut and plug from the INLET end of the new trap. DO NOT open the plug on the OUTLET end.
- 4 Immediately attach the new trap to the gas source tubing using one of the included ferrule sets.

#### CAUTION

**Failure to connect the trap immediately may cause contamination of the adsorbents inside. Reduced adsorption capacity will contribute to elevated levels of contaminants observed by the detector. This may result in the need for additional purge time.**

- 5 Insert the tubing through the nut and ferrule set until the tubing rests firmly against the shoulder in the fitting.
- 6 Finger-tighten the nut, then use a wrench to tighten the nut 3/4 turn for 1/8-inch tubing and 1-1/4 turn for 1/4-inch tubing.
- 7 Wait 3 minutes for the gas pressure inside the new trap to stabilize.
- 8 Increase the gas source pressure to 60 psi.
- 9 Open the outlet fitting and purge the trap for 3 minutes.
- 10 Adjust the gas source pressure to a normal working level. Connect the outlet fitting of the trap to the instrument tubing as described in step 5 and step 6.
- 11 Secure the trap in a vertical orientation. The length of the trap should stand perpendicular to the floor.

Wait for at least 3 minutes to purge out any air that may have entered the instrument tubing line. The trap is now ready for use.



## General Maintenance Tasks

### Installing or removing the nebulizer

#### Schedule

Perform this procedure when you need to access the nebulizer for maintenance.

#### Equipment List

- Clean, powder-free nitrile gloves
- Replacement needle kit
- 1/4-inch x 5/16-inch open-end wrench (Quantity: 2)

#### Removing the nebulizer needle

- 1 Put on clean, powder-free nitrile gloves.
- 2 In MassHunter Data Acquisition, shut off the LC solvent flow and nebulizing gas.
- 3 Disconnect the nebulizer sample line from the nebulizer.
- 4 Disconnect the sample nebulizer gas tubing from the nebulizer.

**WARNING**

**The tip of the nebulizer can be very hot. Do not touch the nebulizer until it is cool.**

- 5 Turn the nebulizer counterclockwise until it disengages from the retaining screws.
- 6 Gently lift the nebulizer out of the spray chamber and place it in a safe location.

#### Replacing the nebulizer needle

- 1 Put on clean, powder-free nitrile gloves.
- 2 Determine your nebulizer type per the user guide or the document that comes with the kit.
- 3 Install the nebulizer in the Nebulizer Adjustment Fixture, turning clockwise to secure the nebulizer to the adjustment fixture.

- 4 Loosen the locknut next to the zero-dead-volume (ZDV) union by placing the 5/16-inch wrench on the nut, and the 1/4-inch wrench on the union, and turning the 5/16-inch wrench clockwise.
- 5 Remove the union from the nebulizer needle holder.
- 6 Remove the union lock nut from the nebulizer.
- 7 Loosen the fastener (locknut, 1.5-mm hex screw or T6 Torx screw) that secures the needle holder in place.
- 8 Loosen the needle holder and pull it out of the nebulizer body. Dispose of the used needle properly.
- 9 For more thorough cleaning, sonicate the nebulizer body. Pour isopropanol or methanol through the inside of the shaft.
- 10 Thread the new needle holder into the nebulizer body.
- 11 Carefully remove the new needle from the shipping tube and adhesive strip.
- 12 Identify the sharp end of the needle.
- 13 Carefully slide the sharp end of the needle through the ferrule until 1 cm of the needle remains at the ferrule.

**CAUTION**

**Do not bend the needle as you slide it into the ferrule. The needle is fragile. A bent needle results in poor alignment with the nebulizer body.**

- 14 Push the needle into the ferrule until the needle is slightly visible flush with the ferrule.
- 15 Reinstall the locknut and the union. Hand-tighten the union.
- 16 Hold the needle holder steady with a 1/4-inch x 5/16-inch open-end wrench, depending on your nebulizer holder style.
- 17 Tighten the union one-half to three quarters of a turn, or until an audible squeak is heard. The ferrule is now compressed.

## Inspecting the nebulizer

### Schedule

Perform this procedure if you have the G1960-67470 Nebulizer Adjustment Kit. Perform this project if there is increased LC back pressure, off-axis spraying, dripping from the nebulizer, or when the reference nebulizer needle is not spraying.

