Agilent

Agilent OpenLab CDS for InfinityLab LC/MSD Series and 6100 Series LC/MS

Quick Start Guide

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What is OpenLab CDS?

OpenLab CDS controls and acquires data from InfinityLab LC/MSD Series and 6100 Series LC/MS single quadrupole (SQ) instruments.

- The InfinityLab LC/MSD and 6120C SQ instruments support ESI, APCI, APPI, and MMI sources.
- The InfinityLab LC/MSD XT and 6130C SQ instruments support ESI, APCI, APPI, MMI, and AJS ESI sources.
- The InfinityLab LC/MSD iQ supports the ESI source only.

What's new in LC/MS Driver 2.3 on OpenLab 2.4?

- The InfinityLab LC/MSD iQ is supported.
- With the InfinityLab LC/MSD iQ only:
  - Auto Acquire mode is available in the Method Editor.
  - You can schedule an Autotune or Checktune.
  - Manual Tune is not supported.
- Early Maintenance Feedback (EMF) is supported.

Functionality of OpenLab CDS

- Tune the SQ instrument. You can run either Checktune or Autotune. If you have an SQ model other than LC/MSD iQ, you can also manually tune the instrument.
- With the LC/MSD iQ only, scheduled tune allows you to set a recurring event, similar to a recurring calendar appointment. You can schedule either a Checktune or an Autotune to run during an idle time, such as at 5:00 AM or on the weekends. You can select how often to run the Checktune or Autotune.
- You can acquire SQ data.

OpenLab Help & Learning

Included with OpenLab CDS is a comprehensive portfolio of manuals, videos, getting started lessons, user applications, and method development tools for your system.

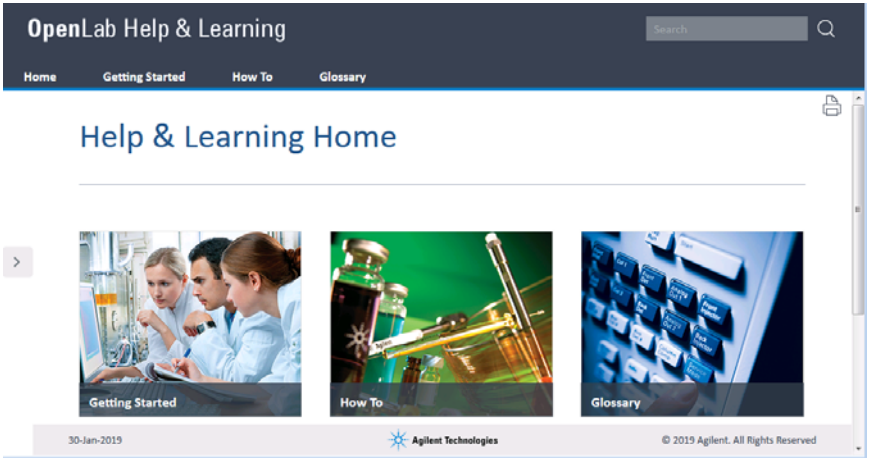


Figure 1. OpenLAB Help & Learning

To start OpenLab Help & Learning

Do one of the following:

Press F1 To get more information about a pane, window, or dialog box, place the cursor on the pane, window, or dialog box of interest and press F1. **OpenLab Help & Learning** is opened.

? Click this button in the title of the program to open **OpenLab Help & Learning** which includes basic tasks, user interface, and reference information.

Click this icon on the desktop. You can also click **Start > All Programs > Agilent Technologies > OpenLab Help & Learning**.

Curricula

You can access the interactive curriculum when you click one of the topics under **Curricula** under **Getting Started**. Each curriculum contains powerful, interactive, on-demand training modules for OpenLab CDS. You can easily learn the functionality at your own pace, whenever you want. The modules walk you through detailed steps of using the OpenLab CDS software.

