

OpenLAB CDS for InfinityLab LC/MSD Series and 6100 Series LC/MS

GETTING STARTED

INSTALL AND CONFIGURE	Click setup.exe on the USB stick to run the installation wizard. Refer to the Installation Guide (in the Resource App) for details.
START SOFTWARE	Turn on the power to the instrument. Start the OpenLAB CDS Acquisition program. In the Instrument Status window, right-click the SQ device and select Pump Down . When done, right-click the SQ device and select On .
PREPARE THE LC MODULES	Purge the LC pump. Follow the directions for purging the pump in the online Help.
PREPARE THE SINGLE QUADRUPOLE	Before acquiring data, you tune the SQ which maximizes sensitivity, maintains acceptable resolution, and ensures accurate mass assignments. First, click the Get Tune Control icon. Run Checktune (🔧). If necessary, run Autotune (🔧).
EDIT METHOD	You edit a method to configure method parameters to use when acquiring data. A method can have different time segments which can have different values for some MS parameters. You change the Time Segment table in any of the SQ > Method sections . In each time segment, you can have different scan segments and source parameters. You edit scan segments in the SQ > Acquisition section.
RUN ACQUISITION METHOD OR SEQUENCE	You can acquire data by running a single sample or by running a sequence of samples. You click either the Single Sample or the Sequence layout. You can override some method values in a sequence.



Instrument Status Window

SQ (SINGLE QUADRUPOLE) DEVICE ON THE DASHBOARD

- Actions from the shortcut menu
- **On** - sets Gas Flow, Nebulizer, and temperatures to setpoints in current method. It does turn on voltages.
 - **Standby** - changes SQ parameters to standby values
 - **Calibrant** - selects whether or not the calibrant is on
 - **LC** - selects whether to direct the LC stream to the MS or to Waste
 - **Vent** - vents the SQ to atmospheric pressure
 - **Pump Down** - pumps down the SQ system to achieve high vacuum
 - **APPI UV Lamp** - turns the UV lamp on or off in the APPI source

SQ TAB

This tab shows status parameters. By noticing significant changes in some of these parameters, you can monitor the health of the instrument. In particular, you can monitor these values: **Rough Vac**, **High Vac**, **Turbo1 Speed**, and **Pump1 Current**.

What’s New in 2.2

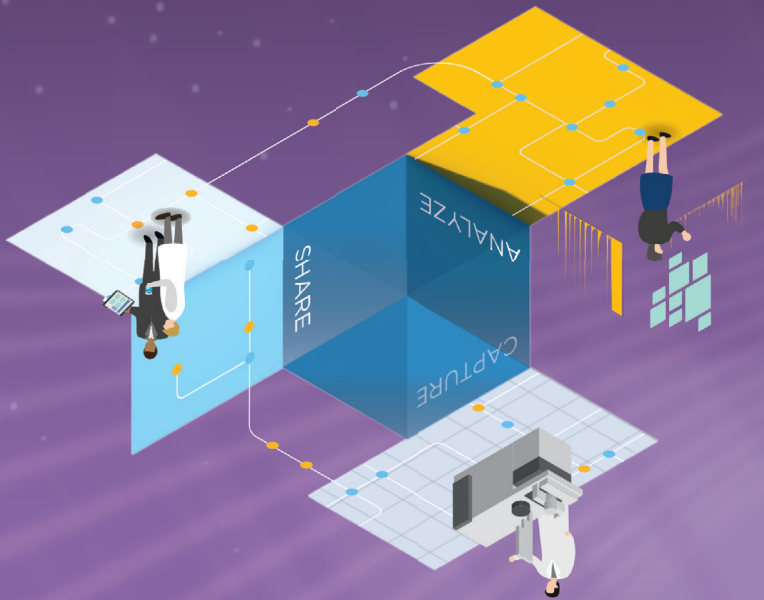
- **Support for InfinityLab LC/MSD Series .**

Resources

- **InfinityLab LC/MSD Series and 6100 Series LC/MS Maintenance Guide**
The animated Maintenance Guide contains instructions to maintain your mass selective detector.
- **Getting Started modules**
LC/MS Tuning and Acquisition Methods
6000 Series LC/MS Hardware
- **Agilent InfinityLab LC/MSD Series System Installation Guide**



Agilent Technologies



Quick Reference

OpenLAB CDS for InfinityLab LC/MSD Series and 6100 Series LC/MS



Agilent Technologies



Part Number G1960-90096



This information is subject to change without notice.

For the latest information please go to:
www.agilent.com/chem/openlabcds

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TIME SEGMENTS PANE

The left pane in each Single Quadrupole Method section contains the **Time Segments** table and other parameters:

- **Ion Source** - the source that is being used in this method.
- **Stop time** - either As Pump/No Limit or the actual Stop time in minutes.
- **Tune file** - the name of the tune file to use when this method is used.
- **Fast scan** - whether or not the selected tune file is a Fast scan tune file.
- **Time Segments** table - You select whether to acquire **Scan**, **SIM**, or **SIM/Scan** data for each time segment. You also specify when the segment starts and how to modify the electron multiplier voltage (V).