### Equipment List

- Clean powder-free nitrile gloves
- G1960-67470 Nebulizer Adjustment Kit
- T6 Torx driver
- 1/4-inch x 5/16-inch open-end wrench (Quantity: 2)

### Parts needed:

- Replacement needed kit

### Steps

- 1 Determine your nebulizer type per the user guide or the document that comes with the kit (need the part number).
- 2 Carefully insert the tip of the nebulizer into the end of the Nebulizer Adjustment Fixture.
- 3 Slide the heads of the two spring loaded socket head cap screws through the mounting holes on the body of the nebulizer.
- 4 Turn the nebulizer body 1/8 turn counter-clockwise.

#### NOTE

If the nebulizer is too tight or too loose, loosen or tighten the nut on the captured screws to adjust the tension on the spring. Turn clock wise to tighten, counter clock wise to loosen.

- 5 Gently push the 40 x Magnifier into the end horizontal position of the Nebulizer Adjustment Fixture. Align the tapered tip of the magnifier to the tip of the nebulizer needle.
- 6 Push the LED Flashlight into the Nebulizer Adjustment Fixture. No tool is needed.
- 7 Turn on the LED Flashlight. The on/off switch is at the end of the flashlight.

**CAUTION**

**Do not hit or touch the end of the nebulizer or you can damage the needle.**

- 8 Gently push the LED Flashlight into the end horizontal position of the Nebulizer Adjustment Fixture.
- 9 Push the 40 x Magnifier into the Nebulizer Adjustment Fixture. No tool is needed. Align the tapered tip of the magnifier to the tip of the nebulizer needle.
- 10 Turn on the LED Flashlight. The on/off switch is at the end of the flashlight.

**CAUTION**

**Do not hit or touch the end of the nebulizer or you can damage the needle.**

- 11 Gently slide and rotate the 40 x Magnifier into or out of the Nebulizer Adjustment Fixture to focus the magnifier on the end of the nebulizer nozzle and needle. For the APCI nebulizer, if needed, remove the pocket clip to focus properly.

**Table 1** Correct needle position

Nebulizer	Distance
Microflow Nebulizer Assembly	0.003 inch
ES Tested Nebulizer	0.000 (flush)
Tested ESI Nebulizer Assembly (older style)	0.003 inch
Tested APCI Nebulizer Assembly	0.000 (flush)

## Adjusting or replacing the nebulizer needle

### Schedule

Perform this procedure if there is increased LC back pressure, off-axis spraying, dripping from the nebulizer, or when the reference nebulizer needle is not spraying.

### Equipment List

- Nebulizer Adjustment Fixture
- Clean, powder-free nitrile gloves
- T6 Torx driver
- 1/4-inch x 5/16-inch open-end wrench (Quantity: 2)
- G1960-67470 Nebulizer Adjustment Kit

### Steps

- 1 Put on clean, powder-free nitrile gloves.
- 2 Determine the nebulizer holder type by consulting the user guide for your model.
- 3 Install the nebulizer in the Nebulizer Adjustment Fixture.
- 4 Loosen the locknut next to the zero-dead-volume (ZDV) union.
- 5 Remove the union from the nebulizer needle holder.
- 6 Remove the union lock nut from the nebulizer.
- 7 Loosen the fastener (locknut, 1.5-mm hex screw, or T6 Torx screw) that secures the needle holder in place.
- 8 Loosen the needle holder and pull it out of the nebulizer body. Dispose of the used needle properly.
- 9 For more thorough cleaning, sonicate the nebulizer body. Pour isopropanol or methanol through the inside of the shaft.
- 10 Thread the new needle holder into the nebulizer body.
- 11 Carefully remove the new needle from the shipping tube and adhesive strip. Identify the sharp end of the needle.
- 12 Carefully slide the sharp end of the needle through the ferrule until 1 cm of the needle remains at the ferrule.

**CAUTION**

**Do not bend the needle as you slide it into the ferrule. The needle is fragile. A bent needle results in poor alignment with the nebulizer body.**

- 13 Push the needle into the ferrule until the needle is slightly visible flush with the ferrule.
- 14 Reinstall the locknut and the union. Hand-tighten the union.
- 15 Hold the needle holder steady with a 3-mm open-end wrench or 1/4-inch x 5/16-inch open-end wrench, depending on your nebulizer holder style.
- 16 Tighten the union one-half to three quarters of a turn, or until an audible squeak is heard. The ferrule is now compressed.
- 17 Pull carefully on the needle to ensure the needle is held firmly in place.
- 18 Insert the needle into the nebulizer shaft.
- 19 Adjust the electrospray needle position before reinstalling the nebulizer in the spray chamber.
- 20 Tighten the fastener (T6 Torx screw) that secures the needle holder in place.