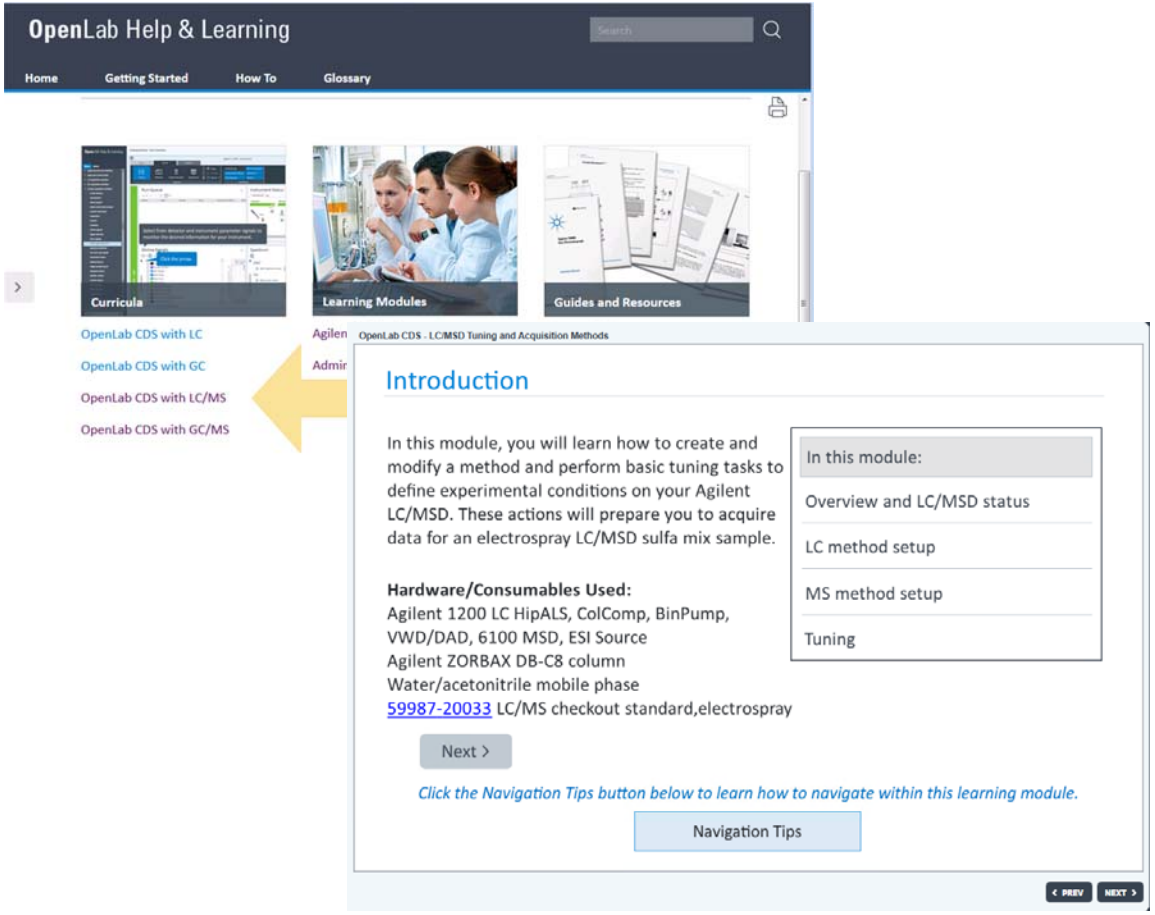


Figure 2. Starting the LC/MS interactive curriculum

How To

In OpenLab Help & Learning under **How To**, you will find hundreds of topics written as detailed step-by-step instructions that walk you through routine tasks.Topics with a Play button include software demonstration videos.

