6230 LC/TOF System
User Guide

with OpenLab CDS Software

Notices

Document Identification

D0146599 Rev. A.00

May 2026

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Software Revision

This guide is valid for OpenLab CDS Acquisition software 3.0 or higher.

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CAUTION

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WARNING

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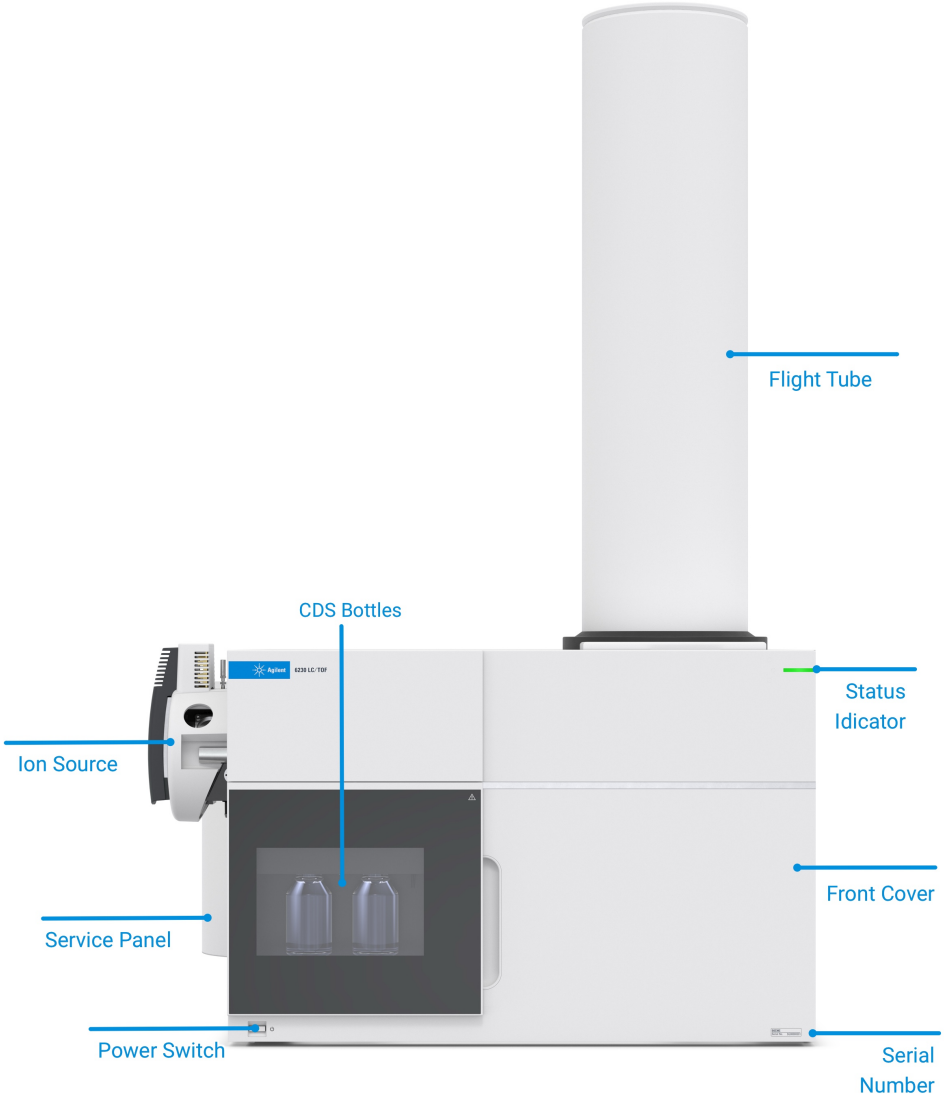
6230 LC/TOF

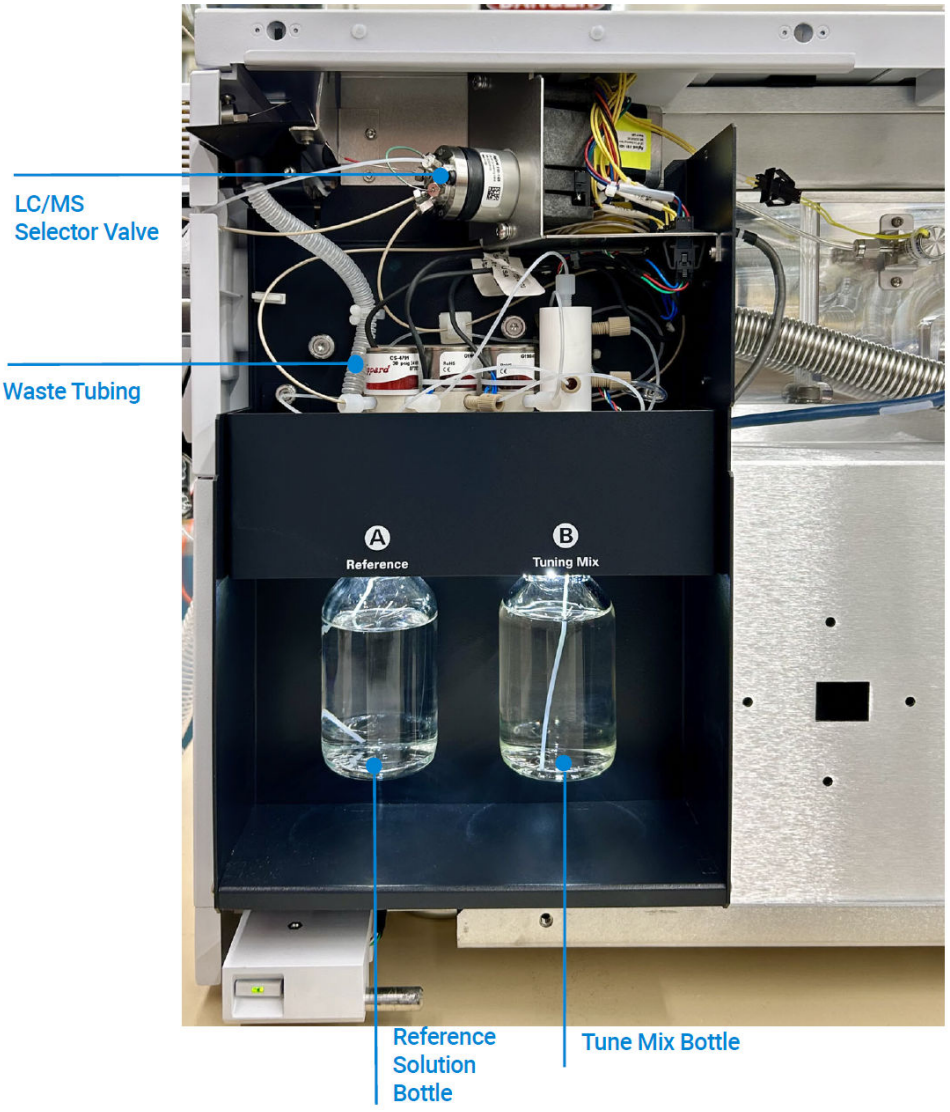
Front view

Figure 1. Front view of 6230 LC/TOF



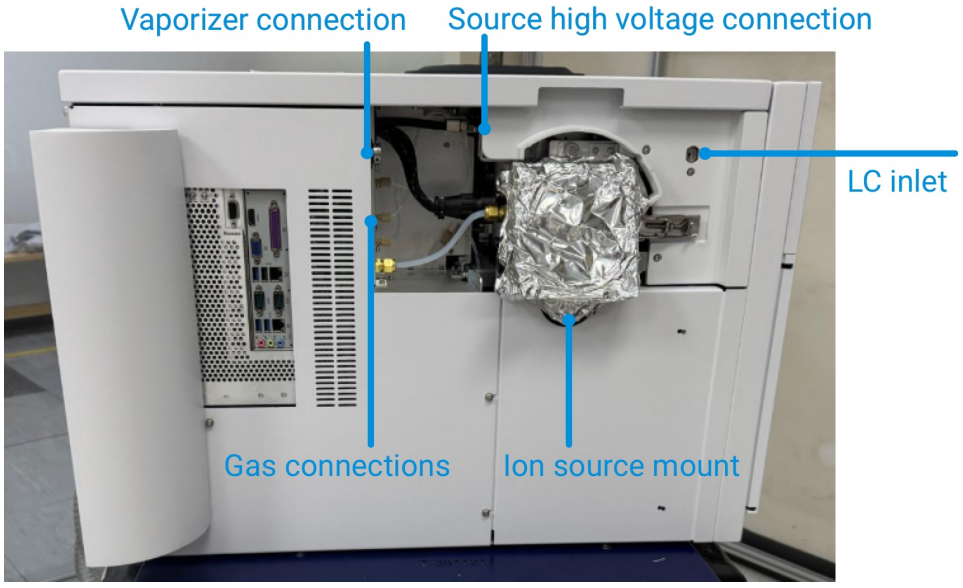
Calibrant Delivery System

Figure 2. Calibrant delivery system



Side view

Figure 3. Side view of 6230 LC/TOF



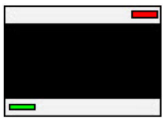
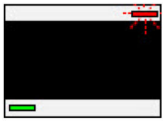
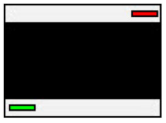

Ion source

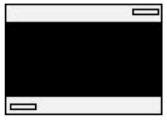
Back view

Figure 4. Back view of 6230 LC/TOF

Instrument Status Indicator Lights

Table 1. Status Indicator Lights on Instrument

	Instrument State = BOOTING (FPGA Loaded) Status LED = Blinking Yellow Power Switch LED = Yellow		Instrument State = ACQUISITION Status LED = Blinking Green Power Switch LED = Green
	Instrument State = BOOTING (LINUX Loaded) Status LED = Yellow Power Switch LED = Green		Instrument State = FAULT Status LED = Red Power Switch LED = Green
	Instrument State = PUMPING DOWN Status LED = Blinking Yellow Power Switch LED = Green		Instrument State = VENTING Status LED = Blinking Red Power Switch LED = Yellow
	Instrument State = STANDBY Status LED = Yellow Power Switch LED = Green		Instrument State = Vented Status LED = Red Power Switch LED = Yellow

	Instrument State = IDLE Status LED = Yellow Power Switch LED = Green		Instrument State = POWERING DOWN Status LED = Off Power Switch LED = Blinking Yellow
	Instrument State = BACKGROUND SCAN Status LED = Green Power Switch LED = Green		Instrument State = Off Status LED = Off Power Switch LED = Off

Instrument Status Indicators in OpenLab Acquisition

In the OpenLab Acquisition software, 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 AIC/workstation 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 to change 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) 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 - Prerun/Injecting: The instrument is on and is preparing to start acquisition.