## Installing the capillary

### Schedule

After cleaning the capillary or when installing a new capillary.

### Equipment List

- Clean powder-free nitrile gloves
- LC/MS-grade isopropanol

### Steps

- 1 Put on clean, powder-free nitrile gloves.
- 2 Lubricate the capillary entrance end with LC/MS-grade isopropanol.
- 3 Carefully insert the capillary straight into the desolvation assembly. The capillary must be aligned correctly so that its end fits into a fixed capillary cap inside the desolvation assembly.

### CAUTION

**Putting vertical and horizontal pressure on the capillary can break it. Spray capillary with isopropanol to lubricate the capillary for easier removal.**

- 4 When 2 to 3 cm of the capillary remains extended from the desolvation assembly, the capillary rests against the rear contact spring, which slightly restricts further insertion of the capillary. Slightly increase the insertion force to push the capillary through the rear contact spring to fully insert the capillary.
- 5 Continue to apply pressure until approximately 1 cm remains extended from the desolvation assembly.

### CAUTION

**Do not twist or turn the capillary cap when you install it or you can damage the metal plating.**

- 6 Install the contact ring and end plate.
- 7 Install the two T10 Torx screws to hold the end plate.
- 8 Lubricate the capillary tip with LC/MS-grade isopropanol.
- 9 Install the capillary cap over the outer end of the capillary.
- 10 Install the spray shield.

**11** Close the spray chamber.



## Removing the capillary (system with a VacShield)

### Schedule

When you need to clean or replace the capillary on a system with a VacShield.

### Equipment List

- Clean powder-free nitrile gloves
- Capillary Puller tool

### Steps

#### WARNING

**The spray chamber operates at very high temperatures. Do not continue until the spray chamber is cool.**

- 1 Put on clean powder-free nitrile gloves.
- 2 Remove the capillary cap from the end of the capillary.
- 3 Screw the capillary puller tool fully into the spray shield mount.
- 4 Push the collet assembly over the capillary and then tighten by holding the puller handle. Turn the collet clamping knob clockwise.
- 5 Pull on the knob until the collet assembly stops moving.
- 6 Visually check that the capillary has been pulled out by the collet by looking through the slots on the tool.
- 7 Rotate the knob assembly counterclockwise slightly, and pull out the assembly to unlock the collet assembly from the puller.
- 8 Pull the tool out.
- 9 Carefully pull the capillary out along its long axis.

#### CAUTION

**The capillary is glass or of similar material, and you can break it by putting vertical or horizontal pressure on it.**

- 10 Loosen the collet clamping knob slightly to loosen the capillary from the capillary puller tool.
- 11 Pull out the capillary from the collet.
- 12 Unscrew the tool from the shield mount.

## Cleaning the capillary

### Schedule

When you observe decreased sensitivity and decreased signal stability.

### Equipment List

- Clean powder-free nitrile gloves
- LC/MS-grade isopropanol
- Alconox powdered precision cleaner
- Deionized (18 MΩ/cm) water
- 100-mL polypropylene graduated cylinder
- 10-mL polypropylene graduated cylinder
- Two 1-mL pipette tips

### Steps

- 1 Put on clean, powder-free nitrile gloves.
- 2 Dissolve 1 gram of Alconox Powdered Precision Cleaner in 100 mL of deionized (18 MΩ-cm) water. This concentration is the recommended concentration for both manual or ultrasonic cleaning.
- 3 If you use a glass graduated cylinder, cover the end of the ion transport capillary with a 1-mL pipette tip to protect the metalized plating.
- 4 Trim the pipette tip to approximately 4 cm so that the capillary can be immersed in the cleaning solution.
- 5 Place the ion transport capillary upright in a graduated cylinder and fill with Alconox Powdered Precision Cleaner solution.
- 6 Sonicate the graduated cylinder that contains the ion transport capillary in an ultrasonic cleaner for 10 to 15 minutes. Do not clean longer than 15 minutes.

### CAUTION

**Sonication should be done under a fume hood.**

- 7 Rinse the capillary and graduated cylinder several times with deionized water.
- 8 Fill the graduated cylinder with deionized water and sonicate for 10 to 15 minutes.