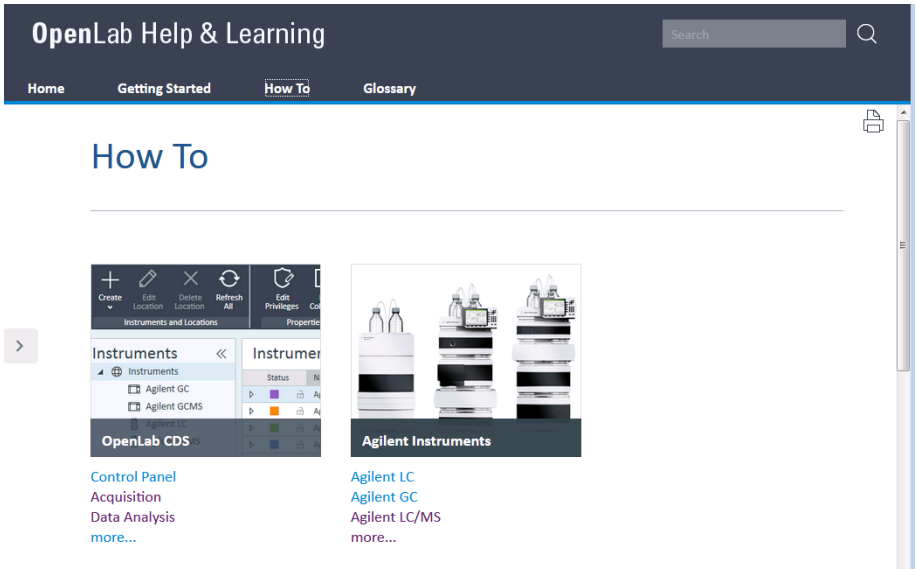


Figure 3. How To section of **Help & Learning**

Installation

To install the OpenLab CDS Help & Learning material on PCs other than those using the OpenLab CDS software, select **Documentation > Install OpenLab Help and Learning Only** from the OpenLab CDS software installation disk.

Included in Help & Learning, under **Get Started**, is the powerful, interactive, on-demand training tool for OpenLab CDS. This can help you easily learn the new functionality at your own pace, whenever you want. The modules walk you through detailed steps of using the Agilent InfinityLab LC/MSD Series and 6100 Series LC/MS software.

In Help & Learning, under **How To**, you will find hundreds of topics written as detailed step-by-step instructions that walk you through routine tasks. Topics with a Play button, include software demonstration videos.

Getting Started

How do I get started?

This *Quick Start Guide* helps you become familiar with the OpenLab CDS user interface.

1. Open the Control Panel.
   - Double-click the **Control Panel** icon on your desktop.
   - Windows 7: Click **Start > All Programs > Agilent Technologies > OpenLab Shared Services > Control Panel**.
   - Windows 10: Click **Start > All Apps > Agilent Technologies > OpenLab Shared Services > Control Panel**.
2. Configure an instrument. See the online Help for information on configuring an instrument.
3. Launch the LC/MS instrument. Click the **Launch** button in the Control Panel.
4. Review this *Quick Start Guide* to learn about the User Interface.
5. Review the *OpenLab CDS with LC/MS interactive curriculum* to learn about:
   - User Interface
   - Acquisition Methods and Tuning
   - Run Submission
   - Data Analysis with Mass Spectrometry
   - Reporting
6. Review the online Help for more specific information about the LC/MS features.

User Interface

Main functional areas

The main Acquisition window consists of two parts: (1) Ribbon and (2) Main Window. The main functional areas are shown in **Figure 4**.

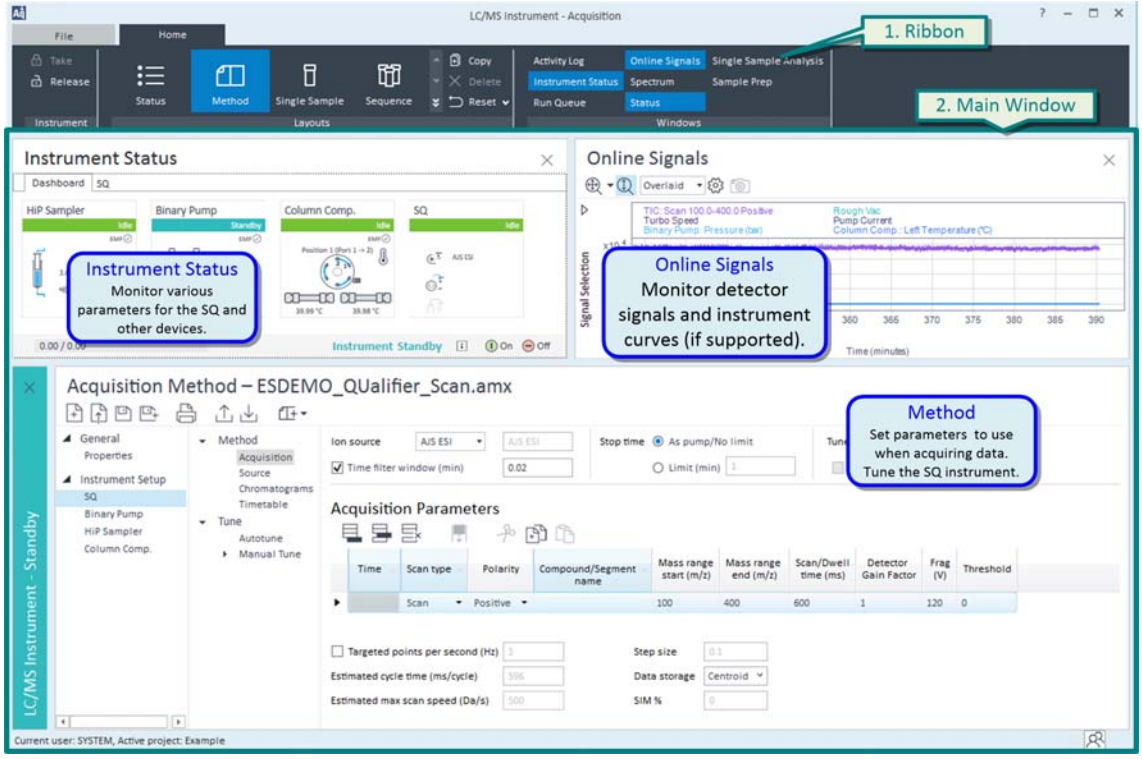
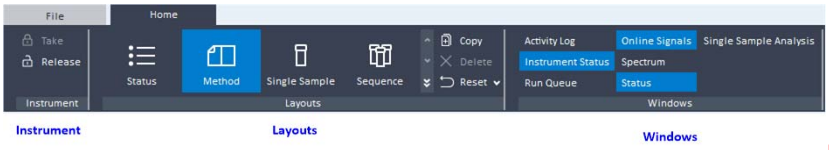