ACQUISITION SECTION

The columns in the Scan Segments table change depending on whether you selected **Scan**, **SIM**, or **SIM/Scan** in the Time Segments table.

SCAN

- **Segment name**, **Start mass**, **End mass**, **Scan time**, **Fragmentor**, and **Polarity**
- **Estimated Cycle time** (ms/cycle) - the estimated calculated time to execute all signals once plus a polarity switch overhead if applicable. It is calculated automatically using the mass ranges and the scan time or peak width.
- **Use same scan table for all time segments** box - whether or not to use the same scan table for all Time Segments of either **Scan** or **SIM/Scan**.

SIM

- **Compound name**, **Mass**, **ISTD?**, **Dwell (ms)**, **Fragmentor**, and **Polarity**.
- **Estimated Cycle Time** - Dwell times added with a polarity switch overhead if applicable.

TOOLBAR

-  - Adds a time segment.
-  - Inserts a time segment.
-  - Deletes the selected time segments.
-  - Copies the selected cells to the other selected cells.
-  - Copies the selected cells to all of the other cells in the column.
-  - Cuts the selected rows from the table and copies to the Clipboard.
-  - Copies the selected rows/cells in the table to the Clipboard.
-  - Pastes the rows/cells from the Clipboard.

SOURCE SECTION

You can specify a unique set of Source Parameters for each time segment. The actual values are shown in a read-only box next to the parameter.

- **Gas Temperature** (°C) - the temperature of the drying gas. It depends on the LC flow rate, the Drying Gas Flow Rate, the type of analysis, and the thermal stability of the sample.
- **Vaporizer** (°C) - the temperature of the vaporizer. This parameter is only available if you have an APCL, APPL, or MMI source.
- **Gas Flow** (L/min) - the flow rate of the nitrogen drying gas through the capillary electrode.
- **Nebulizer** (psi) - the pressure of the nitrogen nebulizing gas through the capillary electrode.
- **Capillary Voltage Positive** (V) - Positive polarity potential
- **Capillary Voltage Negative** (V) - Negative polarity potential
- **Capillary Current** (nA) - Current passing through the capillary electrode (read-only).
- **Corona Current** (µA) - the current from the corona discharge needle to the end plate. This parameter is only used in APCL, MMI-APCL, and MMI-ESI+APCL modes.
- **Corona Voltage** (V) - This value is the instrument actual for an APCL or MMI source. This value is read-only.
- **Charging Voltage** (V) - This value is only available if the source is **MMI**. It is always set to 0 if Ion Mode is **APCL**.
- **Chamber Current** (µA) - This value is read-only and is the instrument actual.
- **Nozzle Voltage** (V) - You enter a value for Positive polarity and Negative polarity. This value is only available for an AJS ESI source.
- **Sheath Gas Temp** (°C) - the temperature for the heater in the AJS ESI.
- **Sheath Gas Flow** (L/min) - the flow rate for the sheath gas in the AJS ESI.

CHROMATOGRAMS SECTION

You select which chromatograms are displayed in the Chromatograms window.

- **TIC** - the Total Ion Chromatogram is the overlap of all of the scan segment TICs in one trace.

- **Channel TIC** - a Channel TIC is a TIC per scan segment. The first TIC is for scan segment 1. The next TIC is for scan segment 2, and so on.
- **EIC** - an Extracted Ion Chromatogram is a chromatogram for only the specified *m/z* or *m/z* range.
- **BPC** - a Base Peak Chromatogram. You can specify masses or mass ranges to exclude.

TIMETABLE SECTION

The Timetable is used to change the position of the diverter valve during a run. You can specify to send the stream from the **LC** to either **Waste** or **MS**. If you divert the stream to **Waste**, then you do not acquire data at that time.

In the Method window, select **SD > Tune > Autotune** to switch to the tune section. This toolbar is displayed at the top of the pane:



Before you run Checktune, Autotune, or manual tune, you click  to lock the SQ for use in tune.

When you are done, you click  to release the SQ for a different use. The tune parameters are saved as a tune file on the instrument.

RUN CHECKTUNE

You run Checktune to check if you need to autotune the SQ.

- Click  .
- Click the **Polarity** and either select or clear the **Fast scan** check box.
- Click  . When the Checktune is done, click .

RUN AUTOTUNE

- Click  .
- Click the **Polarity** and either select or clear the **Fast scan** check box.
- Click  . When the Autotune is done, click .

TUNE THE INSTRUMENT MANUALLY

For many applications, you do not need to manually tune. You might consider manually tuning the SQ in the following situations:

- To achieve maximum sensitivity by sacrificing some resolution
- To tune specifically for the very low end of the mass range (< 150 amu)
- To tune with a compound other than the standard calibrants

MAIN STEPS OF MANUAL TUNING

- Prepare for manual tuning. Click .
- Set acquisition parameters and adjust mass axis.
- Ramp the Fragmentor dynamically.
- Ramp the lenses.
- Optimize the octopole.
- Adjust peak widths and mass axis.
- Optimize Lens2 RF parameters.
- Unlock the SQ instrument. Click .