**Maintenance****Cleaning the capillary**

- 9** Remove the ion transport capillary from the graduated cylinder and remove the pipette tips (if any were used).
- 10** Blow out excess water from the ion transport capillary bore with nitrogen.

## Cleaning a clogged capillary

This EMF item relies on the rough vacuum reading to determine a clog in the capillary/capillary. If the rough vacuum reading falls below a value of 1.4 Torr, the EMF item will be flagged.

### Schedule

When the rough vacuum reading flags an error.

### Equipment List

- Clean powder-free nitrile gloves
- LC/MS-grade isopropanol
- Capillary (new, if replacing)

### Steps

- 1 Put on clean, powder-free nitrile gloves.
- 2 Remove and replace the capillary with a new unit, or reinsert the capillary after cleaning and drying.
- 3 Monitor the rough vacuum level to ensure that it does not fall below 1.4 Torr.

## Flushing the Calibrant Delivery System

### Schedule

When there is suspected contamination of the CDS, low tune response, or possible blockage in the CDS, flushing the Calibrant system may be required.

### WARNING

This procedure risks exposure to hazardous, toxic, or flammable solvents and reagents. Wear appropriate Personal Protective Equipment as described in the material handling and safety data sheet supplied by the chemical vendor, and always follow good laboratory practice.

### Equipment List

- Clean, powder-free gloves
- Ultrapure LC/MS Grade Acetonitrile
- Ultrapure LC/MS Grade Water
- Tuning solution

### Steps

- 1 Stop the LC/calibrant flow to the MS.
- 2 Disconnect sample tubing from the top of the nebulizer and place into a clean beaker or waste bottle.
- 3 Remove the CDS bottle and discard any old tune solution.
- 4 Rinse the CDS bottle with LC/MS grade acetonitrile and then LC/MS grade water.

### NOTE

In the case of a highly contaminated bottle, the bottle can be cleaned with Alconox and hot water (60 to 70 °C), then rinsed as per step 4.

- 5 Flush the CDS with 50/50 (v/v) LC/MS grade acetonitrile and LC/MS grade water:
  - a Fill the rinsed CDS bottle with approximately 20 to 30 mL of the acetonitrile/water mixture.
  - b Install the bottle and turn on the calibrant flow.
  - c Run the calibrant flush for at least 10 min.
- 6 Reattach the sample tubing to the top of the nebulizer.

- 7 Repeat step 5 with just LC/MS grade acetonitrile and flush for at least 10 min.

**NOTE**

To confirm cleaning procedures, monitor the MS spectrum and watch the contamination decrease over time.

- 8 Discard any remaining solvent and add fresh tune solution to the bottle.
- 9 Flush the fresh tune solution through the CDS for 5 min. Monitor tune ions to ensure that response is adequate.

## Replacing the electron multiplier horn (Ultivo only)

### Schedule

When sensitivity is poor and autotune consistently sets the detector gain to its maximum value.

### Equipment List

- Clean, powder-free nitrile gloves
- Long-nose pliers
- Electron multiplier horn

### CAUTION

**Take care when you perform this procedure. Damages that you cause during maintenance are not covered under warranty. If you need assistance, contact Agilent support.**

### Steps

- 1 Remove the left side cover.
- 2 Remove the detector horn carrier.
- 3 Disconnect the signal wire from the electron multiplier horn.
- 4 Open the retaining clip.
- 5 Remove the electron multiplier horn.
- 6 Install the new electron multiplier horn.
- 7 Close the retaining clip.
- 8 Connect the signal wire to the pin on the electron multiplier horn.
- 9 Install the detector horn carrier.
- 10 Install the left side cover.

## Replacing the MS selection valve rotor seal (Ultivo only)

### Schedule

After 10,000 diverter valve switches.

### Equipment List

- 9/64-inch hex key
- MS selection valve rotor seal

### Steps

- 1 Stop the flow of LC solvent to the instrument.
- 2 Open the Calibrant Delivery System (CDS) door.
- 3 Make a note of which port is plumbed to which tubing & unplug all the connections of MS selection valve.
- 4 Use the 9/64-inch hex key to remove the three hex head screws from the stator face of the selection valve.
- 5 Remove the rotor seal and replace it with a new one. Be sure to install it in the proper orientation.
- 6 Use the 9/64-inch hex key to fix the three hex head screws from the stator face of the selection valve.
- 7 Plug in all the connections of the MS selection valve.
- 8 Close the CDS door.