Figure 4. The main functional areas of OpenLab CDS Acquisition window.

Ribbon

The Ribbon is located at the top of the program and has three groups: Instrument, Layouts, and Windows.



Instrument Use the buttons in this group to take and release control of the instrument. You need to first take control of the instrument to run Autotune or Checktune or to acquire data. In this image, this Acquisition program has control of the instrument. You typically do not change this option.

Layouts Select a layout in this group to automatically show the windows that are typically needed for a task. For example, if you click the **Method** button, the windows that are needed when you are editing a method are automatically displayed.

Four default layouts are available to select. A layout contains information about the size and position of each of the Acquisition windows. Each layout has a different window that is always visible. Each layout has a different set of other windows that are visible by default. You can copy a layout and modify the copy.

- **Status layout** - The Instrument Status window is always visible.
- **Method layout** - The Acquisition Method window is always visible.
- **Single Sample layout** - The Single Sample Analysis window is always visible.
- **Sequence layout** - The Sequence window is always visible.

Windows You can display or hide some windows in the selected layout. The windows that are currently shown have a blue background. In the Method layout, these windows are shown by default: **Instrument Status**, **Online Signals**, and **Status**. The Spectrum window is also described in **"Main Window"** on page 9. You can click these buttons to hide or show any of these windows.

In the **Method** layout, the **Acquisition Method** window is always shown, so it is not listed in the Windows section.

Main Window

The main window (**Figure 4** on page 7) is further divided into additional windows. The following windows have features that are specific to the LC/MS instrument. See the online Help for more information.

- Acquisition Method
- Instrument Status
- Online Signals
- Spectrum

Acquisition Method window

In the SQ part of the Acquisition Method, you can do two major tasks: tune the instrument and edit the method. The user interface in this window changes depending on the type of instrument that you have.

LC/MSD, LC/MSD XT, and 6100 Series LC/MS

If you have an LC/MSD, LC/MSD XT, or 6100 Series LC/MS, then the SQ section in the Method Editor has 2 parts:

- **Method** - The SQ parameters are available in four different sections: Acquisition, Source, Chromatograms, and Timetable. You can see the MS Global Parameters at the top of each section.
- **Tune** - You can run either **Checktune** or **Autotune**. You can also run **Manual Tune**. You can save a tune file to a different name.