Blue - Running, postrun: 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

NOTE

APCI and MMI ion sources are currently compatible with MassHunter Acquisition software only. For more information on those ion sources, see https://www.agilent.com/en/product/liquid-chromatography-mass-spectrometry-lc-ms/lc-ms-ion-sources.

Electrospray Ionization Dual 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 the ions are ejected (desorbed) into the gas phase. These ions are attracted to and pass through a capillary sampling orifice into the mass analyzer.

The dual-nebulizer ESI source contains a second nebulizer dedicated to the continuous introduction of a reference mass to ensure superior mass accuracy.

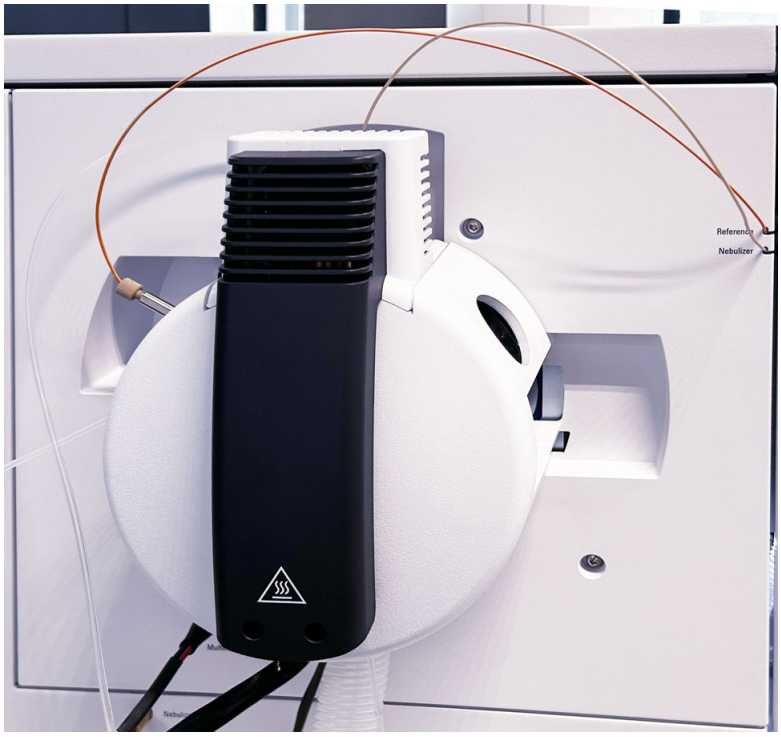
Figure 5. Dual ESI source with cover

Agilent Jet Stream (Dual AJS ESI) source

The Agilent Jet Stream (Dual AJS ESI) source:

- Uses the same ionization technique as the ESI source.
- Uses thermal gradient focusing technology, which is a process in which super heated nitrogen (N2) is used to improve ion generation and desolvation.
- Improves sensitivity 5x or more for many small-molecule compounds that undergo electrospray ionization.
- Utilizes a second sprayer to improve reference mass stability over a wide range of LC conditions.

Figure 6. Dual AJS ESI with cover



Atmospheric Pressure Chemical Ionization (APCI) source

In Atmospheric Pressure Chemical Ionization (APCI), the LC mobile phase is sprayed through a heated vaporizer (typically 250 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 7. APCI source with cover

2 Tuning

The tuning process determines the appropriate values to use for various instrument parameters to obtain the best results. The goal of this process is to optimize abundance, resolution, mass accuracy, and mass selection performance. Tuning works by infusing a sample with known masses into the source and then observing the mass peaks. Values of desired parameters are changed from a low value to a high value (or vice versa), keeping all other parameters constant, and the parameter values with the best results are selected.

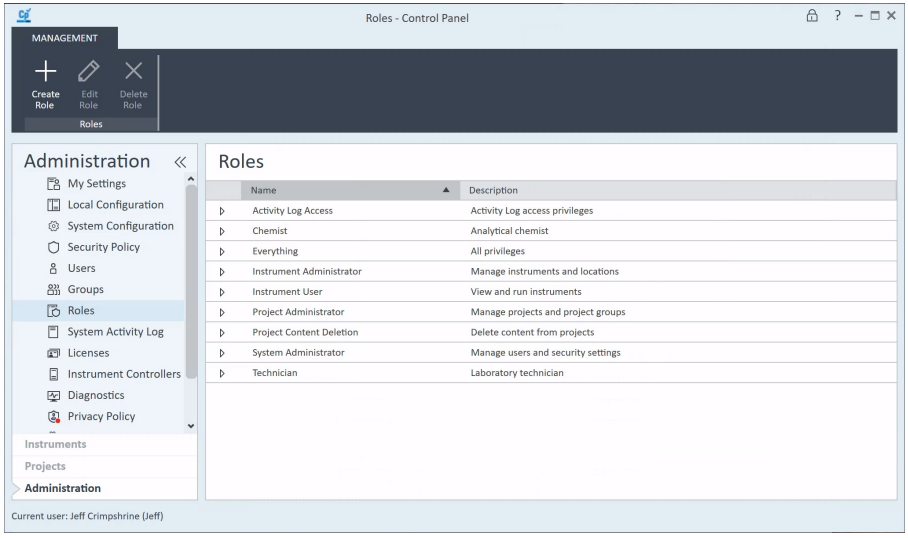
Roles

OpenLab Control Panel provides multiple roles available in the configuration when Authentication is enabled. Roles are collections of privileges that can be assigned to users or groups. Create a new role or use roles available in your system. The Control Panel includes the following roles:

- Everything
- System Administrator
- Instrument Administrator
- Project Administrator
- Instrument User
- Lab Manager

Additional roles are available depending on your OpenLab configuration.

The roles are described in the Control Panel on the Roles page.



NOTE

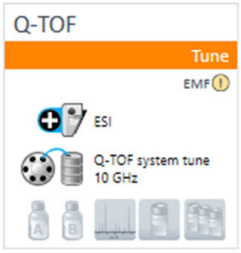
Only the Everything role has access to all roles and privileges. By default, only the Lab Manager role has the privilege to configure tunes. Other roles do not have access to this configuration and are only able to perform tunes from a predefined list configured by the Lab Manager. See OpenLab Control Panel help for more information on authentication, roles, and privileges.

Configure Tune

A tune can only be run on instrument modes that have first been configured and enabled in the Configure Tune section. System tune is always enabled by default.

1. In Acquisition, click **Method Editor** in the Windows section of the Ribbon to display the Method Editor window.
2. In the Method Editor window, click the **MS Q-TOF** tab.
3. Click **Tune > Configure Tune** in the left pane.
   A list of instrument modes and tunes is displayed.
4. Click Tune control **Tune control**.
   This button locks control of the TOF instrument and changes the status of the instrument to Tune. A single sample run or a sequence cannot be started when Tune has control of the instrument.

   Figure 8. Tune Status

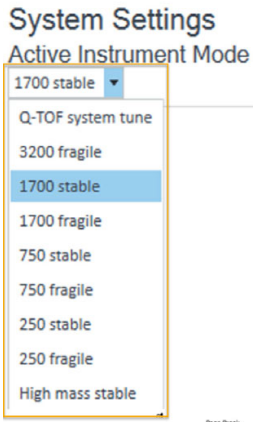
   When clicked, tune setpoints are applied. If an action is not selected within the timeout period of three minutes, the system will go back to the method setpoints.
5. Toggle the **Selected** switch to select specific instrument modes and tunes.
6. Click the +/- button to select a specific Polarity for the instrument mode. There are three states to choose from, +, -, and +/-.

7. Click the Spectrum mode drop-down and select **High res.** or **Dynamic range**. The combination of Slicer in Sensitivity and Spectrum mode in High res. is not compatible.
   For more information on Spectrum mode settings, see the LC/MS (Q-)TOF Driver help.
8. (Optional) Double-click in the **Description** field to modify the default description of the predefined instrument modes.

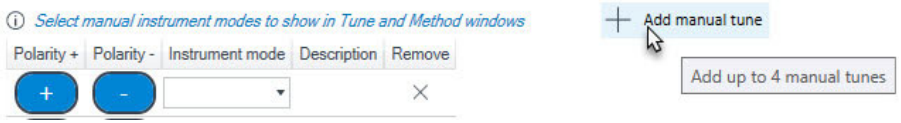
NOTE

System tune is always selected as this tune uses the default values as the starting point and includes all the elements involved in mass resolution.

9. Click the Active Instrument Mode drop-down under System Settings to view the changes.



10. Click Tune control **Tune control** to release control of the TOF instrument.
    Settings are selected using instrument mode and polarity.
    In addition to these predefined instrument modes/tunes, the lab manager role allows the creation of up to 4 manual tunes that are made visible to operator and lab technician, if needed.



Dilute the Agilent Tuning Mix

Introduction

Depending on LCMS system model, ion source, and tune type, the tuning mix may need to be diluted before use. The goal of diluting the tuning mix is to produce peaks in an abundance range optimal for the automatic tuning algorithms. Negative polarity may require a different dilution recipe because many of the tuning mix ions tend to be more abundant in negative polarity.

ESI-L Low Concentration Tuning Mix typically requires the addition of HP-0321 from the Biopolymer Reference Mass Kit (G1969-85003).