## Cleaning the corona needle

### Schedule

When you observe decrease sensitivity, decreased signal stability and increase corona voltage during APCI operation.

### Equipment List

- Clean, powder-free nitrile gloves
- Clean lint-free cloth
- LC/MS-grade isopropanol
- 4000 grid abrasive paper

### Steps

- 1 Before beginning any steps in this maintenance procedure, put on clean, powder-free nitrile gloves.

#### WARNING

**The needle and related parts can be very hot. Do not touch the needle or related parts until they are cool.**

- 2 Pull the corona needle assembly out of the spray chamber.

#### CAUTION

**Do not bend or blunt the tip of the needle, it will decrease system performance. Sharpening the needle is not needed.**

- 3 Fold a piece of 4000 grit abrasive paper over the base of the needle.
- 4 Pull and twist the 4000 grit abrasive paper along the needle and off the tip of the needle.

#### CAUTION

**Do not hit tip of the corona needle. The tip can bend, which can decrease system performance.**

- 5 Starting at the base of the needle, wipe the needle with a clean lint-free cloth. The cloth can be dry or dampened with LC/MS-grade isopropanol.
- 6 Reinstall the corona needle assembly in the spray chamber.

## Replacing the corona needle

### Schedule

Perform this procedure when symptoms indicate poor corona needle performance and cleaning the needle does not restore performance.

### Equipment List

- Clean, powder-free nitrile gloves
- Corona needle

### Steps

- 1 Before beginning any steps in this maintenance procedure, put on clean, powder-free nitrile gloves.
- 2 Pull the corona needle assembly out of the spray chamber.
- 3 Remove the needle collar from the corona needle shaft.
- 4 Remove the old corona needle from the collar.
- 5 Install a new corona needle, with its integral ferrule, in the collar.
- 6 Turn the collar onto the needle holder and tighten it by hand.

### CAUTION

**Do not hit tip of the corona needle. The tip can bend, which can decrease system**

- 7 Reinstall the corona needle assembly in the spray chamber.

## Disinfection

### Schedule

To prevent the spread of respiratory illness, disinfect your instrument as needed.

### Equipment List

- Clean, powder-free nitrile gloves
- Clean lint-free cloth
- Gown
- Isopropanol
- Mask

### Steps

- 1 Put on personal protective gear (gloves, mask, gown).
- 2 Make sure your instrument is cooled to room temperature.
- 3 Dampen a clean lint-free cloth with the 70:30 isopropyl alcohol:water mix.
- 4 Gently wipe external surfaces to be cleaned using moistened cloth. Do not allow any liquid to drip into the instrument.
- 5 Wipe the outer surface of cables and their connectors but do not touch the electrical connections (for example pins and plugs inside the cable or connection port).
- 6 Use one cloth per instrument to prevent cross contamination.
- 7 Dispose of the cloth appropriately.
- 8 Allow all surfaces to completely air-dry. No moisture should be present on the instrument surfaces.
- 9 Discard the gloves and other personal protective equipment or clean them in an approved process, then wash your hands.

## Source Maintenance

### Changing to a source that uses a different tuning mix

#### Schedule

Every time you change a source that uses a different tuning mix.

#### Equipment List

None

#### Steps

- 1 Right-click the TQ device pane and select **Calibrant**.
- 2 Run the calibrant for 5 minutes.
- 3 Perform a checktune. See **"Calibrating the LC/TQ (Checktune)"** on page 44.
- 4 If the checktune results are not acceptable, run autotune on a supported tuning source. See **"Calibrating the LC/TQ (Autotune)"** on page 48.
- 5 When the instrument is ready, load or create the method to use with the source.
- 6 Change the method settings for the new source.

### Installing and removing sources

#### Schedule

Every time you change a source that uses a different tuning mix.

Before you begin:

- Do a complete autotune (see **"Calibrating the LC/TQ (Autotune)"** on page 48). If an autotune is not available, do a checktune (see **"Calibrating the LC/TQ (Checktune)"** on page 44).
- If the tune report does not show good results, tune the instrument. If needed, change the source to one that supports autotune.

- Put the system in Standby mode.

**NOTE**

In the tune view or context, turn down the gas temperature as low as possible. Leave the gas flow on for 30 minutes to cool the source.