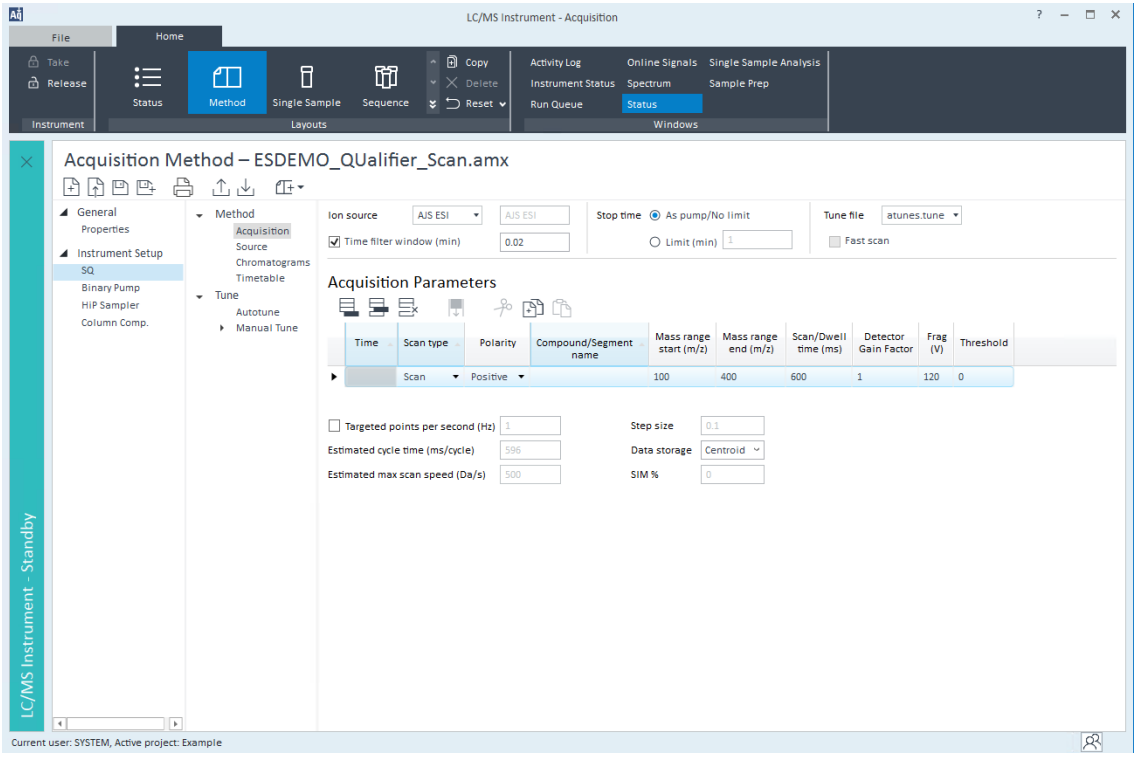


Figure 5. SQ > Method > Acquisition section of the Acquisition Method window for an LC/MSD or LC/MSD XT.

LC/MSD iQ If your instrument is an LC/MSD iQ, then the SQ section in the Method Editor has 3 sections:

- **Auto Acquire** - This mode automatically sets optimized instrument parameters and does not require a lot of input. You specify the liquid chromatography method, SIM ions, and/or m/z range for Scan. You set the **Targeted points per second** parameter based on the chromatography knowledge so that each peak has 10 to 12 points across the peak for best accuracy and quantitation. Source and ion optic parameters are then automatically set. You can view the actual values in the method report.
- **Advanced Acquire** - If you switch to this mode, then you are able to edit other parameters. The parameters are shown in four different sections. However, once you have switched to the Advanced Acquire user interface and saved the method, you will permanently change the method to Advanced Acquire, and you will not be able to change that method back to Auto Acquire mode. To make a new Auto Acquire method, select “new method.”
- **Tune** - You can run either **Checktune** or **Autotune**. A single tune file is used which runs in both polarities and all scan speeds. Manual Tune is not available.

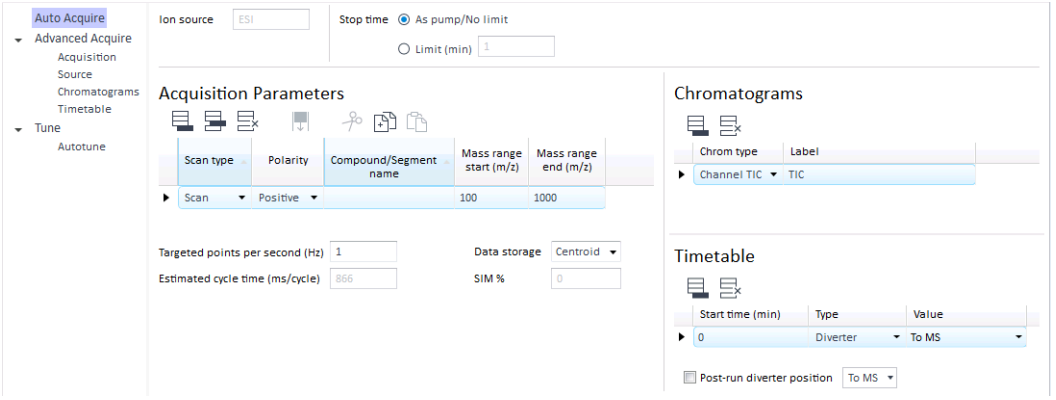


Figure 6. SQ > Auto Acquire section of the Acquisition Method window for an LC/MSD iQ