Dilution Instructions

Before you begin, gather the following materials:

- G1969-85000 ESI-L Low Concentration Tuning Mix
- G1969-85003 Biopolymer Reference Mass Kit, which contains the HP-0321 solution (for Dual AJS ESI)
- G1969-85020 MMI-L Low Concentration Tuning Mix (for Multimode source)
- HPLC-grade acetonitrile (must be suitable for HPLC, spectrophotometry, and pesticide residue analysis)
- Water, 18 MΩ-cm resistivity or better and free of organics
- Glass CDS bottle (p/n 9300-2576) and cap (p/n 9300-2575)

Guidelines:

- The materials shipped with the instrument are of sufficient purity for this purpose.
- In the final tune report, make sure all abundances listed in the report are between 50,000 and 650,000 counts for proper correction of the mass.

- Dilute tune mix when there is an error message that instructs you to, or when the tune report shows calibration abundances greater than 750,000 counts. Dilution of the tuning mix up to 200-fold is sometimes needed for instruments with exceptional sensitivity. Be careful when diluting at amounts greater than 50-fold because contamination and sodium trifluoroacetate adducts can become problematic at higher dilutions.
- The amount of water added affects the response of 118 m/z, with higher amounts yielding a greater response and vice versa. Up to 5% (v/v) of water can be added. Do not add more water than that because some components of the tuning mix can precipitate under these conditions.
- If tune mass abundances are less than 10,000 counts, the tuning mix is overdiluted. Dilutions at this level can result in poor mass accuracies.
- Adding the components in the order listed helps avoid precipitation of any components of the tuning mix.
- Store the tuning mix in the refrigerator when it is not being used for extended periods of time.

Instructions:

- To make dilutions add components in the tables below, in the order listed, to a clean glass CDS bottle, then mix the contents thoroughly and install the bottle on the instrument. The recipes below will make 100 mL of diluted tuning mix.

Dilution guidance for the 6230 LC/TOF

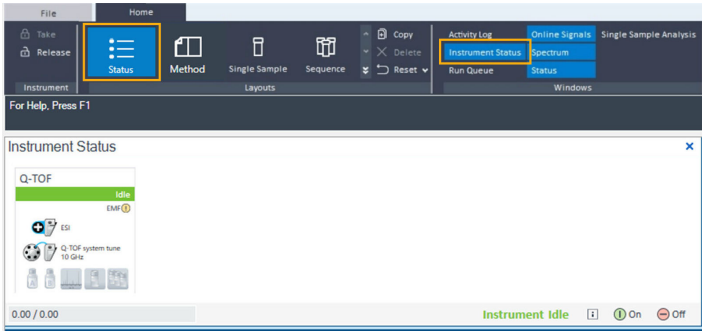
6230 LC/TOF with ESI or Dual ESI Source	Positive and Negative Mode
Undiluted Tuning Mix	25 mL ESI-L
Acetonitrile	71.25 mL
Water	3.75 mL

6230 LC/TOF with Dual AJS ESI Source	Positive Mode	Negative Mode
Undiluted ESI-L Tuning Mix	10 mL ESI-L	2.5 mL ESI-L
Acetonitrile	85.5 mL	95.6 mL
Water	4.5 mL	1.9 mL
0.1 mM HP-0321 (included in the Biopolymer Reference Mass Kit)	5 µL	N/A

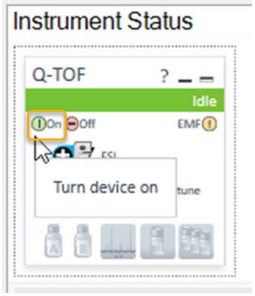
6230 LC/TOF with Multimode Source	Positive and Negative Mode
Undiluted MMI-L Tuning Mix	25 mL MMI-L
Acetonitrile	71.25 mL
Water	3.75 mL

Starting the instrument

1. Follow the procedures in "Starting Up and Shutting Down the Instrument" to begin operation of the instrument.
2. If the Instrument Status window is not visible in the OpenLab Acquisition software:
   - Open the Status layout.
   - On the ribbon, click **Instrument Status** in the **Windows** section.



3. Hover over the TOF device pane and click **On**.



4. Monitor baseline and adjust the plot if necessary. See "Monitoring baseline and adjusting plot".

Mass Calibration

Mass Calibration performs a TOF mass calibration on the active instrument mode by infusing a solution with known masses into the source and measuring the actual flight times for ions of the masses.

For optimum performance, run a mass calibration before analysis each day, or after changing high-voltage manual tune parameters or adjusting the mass range. During normal operation, mass calibration takes approximately 5 minutes. To ensure the mass accuracy of your data, a mass calibration is required when selecting a different active instrument mode.

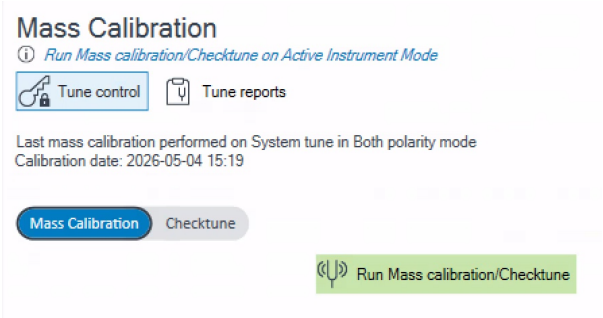
NOTE

Only the active instrument mode can be calibrated.

A mass calibration can only be run on instrument modes that have first been configured and enabled in the . System Tune is always enabled by default.

Follow these steps to perform a mass calibration:

1. In the Method Editor window, click the **MS TOF/Q-TOF** tab.
2. Click **Tune > Mass Calibration** in the left pane.
3. Click Tune control **Tune control**.
4. Select **Mass Calibration**.



5. Click **Mass calibration/Checktune**. When the tune completes, review the report.

6. Click  **Tune control** to release control of the LC/TOF instrument.

Checktune

Checktune is used to determine whether the instrument is correctly tuned by applying the current tune parameters to the source and detector to confirm that the signal intensity and resolution is within the expected range. A checktune performs a TOF mass calibration and checks the detector for the currently selected active instrument mode. A checktune is automatically performed when running an autotune.

During normal operation, a checktune will take approximately 20 minutes.

A checktune can be run with the following ion sources:

- ESI
- Dual AJS ESI

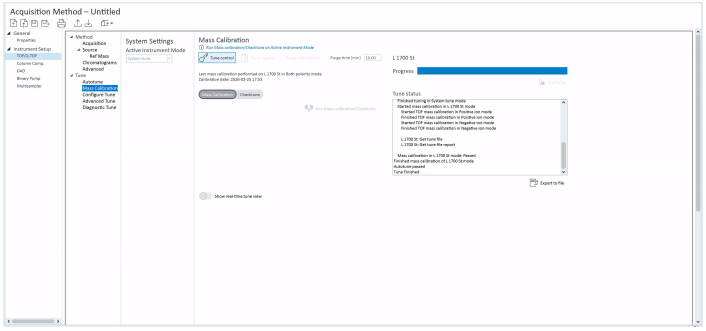
NOTE

A checktune is only run on the currently selected instrument mode in the Active Instrument Mode drop-down.

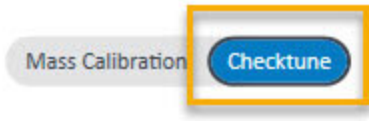
A Checktune can only be run on instrument modes that have first been configured and enabled in the . System Tune is always enabled by default.

Follow these steps to perform a checktune:

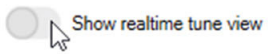
1. In the Method Editor window, click the **MS TOF/Q-TOF** tab.
2. Click **Tune > Mass Calibration** in the left pane.
3. Click Tune control **Tune control**.



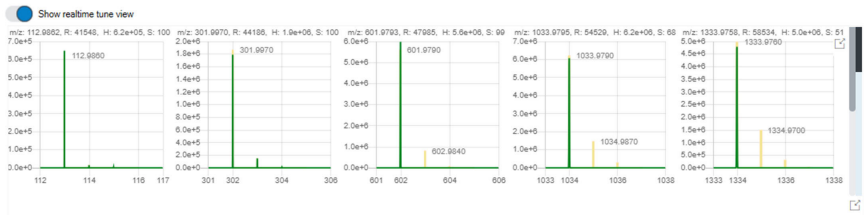
4. Select **Checktune**.



5. Activate **Show realtime tune view** to view the real time data acquisition.



6. Click Run Mass calibration/Checktune. View the progress of the tune in the Real Time tune results.



7. When the tune completes, review the report.
8. Click Tune control **Tune control** to release control of the LC/TOF instrument.

Autotune

Autotune is an automated tuning program that adjusts the MS for good performance over the entire mass range. During an autotune, the tuning mix is delivered by the calibrant delivery system, which is switched on automatically during the tune.

During normal operation, the base System tune takes approximately 2 hours. Autotune takes longer to complete when additional instrument modes are enabled. Perform an autotune on a monthly basis to ensure that TOF resolution and sensitivity are optimized.

An autotune can be run with the following ion sources:

- ESI
- Dual AJS ESI

Autotune can only be run on instrument modes that have first been configured and enabled in the . System Tune is always enabled by default.