Once complete, proceed to the desired source removal and installation instructions.

## Electrospray Ionization (ESI) source

### Removing

- 1 Disconnect the nebulizer sample line.
- 2 Disconnect the heating cable.
- 3 Disconnect the sheath gas line at the connector and unplug it.
- 4 Disconnect the AJS HV cable delivering AJS nozzle voltage.
- 5 Disconnect the Multimode cable delivering AJS nozzle voltage.
- 6 Open the latch of spray chamber.
- 7 Open the latch of spray chamber.

### WARNING

**The spray chamber operates at very high temperature. Do not continue until the spray chamber is cool.**

- 1 Open the spray chamber.
- 2 Remove the ion source by lifting it along the axis of its hinges.

### WARNING

**The spray shield can be hot. Be careful not to burn yourself when you remove the spray shield.**

- 3 If you are changing to a different source type, remove the spray shield

### Installing

- 1 Install the spray shield, making sure the small hole is at the top of the "12 o'clock position". If needed, use a T10 Torx screwdriver to loosen the two screws in the end plate.
- 2 Rotate the ESI spray shield clockwise until the hole is in the correct position.
- 3 Gently tighten the Torx screws again.
- 4 Install the source.
- 5 Close the source.
- 6 Connect the MultiMode cable delivering AJS nozzle voltage.
- 7 Connect the heater cable.
- 8 Connect the sample nebulizer gas tubing.
- 9 Connect the nebulizer sample line.

**10** Connect the reference nebulizer sample line and sample nebulizer gas tubing.

**In the MassHunter Data Acquisition program:**

- 1** Turn on the LC/MS instrument.
- 2** While you wait for the set points to equilibrate, prepare and install the calibrant for the new ion source.
  - a** Rinse a clean calibrant bottle with LC/MS-grade acetonitrile.
  - b** Pour the appropriate ESI Calibrant into the calibrant bottle for your instrument.
  - c** Install the calibrant bottle into the calibrant delivery system.

**When all set points are equilibrated:**

- 1** In the tune view or context, turn on the calibrant.
- 2** Purge the calibrant line for 5 minutes.
- 3** Do a complete autotune. If an autotune is not available, do a checktune. If the tune report does not show good results, tune the instrument. If needed, change the source to one that supports autotune.
- 4** If the checktune results are not acceptable, run autotune on a supported tuning source.
- 5** When the instrument is ready, load or create the method to use with the ion source.
- 6** Change the method settings for the new ion source.

## Agilent Jet Stream (AJS ESI) source

### Removing

- 1 Disconnect the nebulizer sample line and sample nebulizer gas tubing.
- 2 Disconnect the heating cable.
- 3 Disconnect the sheath gas line at the connector and unplug it.
- 4 Disconnect the AJS HV cable delivering AJS nozzle voltage.
- 5 Disconnect the Multimode cable delivering AJS nozzle voltage.
- 6 Open the latch of the spray chamber.
- 7 Open the latch of spray chamber.

### **WARNING**

**The spray chamber operates at very high temperature. Do not continue until the spray chamber is cool.**

- 8 Open the spray chamber.
- 9 Remove the ion source by lifting it along the axis of its hinges.

### **WARNING**

**The spray shield can be hot. Be careful not to burn yourself when you remove the spray shield.**

- 10 If you are changing to a different source type, remove the spray shield

### Installing

- 1 Install the spray chamber.
- 2 Close the spray chamber.
- 3 Connect the MultiMode cable delivering AJS nozzle voltage.
- 4 Connect the heater cable.
- 5 Connect the sample nebulizer gas tubing.
- 6 Connect the nebulizer sample line.
- 7 Connect the reference nebulizer sample line and sample nebulizer gas tubing.



**Maintenance****Agilent Jet Stream (AJS ESI) source****In the MassHunter Data Acquisition program**

- 1 Turn on the LC/MS instrument.
- 2 While you wait for the set points to equilibrate, prepare and install calibrant for the new ion source.
  - a Rinse a clean calibrant bottle with LC/MS-grade acetonitrile.
  - b Pour the appropriate ESI Calibrant into the calibrant bottle for your instrument.
  - c Install the calibrant bottle into the calibrant delivery system.