Instrument Status window

In the SQ device pane you can see the following information:

- Polarity of Scan segments in the Acquisition Parameters table in the Acquisition Method window
- Source
- LC Stream diverter valve position (**MS** or **Waste**)
- Calibrant on or off

Context menu

If you right-click the SQ device, you can use any of the following commands:

- **On** - Turns the SQ device On.
- **Standby** - Puts the SQ device in Standby.
- **Calibrant** - Toggles whether the calibrant is On or Off.
- **LC** - Sends the calibrant either to the MS or to Waste.
- **Vent** - Vents the instrument.
- **Pump Down** - Pumps down the instrument.
- **APPI UV Lamp** - Turns the APPI lamp on or off. This feature is only available for an LC/MSD, LC/MSD XT, or 6100 Series LC/MS when an APPI source is installed.
- **Schedule Tune** - Opens the Schedule Tune dialog box so that you can schedule an Autotune or a Checktune. This feature is only available for an LC/MSD iQ.
- **Maintenance** - Opens the Maintenance dialog box so that you can enable or disable some of the Early Maintenance Feedback (EMF) counters. This feature is only available for an LC/MSD iQ.
- **Review Tune Report** - Opens the selected tune report.

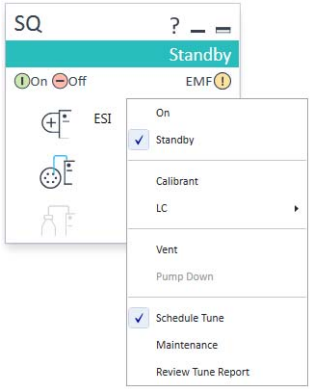


Figure 7. Context menu for the SQ device in the Instrument Status window for an LC/MSD iQ

Online Signals window

You can select which SQ signals you want to observe in this window. Each signal is plotted in a different color, and the legend at the top of the window shows the color for each signal.

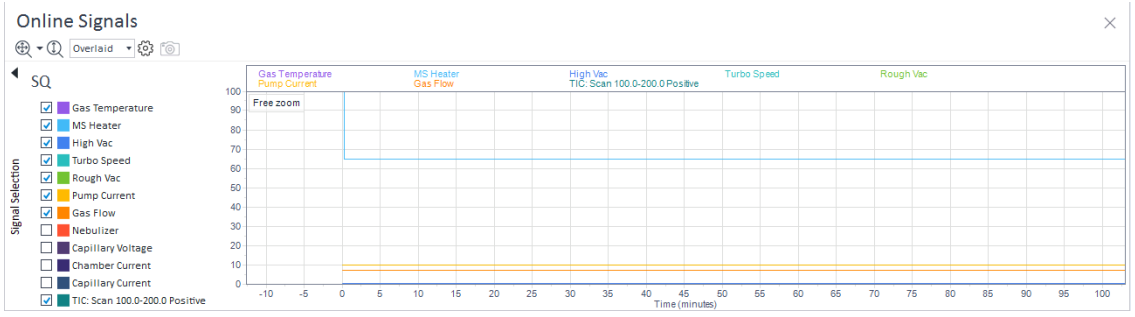


Figure 8. Online Signals window

Spectrum window

This window shows spectra from the different devices. It shows MS spectra during both Tune and Acquisition.

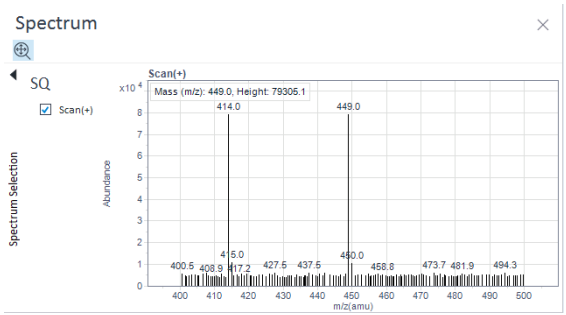


Figure 9. Spectrum window

In This Book

The *Agilent OpenLab CDS for InfinityLab LC/MSD Series and 6100 Series LC/MS Quick Start Guide* presents an overview of the OpenLab CDS program.

This guide is valid for LC/MS Driver 2.3 or higher on OpenLab 2.4 or higher, until superseded.

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