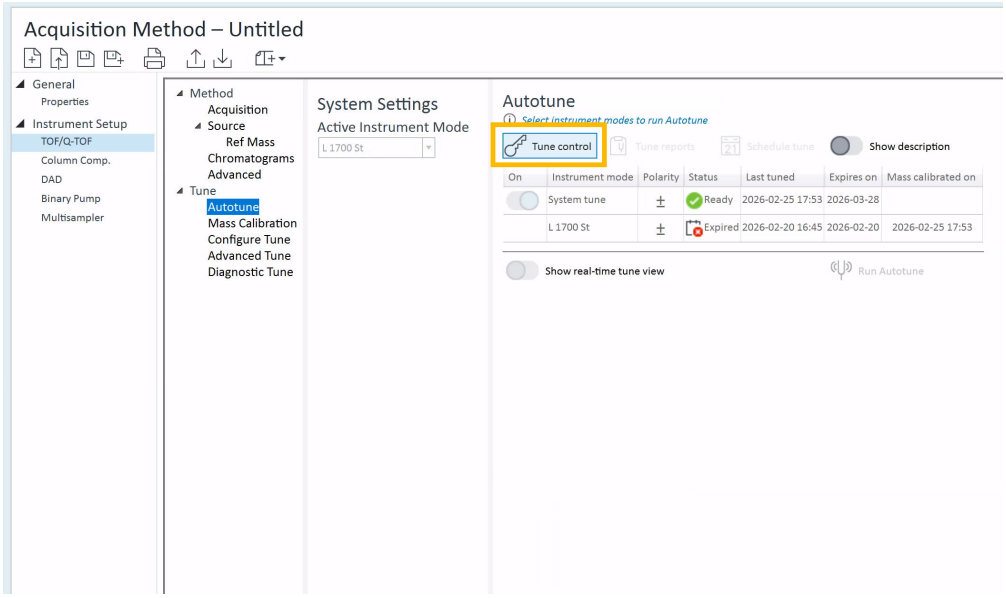
NOTE

Autotune will perform an autotune on all instrument modes enabled in the Autotune table. Autotune will also perform a checktune and mass calibration on the currently selected instrument mode in the Active Instrument Mode drop-down.

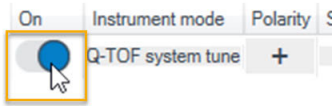
Follow these steps to perform an autotune:

1. In the Method Editor window, click the **MS TOF/Q-TOF** tab.
2. Click **Tune > Autotune** in the left pane.

3. Click Tune control **Tune control**.



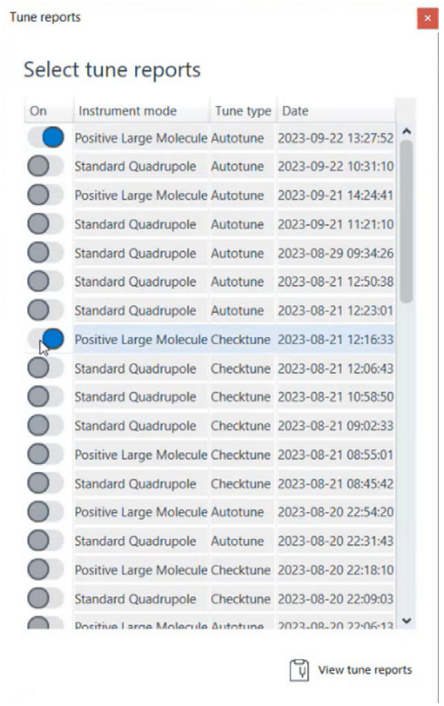
4. Use the toggles in the On column of the Autotune table to enable one or more instrument modes.



5. (Optional) Activate **Show realtime tune view** to view the real time data acquisition.
6. Click **Autotune**.
7. When the tune completes, review the report.
8. Click Tune control **Tune control** to release control of the LC/TOF instrument.

Generating a Detailed Tune Report

1. In the Method Editor window, click the **MS TOF/Q-TOF** tab.
2. Click **Tune > Autotune** in the left pane.
3. Click Tune control **Tune control**.
4. Click **Tune Reports**. If this button is not available, run an autotune, checktune, or mass calibration first.
5. Use the toggles to select reports for viewing.



6. Click **Tune Reports** to generate PDFs for viewing in a PDF viewer.
7. Click Tune control **Tune control** to release control of the TOF instrument.

Advanced Tune

In the Advanced Tune section, launch Advanced Tune View to create a manual tune.

NOTE

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

1. In Acquisition, in the Method Editor window, click the **MS TOF/Q-TOF** tab.
2. Click **Tune > Advanced Tune** in the left pane.
3. Click Tune control **Tune control**.
4. Click Launch advanced tune view . The Advanced Tune View opens.

For more information on creating a manual tune, click the **Help** tab in Advanced Tune View.

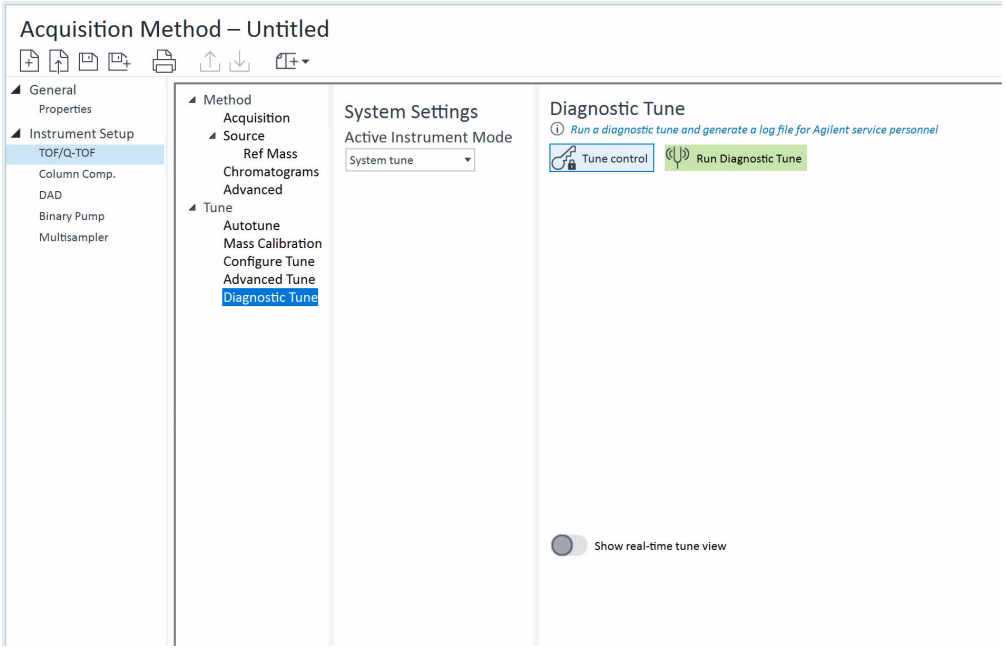
Diagnostic Tune

Diagnostic Tune is only performed when an autotune has failed, and should only be run at the request of Agilent service personnel. During normal operation, Diagnostic Tune will last approximately 3 hours and will create a log file when finished.

A diagnostic tune can only be run on instrument modes that have first been configured and enabled in the . System Tune is always enabled by default.

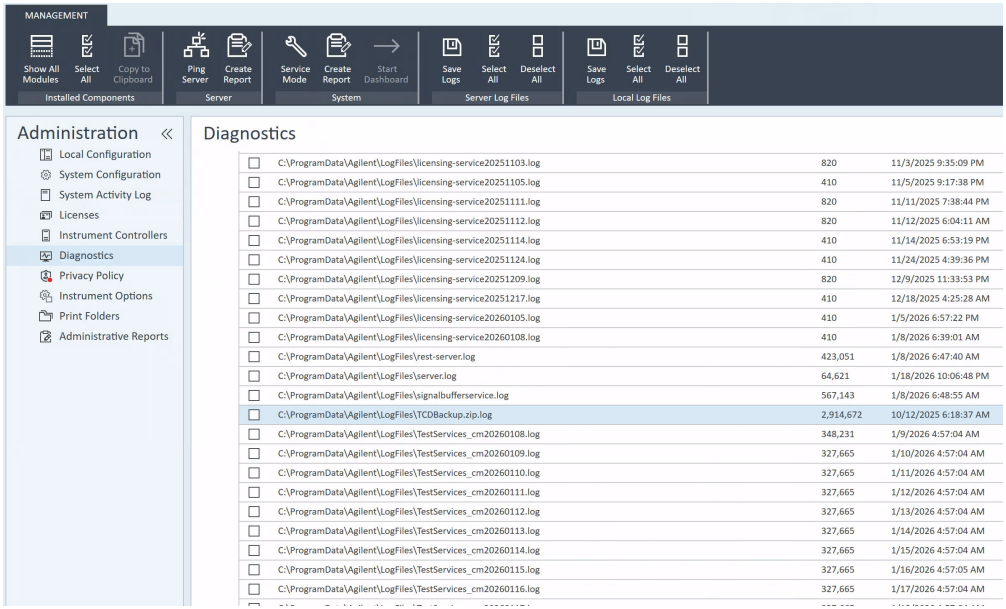
Follow these steps to perform a diagnostic tune:

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



3. Click Tune control **Tune control** in the toolbar to lock control of the instrument.

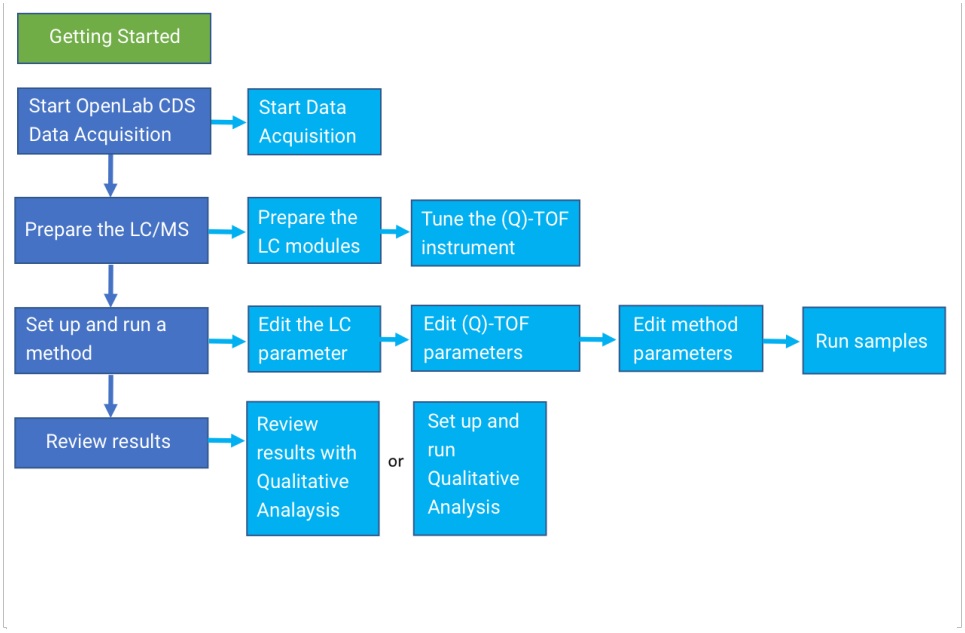
4. Click Run Diagnostic Tune to start a diagnostic tune.
   The Progress bar and Tune status window displays the progress and status of the tune.
5. In OpenLab Control Panel, navigate to the **Control Panel > Administration > Diagnostics** page.
   The file path for the log is
   C:\ProgramData\Agilent\LogFiles\TCDbackup.zip.log



3 Basic Operation

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 the Instrument

1. Turn on the power to the instrument
2. Pump down the TOF.
3. In the Instrument Status window, right-click the **TOF** device, and select **On**.