**When all set points are equilibrated**

- 1 In the tune view or context, turn on the calibrant.
- 2 Purge the calibrant line for 5 minutes.
- 3 Do a complete autotune. If an autotune is not available, do a checktune. If the tune report does not show good results, tune the instrument. If needed, change the source to one that supports autotune.

## Atmospheric Pressure Chemical Ionization (APCI) source

### Removing

- 1 Disconnect the nebulizer sample line.
- 2 Disconnect the sample nebulizer gas tubing.
- 3 Disconnect the heater cable.
- 4 Disconnect the corona needle voltage cable.
- 5 For APPI, disconnect the heater cable.
- 6 Disconnect the serial output cable.
- 7 Disconnect the external power supply cable.
- 8 Open the latch of spray chamber.

### **WARNING**

**The spray chamber operates at very high temperature. Do not continue until the spray chamber is cool.**

- 9 Open the spray chamber.
- 10 Remove the ion source by lifting it along the axis of its hinges.

### **WARNING**

**The spray shield can be hot. Be careful not to burn yourself when you remove the spray shield.**

- 11 If you are changing to a different source type, remove the spray shield.

### Installing

- 1 Make sure the small hole is at the top ("12 o'clock position").
- 2 If needed, use a T10 Torx screwdriver to loosen the two screws in the end plate.
- 3 Rotate the ESI spray shield clockwise until the hole is in the correct position.
- 4 Gently tighten the Torx screws again.
- 5 Install the ion source, sliding it along the axis of its hinges.
- 6 Close the spray chamber.
- 7 Close the spray chamber latch.

**Maintenance****Atmospheric Pressure Chemical Ionization (APCI) source**

- 8 checktuneConnect the heater cable.
- 9 Connect the corona needle voltage cable.
- 10 Connect the sample nebulizer gas tubing.
- 11 Connect the nebulizer sample line.

**In the MassHunter Data Acquisition program**

- 1 Select the new source.
- 2 Turn on the LC/MS instrument. While you wait for the set points to equilibrate, prepare and install the calibrant for the new source.
- 3 Rinse a clean calibrant bottle with LC/MS-grade acetonitrile.
- 4 Pour the APCI Calibrant into the calibrant bottle.
- 5 Install the calibrant bottle into the calibrant delivery system.

**When all set points are equilibrated**

- 1 In the tune view or context, turn on the calibrant.
- 2 Purge the calibrant line for 5 minutes.
- 3 Do a complete autotune. If an autotune is not available, do a checktune. If the tune report does not show good results, tune the instrument. If needed, change the source to one that supports autotune.

## Multimode Ionization (MMI) source

### Removing

- 1 Disconnect the nebulizer sample line.
- 2 Disconnect the sample nebulizer gas tubing.
- 3 Disconnect the heater cable.
- 4 Disconnect the charging electrode cable.
- 5 Disconnect the corona needle voltage cable.
- 6 Open the latch of spray chamber.

### **WARNING**

**The spray chamber operates at very high temperature. Do not continue until the spray chamber is cool.**

- 7 Open the spray chamber.
- 8 Remove the ion source by lifting it along the axis of its hinges.

### **WARNING**

**The spray shield can be hot. Be careful not to burn yourself when you remove the spray shield.**

- 9 If you are changing to a different source type, remove the spray shield.

### Installing

- 1 Install the appropriate spray shield.
- 2 Make sure the dowels are at 6 and 9 o'clock positions.
- 3 Install the spray chamber.
- 4 Close the spray chamber.
- 5 Close the latch of spray chamber.
- 6 Connect the corona needle voltage cable.
- 7 Connect the charging electrode cable.
- 8 Connect the heater cable.
- 9 Connect the sample nebulizer gas tubing.
- 10 Connect the nebulizer sample line.

**Maintenance****Multimode Ionization (MMI) source****In the MassHunter Data Acquisition program**

- 1 Turn on the LC/MS instrument.
- 2 While you wait for the set points to equilibrate, prepare and install calibrant for the new source.
  - a Rinse a clean calibrant bottle with LC/MS-grade acetonitrile.
  - b Pour the MMI Calibrant into the calibrant bottle.
  - c Install the calibrant bottle into the calibrant delivery system.

**When all set points are equilibrated**

- 1 In the tune view or context, turn on the calibrant.
- 2 Purge the calibrant line for 5 minutes.
- 3 Run an autotune. If an autotune is not available, run a checktune. If the tune report does not show good results, tune the instrument. If needed, change the source to one that supports autotune.

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