Putting the instrument in Standby

In OpenLab Acquisition, right-click the **TOF** device in the **Instrument Status** window, and select **Standby**.

Turning off the instrument

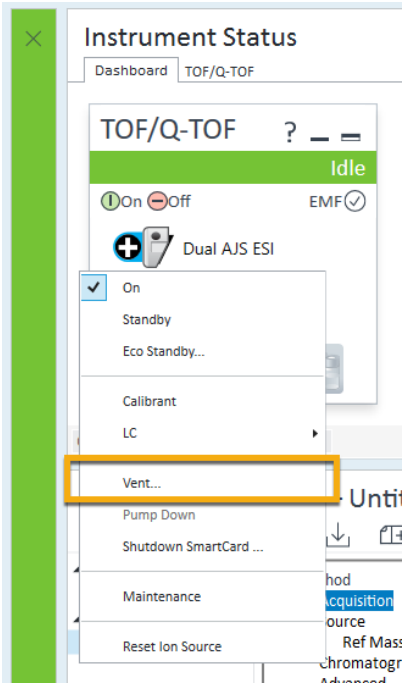
Before turning off the instrument, complete any data acquisition steps and save your data.

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. Put the TOF instrument in Standby. See “Putting the instrument in Standby”.

2. In OpenLab Acquisition, right-click the **TOF** device in the **Instrument Status** window, and select **Vent** to vent the system. Click **Yes** to continue.



3. Wait until the instrument completely vents.
4. Close the OpenLab Acquisition software and shut down the computer.
5. Turn off the power to the instrument.

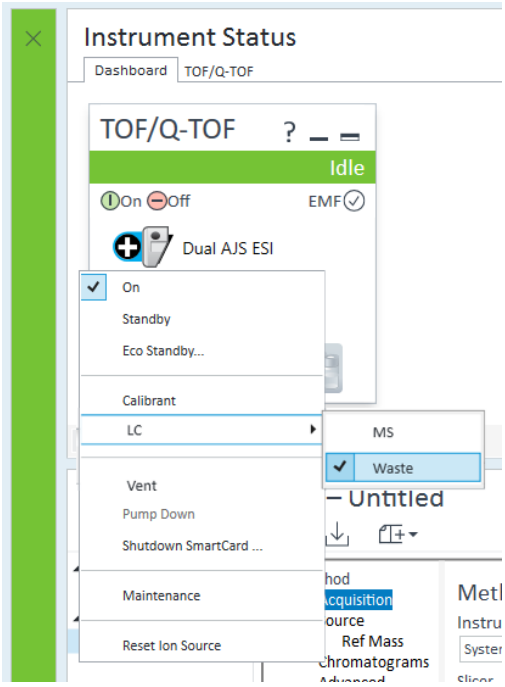
Preparing the LC Modules

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.

1. Right-click the **TOF** device in the Instrument Status window.
2. Select **LC > Waste**.



3. Purge the LC pump.

- Follow the specific user guide directions for purging the installed pump model.

4. Set up to condition or equilibrate the column.
   a. In the Method layout, click **Download to instrument** to download the method parameters to the instrument.
   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.

Preparing the 6230 LC/TOF

Performing a checktune or autotune

See Chapter 2, "Tuning".

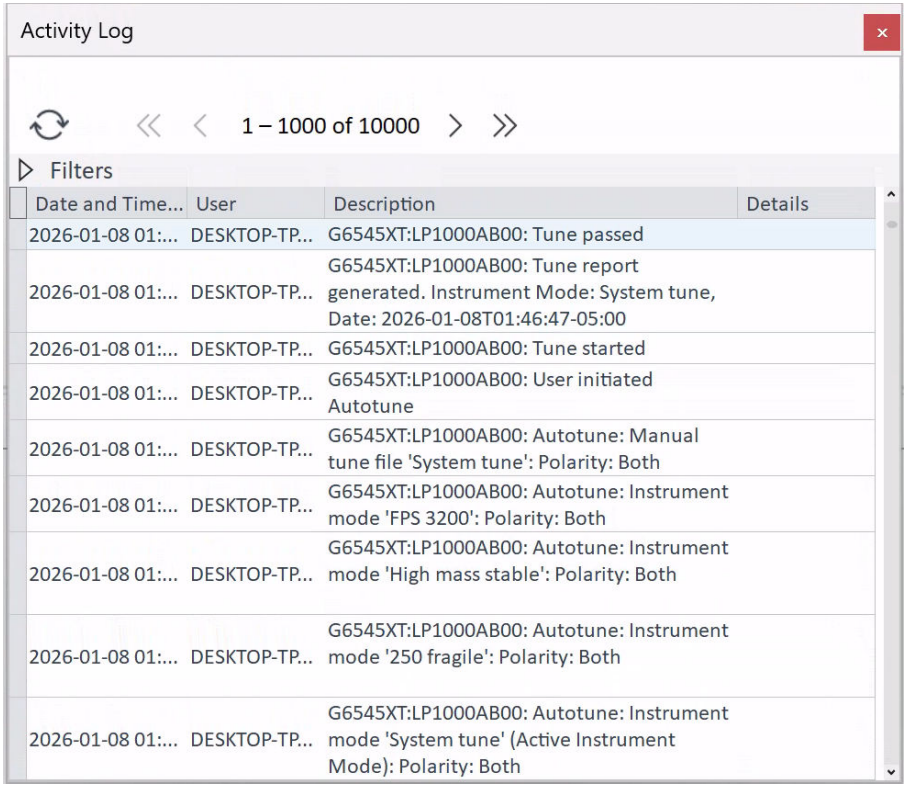
Switching LC stream to MS

After you condition the column and tune the instrument, switch the LC stream from **Waste** to **MS**. See “Switch LC stream to Waste” for more information.

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 **Activity Log** from the Windows section in the ribbon, and view the logged events.



Create an Acquisition Method

1. Open the **Method** layout.
2. Enter values for all of the LC modules under **Instrument Setup** in the left pane.
3. Click **New Method** .
4. Enter your instrument's method parameters as applicable. For details on entering these parameters, place your cursor in the instrument parameters area and press **F1**.
5. To download the settings to the instrument, click .
6. To save the method, click **Save As**. Name the method and click **OK**.

Setting Up and Running a Single Sample

Enter the information in the Single Sample Analysis window before running the method; once the run has started, this information cannot be changed. The information in this window is not part of the method, and it is not saved when the method is saved. When you are running a sequence, enter the information in the Sequence window.

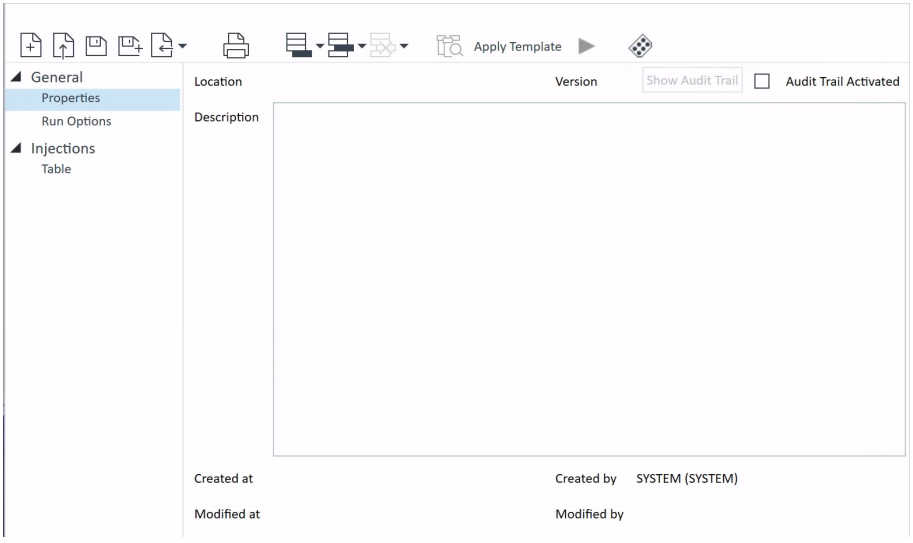
1. Click the **Single Sample** layout.
2. Enter the **Sample name**. The **Sample name** appears on any reports generated. Use the tokens to simplify this entry.
3. Select the **Acq. method**. This method is used to acquire the data. Click **browse** to open and select an acquisition method. An acquisition method has the extension .amx.
4. Select the **Proc. method**. This method is used to process the data. Click **browse** to open and select a processing method. A processing method has the extension .pmx.
5. Select the **Result path**. This path indicates where the data file will be saved. Click **browse** to open and select the directory path.
6. Enter the **Result** name. Use the tokens ▷ to simplify this entry. A token is a parameter in the system. Include any of the following in any order: **Acq. method**, **Increment number**, **Instrument name**, **Local date & time**, **Proc. method**, **Sample name**, **Short local date & time**, **Username**, and **Vial**. When the run is started, the file name is determined based on the selected parameters.
7. Enter the **Autosampler** information:
   a. Select the **Injection source**.
   b. Enter the **Injection volume**.
   c. Enter the **Vial**.
8. Review the **Processing Section**. Click ▷ if the Processing Section is hidden.
9. *Optional*. Enter the **Sample Description**. Click ▷ if the Sample Description box is hidden.

10. Click **Run**.

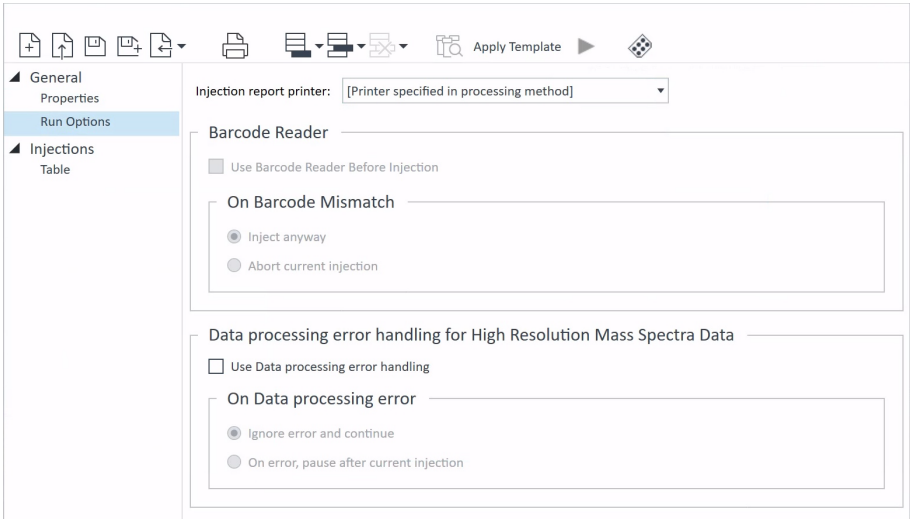
Setting Up and Running a Sequence

A sequence can only be run after an acquisition method has been developed.

1. Click the **Sequence** layout.
2. In the Sequence window, enter the **Properties** information.
   a. In the navigation pane at the left of the window, click **General > Properties**.
   b. Select or clear **Audit Trail Activated**. Audit Trail cannot be turned off once it has been enabled.
   c. Enter the **Description** for the sequence.

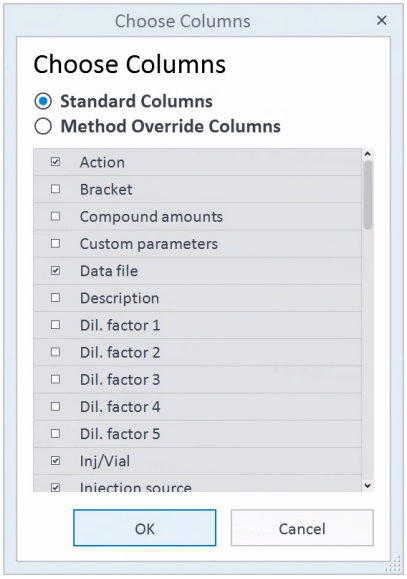


3. Enter the **Run Options** information:
   a. In the navigation pane at the left of the window, click **General > Run Options**.
   b. Select or clear **Use Barcode Reader Before Injection**.
   c. Click either **Inject anyway** or **Abort current injection**.



4. *Optional*. Add a column to the Sequence table.
   a. In the navigation pane at the left of the window, click **Injections > Table**.

b. In the upper left corner of the Sequence table, click . The Choose Columns dialog opens.



c. Select the desired column (or columns).

d. Click **Method Override Columns**.

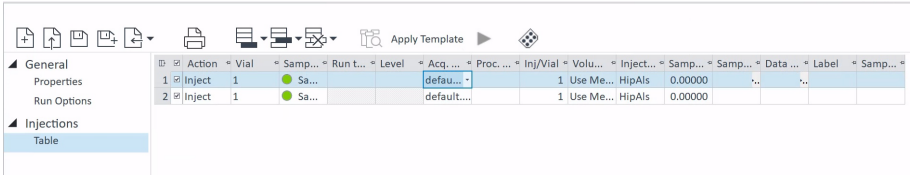
e. Select the desired override column (or columns).

f. Click **OK**.

5. Enter the **Table** information:

a. In the navigation pane at the left of the window, click **Injections > Table**.

b. Enter the information for each injection.



6. Select the rows to submit as part of the run. By default, all rows are selected.
7. To save your results to a sub-folder inside your Results folder, change the **Result Path** by clicking browse and creating a new folder. Results cannot be saved to an existing .sirslt folder.

8. The **Result name** defaults to the last filename used for this instrument and project. Enter a filename by typing in the field or using tokens. If left blank, the instrument name and local date & time is used for the filename.
9. Select to **Save result as**:
   - **Separate single injections** to save each sample injection in the sequence as an individual result set. When using this option, result set names will be based on the value of the **data file** column for each sequence row. For example:
     - DataFileName: A1
     - DataFileName: B1
     - DataFileName: A2
     - DataFileName: B2
10. *Optional*. Click Validate to validate the sequence against the specified acquisition method. The columns validated are **Acq. method**, **Volume**, and any override parameters. If invalid entries are found, correct those entries.
11. Click Run. If this is a new "Untitled" sequence, the sequence file is saved as the instrument name + the local date and time.
    Submitted sequences are placed in the **Run Queue**, where runs can be stopped or paused, and sequences can be edited. A result folder (.rslt) is created when the run is added to the Run Queue.

Run a sequence to optimize a parameter

Use a sequence to optimize a method parameter. For example, to find a good overall Gas Temperature for your compounds, first, add a method override column to the sequence and override the Fragmentor voltage or one of the source parameters. Then, add multiple rows to the Sequence table which run the same sample. For each row in the Sequence table, vary the parameter that you want to optimize. For example, add five rows to the table and set the Gas Temperature to 250, 260, 270, 280, and 290. By comparing the data files, it is possible to determine which Gas temperature is best for your compounds.

1. Click the **Sequence** layout.
2. In the Sequence window, enter the Properties and Run Options information. For more information, see step 2 and step 3 in "Setting Up and Running a Sequence".
3. Add a column to the Sequence table.
   a. In the navigation pane at the left of the window, click **Injections > Table**.
   b. In the upper left corner of the Sequence table, click . The Choose Columns dialog opens.
   c. Click **Method Override Columns**.
   d. Select the column (or columns) that you want to display. Only one parameter can be optimized at a time, but multiple overrides can be added to a method.
      If you add a Method Override column and enter values in the column, then even if the column is hidden, the method override will work. To remove the override, clear the values in the Method Override column.
   e. Click **OK**.
4. Enter the **Table** information:
   a. In the navigation pane at the left of the window, click **Injections > Table**.
   b. Enter the information for each injection.
   c. Repeat that row several times. Most of the values in these rows are the same. Only vary the sample name, the data file name, and the parameter that you want to optimize. Only one parameter can be optimized at a time.

d. For the parameter that you want to optimize, set the parameter in the first row to the lowest value that you want to check. The first data file contains the data with the parameter at this value.

e. In the second row, set the parameter to a slightly larger value. The second data file contains the data with the parameter at this higher value.

f. Continue to increase the value for that parameter in subsequent rows.

5. Continue with step 6 in "Setting Up and Running a Sequence".

6. Review the data files to determine the optimum value for that parameter for your sample.

4 Maintenance

Maintenance Overview

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

The difference 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.

OpenLab Acquisition for LC/MS systems tracks the number of injections and the number of days since a maintenance activity was performed for your LC/TOF 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.

LC/MS Maintenance Video Series

Procedures notated with the Video Support icon are linked to videos intended to support written content. These links are also found in the online help and/or the instrument user guides. Refer to these videos for supplemental instructions. View the full series at https://aglt.co/LCMSMaintenance.

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 is not 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 that 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

- ESI-X 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

Video Support

For more information, scan the QR code, or visit: https://aglt.co/D0115679.

Perform this maintenance:

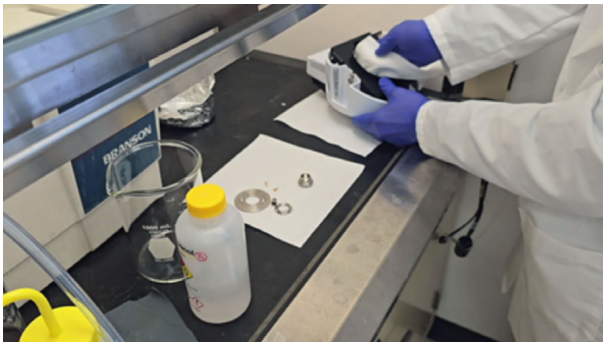
- Weekly.
- Whenever symptoms indicate that contamination exists in the spray chamber.
- If the spray shield or capillary cap shows significant discoloration not removed by daily cleaning.

Tools needed:

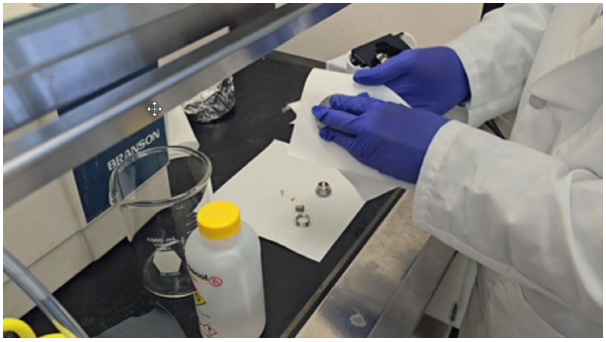
- Clean powder-free nitrile gloves
- Clean lint-free cloth
- LC/MS-grade isopropanol
- LC/MS-grade water
- Clean wash bottle
- 4000 grit sandpaper

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 ion source connections to the instrument.
4. Open the latch of spray chamber.
5. Open the spray chamber.
6. Remove source and put the source under a fume hood.
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.

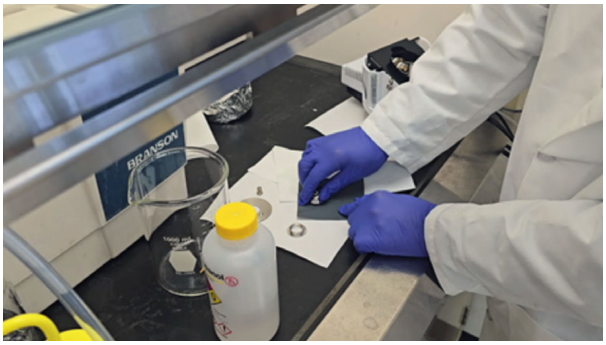


9. Make sure you wear clean gloves. Use a tech wipe to hold the parts as you remove them. They will be warm.



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. (Optional) Abrasive cleaning for persistent contaminants: 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 spray chamber parts and source on the instrument.
19. Reinstall the spray chamber on the instrument.
20. Connect all cables and tubing to the instrument.
21. Connect the nebulizer sample line and sample nebulizer gas tubing to the nebulizer.

Cleaning the nebulizer - weekly

Video Support

For more information, scan the QR code, or visit: https://aglt.co/D0115677.

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 that 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

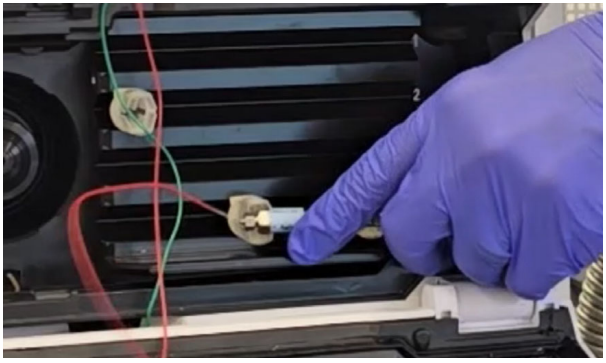
Check the nebulizer weekly. If needed, flush traces of samples and buffers out of the tubing, valves, and nebulizer.

Equipment List

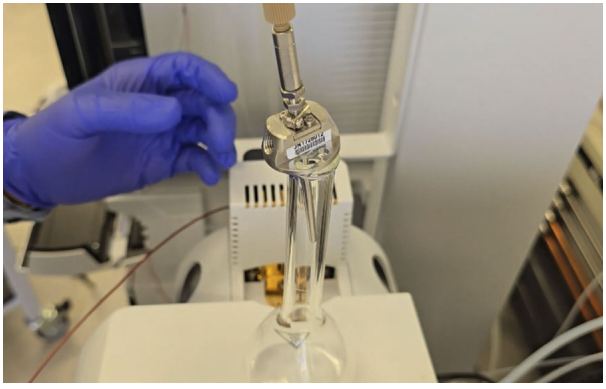
- LC/MS-grade methanol
- LC/MS-grade water

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

Periodic Tasks

Periodic maintenance tasks must be performed on the vacuum pumps contained in the instrument. For more information, see https://www.agilent.com/en/product/vacuum-technologies.

General Maintenance Tasks

Replacing the nebulizer needle

Video Support

For more information, scan the QR code, or visit: https://aglt.co/D0115676.

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" Nebulizer adjustment fixture (GT430-20470)-inch x 5/16-inch open-end wrench (Quantity: 2)

Removing the nebulizer

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

WARNING

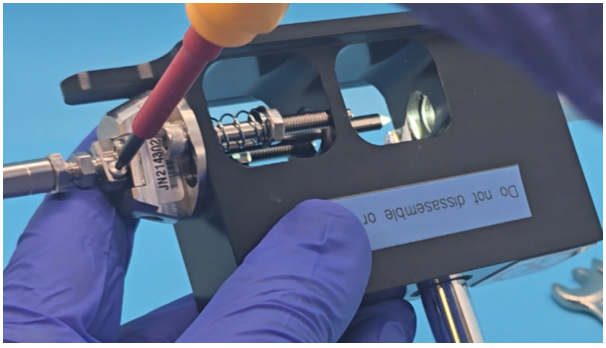
The tip of the nebulizer can be very hot. Do not touch the nebulizer until it is cool.

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

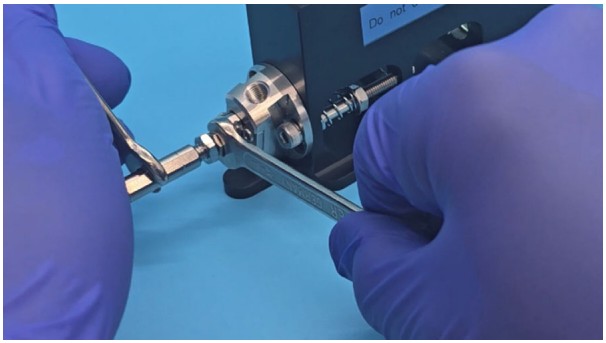
Replacing the nebulizer needle

1. Determine your nebulizer type per the user guide or the document that comes with the kit.
2. Install the nebulizer in the Nebulizer Adjustment Fixture, turning clockwise to secure the nebulizer to the adjustment fixture.

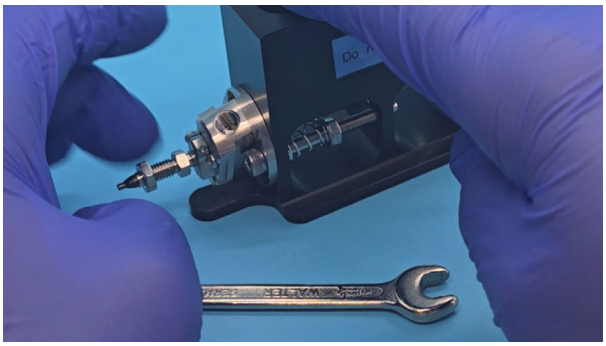
3. Loosen the fastener (locknut, 1.5-mm hex screw, or T6 Torx screw) that secures the needle holder in place.



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.

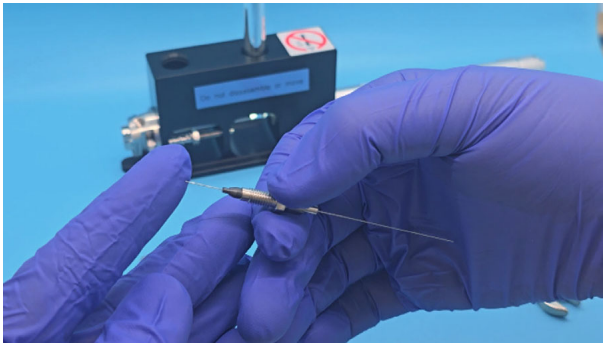


7. Loosen the needle holder and pull it out of the nebulizer body. Dispose of the used needle properly.
8. For more thorough cleaning, sonicate the nebulizer body. Pour isopropanol or methanol through the inside of the shaft.
9. Carefully remove the new needle from the shipping tube and adhesive strip. Identify the sharp end of the needle.

10. Carefully slide the sharp end of the needle through the ferrule until 1 cm of the needle remains at the ferrule.

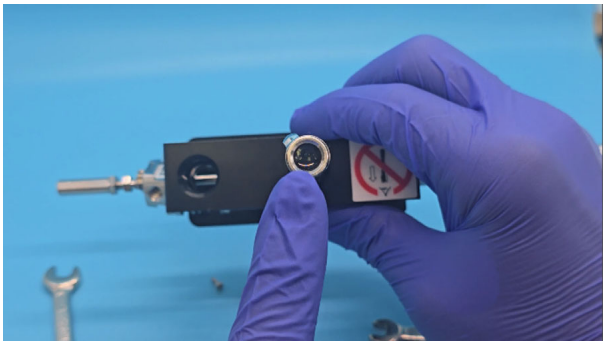
CAUTION

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.



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

15. Adjust the electrospray needle position before reinstalling the nebulizer in the spray chamber.



16. Tighten the fastener (T6 Torx screw) that secures the needle holder in place.

Inspecting and adjusting the nebulizer needle

Video Support

For more information, scan the QR code, or visit: https://aglt.co/D0115675

Schedule

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

- Nebulizer Adjustment Fixture (GT430-20470) or Nebulizer adjustment kit (G1960-67470)
- Clean powder-free nitrile gloves
- T6 Torx driver
- 1/4-inch x 5/16-inch open-end wrench (Quantity: 2)

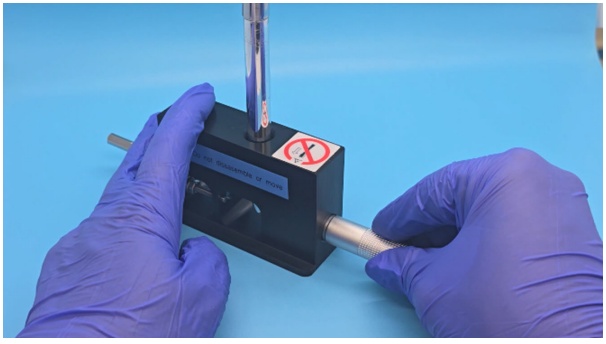
1. Put on clean, powder-free nitrile gloves.
2. Insert the tip of the nebulizer into the end of the Nebulizer Adjustment Fixture.
3. Slide the heads of the two spring loaded socket head cap screws through the mounting holes on the body of the nebulizer.

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. Push the 40 x Magnifier into the vertical end position of the Nebulizer Adjustment Fixture.
6. Align the tapered tip of the magnifier to the tip of the nebulizer needle.
7. Push the LED Flashlight into the Nebulizer Adjustment Fixture.



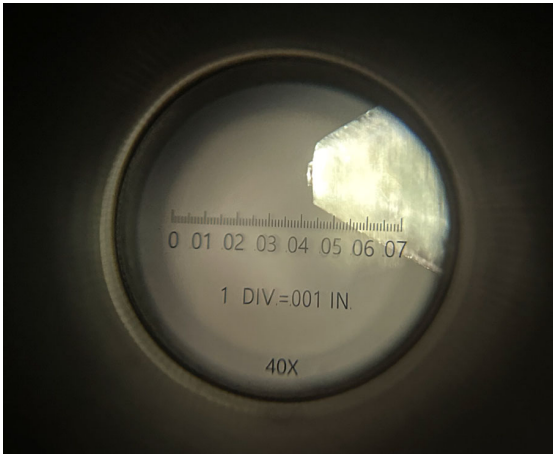
8. Turn on the flashlight and, while looking down the magnifier, adjust the height of the magnifier until the tip of the nebulizer is clearly in focus.

Table 2. 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

The distance shown is the distance that the needle tip protrudes from the tip of the nebulizer assembly in inches.
Note the scale shown in the magnifying lens is also in inches, with one division equaling 0. 001 inches.

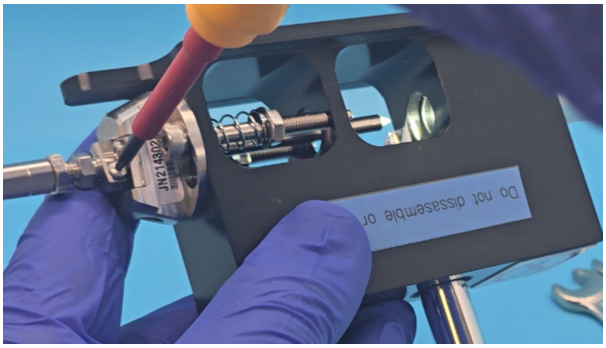
Figure 9. Correctly adjusted nebulizer needle.



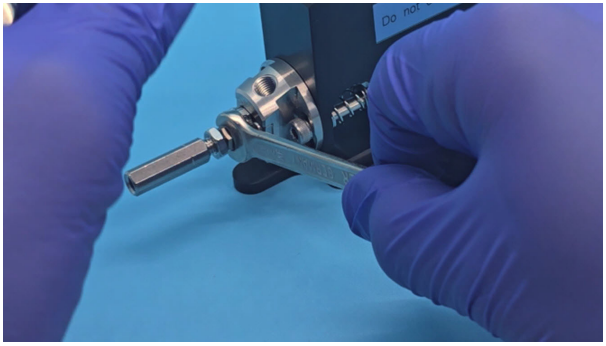
NOTE

If the needle tip looks pitted, clogged with salt, corroded, or is not square and has jagged edges then the needle will need to be replaced.

9. Using either a T6 Torx driver or 1.5 mm hex wrench, loosen the lock screw on the head of the nebulizer assembly. The nebulizer lock screw is either a T6 Torx or 1.5 mm hex bolt



10. Using the 1/4" end of the open-end wrench, rotate the needle assembly while looking down the magnifier. Turning the nut with either push the needle out or drawn it into the nebulizer tip. Adjust the needle so that the distance matches the specified distance for your nebulizer type.



11. If the needle distance looks correct, reverse the position of the magnifier and the flashlight so the flashlight is in the top port and the magnifier is in the side port of the fixture. Check that the needle tip is also centered (concentric) with the tip of the nebulizer assembly. If it is a long way off center after optimizing the distance, then the needle may need to be replaced.

12. Once the position of the needle has been optimized, carefully tighten the lock screw loosened earlier, while checking that the position of the needle has not moved during tightening.
13. The nebulizer needle adjustment is now complete.

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 the 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.

Cleaning the capillary

Video Support

For more information, scan the QR code, or visit: https://aglt.co/D0115670.

Schedule

When you observe decreased sensitivity and decreased signal stability. If sensitivity and signal stability do not fully recover after cleaning, a new ion injector should be purchased.

Equipment List

- Clean powder-free nitrile gloves
- Concentrated Citranox detergent solution (5188-5359)
- Deionized (18 MΩ/cm) water
- 100 mL glass graduated cylinder
- Two 1-mL pipette tips

CAUTION

Cleaning in Alcanox detergent may cause damage to the ion injector, hence the recommendation to clean with Citranox.

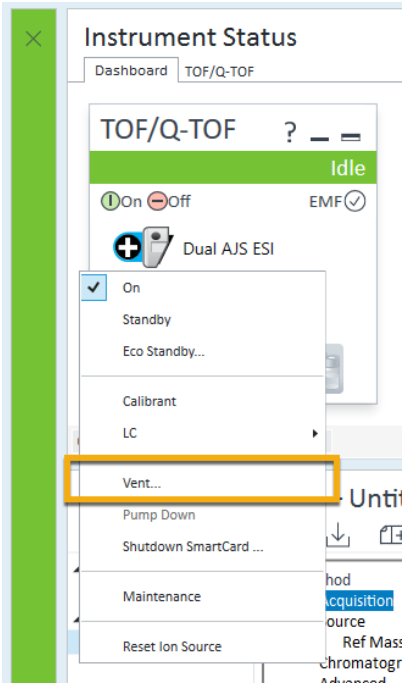
Steps

1. Put on clean, powder-free nitrile gloves.

CAUTION

Ensure the source heated zones are cool before working on the instrument.

2. In OpenLab Acquisition, right-click the instrument icon in the Instrument Status window and select **Vent** to vent the system.

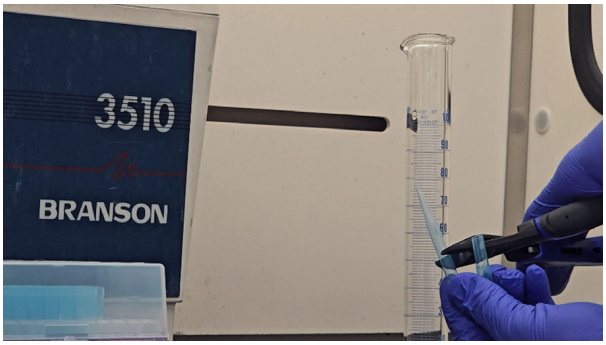


3. Dilute 2 mL of concentrated Citranox solution in 100 mL of deionized water (2% by volume).

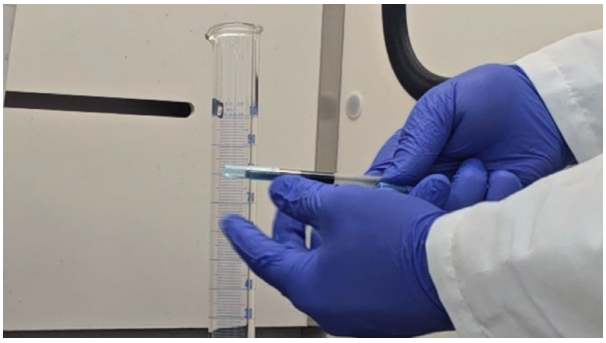
CAUTION

All cleaning and sonication should be done under a fume hood.

4. Trim the pipette tip to approximately 4 cm so that the capillary can be immersed in the cleaning solution.



5. 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.



6. Place the ion transport capillary upright in a graduated cylinder and fill with 2% Citranox solution.

7. 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.

8. Rinse the capillary and graduated cylinder several times with deionized water.
9. Fill the graduated cylinder with deionized water and sonicate for 10 to 15 minutes.
10. Repeat steps 8 and 9 two more times.
11. Remove the ion transport capillary from the graduated cylinder and remove the pipette tips (if any were used).
12. 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 re-insert 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 (CDS)

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 the 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. Re-attach 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 that response is adequate.

Replacing the valve rotor seal

Video Support

For more information, scan the QR code, or visit: https://aglt.co/D0115686.

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 via the acquisition software.
2. Disconnect the nebulizer sample line and sample nebulizer gas tubing.
3. Open the spray chamber.
4. Remove the front and top covers. Some instrument covers require disconnection of the LED ribbon cable located on the front cover.

   NOTE

   The images shown are for illustration purposes only and may not be an exact representation of the product or instrument.
5. Make a note of which port is plumbed to which tubing and unplug all the connections of MS selection valve.
6. Remove the LC PEEK (polyether ether ketone) tubing from the MS inlet, near the spray chamber.
7. Unplug the connections of waste and nebulizer sample line.
8. Use the 9/64-inch hex key to remove the three hex head screws from the stator face of the selection valve.
9. Remove the rotor seal and replace it with a new one. Be sure to install it in the proper orientation.

10. Use the 9/64-inch hex key to fix the three hex head screws from the stator face of the selection valve.
11. Plug in all the connections of the MS selection valve.
12. Install the upper left front cover or ion funnel cover.
13. Fix all the screws that hold the upper left front cover or ion funnel cover.
14. Plug in the connection of CDS liquid line.
15. Plug in the connections of waste line and PEEK tubing.
16. Attach the top and front covers.
17. Close the latch of the spray chamber.
18. Connect the sample nebulizer gas tubing and nebulizer sample line.

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 the tip of the corona needle. The tip can bend, which can decrease the 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 that 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

None

Steps

1. Right-click the Q-TOF device pane and select **Calibrant**.
2. Run the calibrant for 5 minutes.
3. Perform a checktune. See "Mass Calibration".
4. If the checktune results are not acceptable, run autotune on a supported tuning source. See "Mass Calibration".
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 "Autotune"). If an autotune is not available, do a checktune (see "Mass Calibration").
- 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.

WARNING

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 OpenLab Acquisition software:

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 sample lines and gas tubing lines from both the sample and reference nebulizers.
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.

WARNING

The spray chamber operates at very high temperatures. 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 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.

In the OpenLab Acquisition software:

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.

5 Compliance

Sustainability Information

Packaging End-of-Life

The Agilent 6230 TOF 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 pallets 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 6230 LC/TOF LC/MS system customers in US, EU, and UK markets. See 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 Industrial, Scientific and Medical (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 기기로 서 가정용 환 경에서 사용하는 경우 전파간섭의 우려가 있습니다 .

※ 사용자 안내문은 " 업무용 방송통신기자재 " 에만 적용한다 .

국립전파연구원

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 Lp < 70 dB(A) according to DIN EN ISO 7779.

Schalldruckpegel

Schalldruckpegel LP <70 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 see https://www.agilent.com/environment/product/index.shtml for more information.

6 Additional Resources

User Documentation

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

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

Agilent TOF 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/LCQTOFSupplies.

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:

https://www.agilent.com/en/support

Agilent Community

To get answers to your questions, join over 10,000 users in the Agilent Community. Review curated support materials organized by platform technology. Ask questions to industry colleagues and collaborators. Get notifications on new videos, documents, tools, and webinars relevant to your work.

https://community.agilent.com/

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D0146599 Rev. A.00

May 2026