

High-Resolution Mass Spectrometry Data Acquisition Powered by Unified OpenLab CDS System

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Introduction

High-resolution mass spectrometry (HRMS) is a critical capability for late-stage development and QA/QC laboratories in the biopharma industry, where precision, reproducibility, and compliance are non-negotiable. The latest release of Agilent OpenLab CDS software (version 3.0) expands its reach to support Agilent liquid chromatography/time-of-flight (LC/TOF) and liquid chromatography/quadrupole time-of-flight (LC/Q-TOF) mass spectrometry (MS) instruments, integrating both chromatography and mass spectrometry workflows into a single, cohesive platform.

By unifying data acquisition for both chromatography and MS, OpenLab CDS delivers an easy-to-use, easy-to-learn, standardized user experience with a consistent data format, reducing training needs and minimizing operational errors.¹ The scalable client-server architecture ensures centralized control, secure data access, and seamless collaboration between teams across different locations.

This technical overview explains the general benefits of the OpenLab ecosystem and introduces new features that enable you to perform high-resolution mass spectrometry analyses within the ecosystem. This includes:

- Scheduled preconfigured instrument tuning for optimized performance and reduced downtime.
- Seven acquisition modes to support a wide range of targeted and untargeted analytical strategies.
- Real-time spectral viewing by multiple clients through a robust signal buffer service.
- Advanced sequence management with new task and wait actions for improved workflow flexibility.
- Integrated acquisition-to-analysis tools such as sample custom parameters, unattended data analysis, automated error handling, snapshot viewing, and batch data reprocessing.

OpenLab ecosystem

OpenLab CDS delivers a single software platform for GC, GC/MSD, LC, LC/MSD, and now LC/TOF and LC/Q-TOF, ensuring a consistent user experience across selected chromatography and MS workflows (Figure 1). This comprehensive solution supports the entire laboratory lifecycle:

- Instrument and user management
- Data acquisition, analysis, and reporting
- Centralized data management with advanced data integrity controls

Built-in compliance features provide the ability to safeguard data integrity and security, manage role-based access, trace every step of data creation, and streamline audit trail review, helping laboratories meet strict regulatory requirements.²

Client-server configuration

Unlike disparate workstation islands, OpenLab CDS client-server configuration (Figure 2) connects instruments, workstations, and users into a unified environment that³:

- Offers centralized data storage and sharing via secure, network-connected servers.
- Enables centralized management of users, roles, and instrument configurations.
- Provides centralized control over methods, sequences, and templates.
- Offers remote access for flexible, hybrid work arrangements.
- Supports real-time collaboration between teams at different sites.
- Facilitates centralized monitoring of active acquisitions and instrument status.

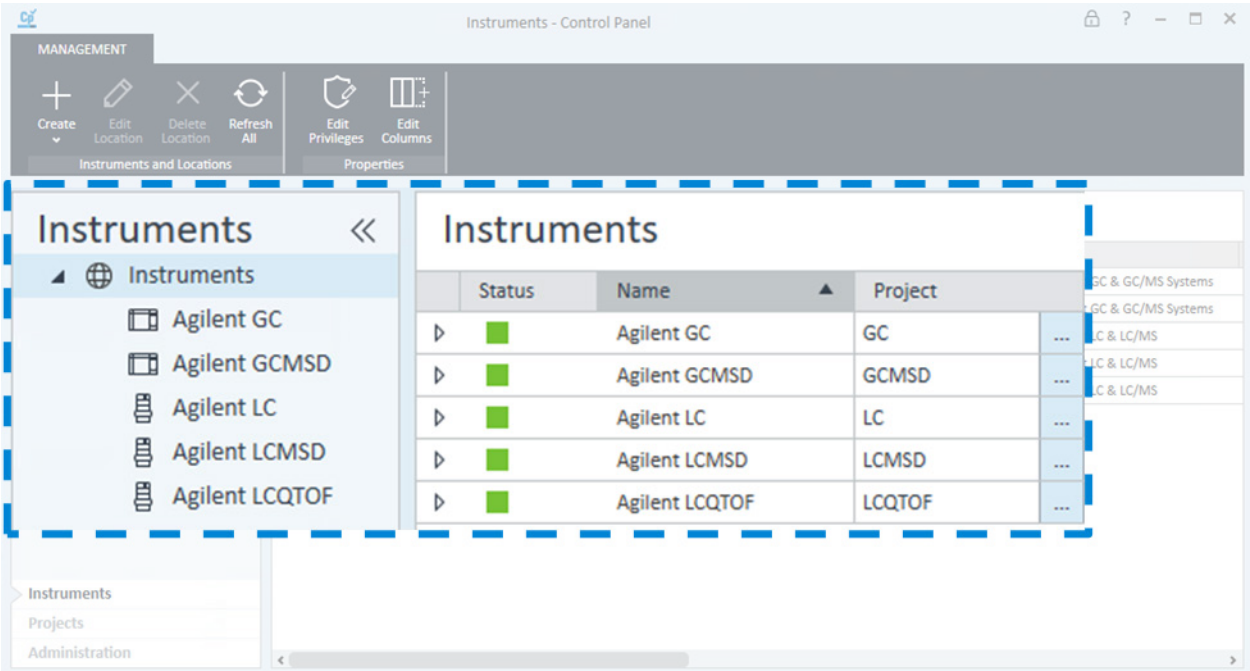


Figure 1. Instruments configured in OpenLab CDS software.

Advanced features include centralized sharing of validated acquisition methods, protein or oligonucleotide sequences, and chemical data dictionaries ensure that all analysts work from a single source of truth.

OpenLab CDS client-server deployments also provide operational resilience by allowing instruments to continue data acquisition even when the server connection is temporarily disrupted, and the ability to submit new analytical tasks (i.e. failover for LC/(Q-)TOF) (Figure 3).

Note: For LC/TOF and LC/Q-TOF, unattended data analysis is not available in failover mode. Detailed information on this mode for instruments other than LC/TOF and LC/Q-TOF can be found in the corresponding users guide.⁴

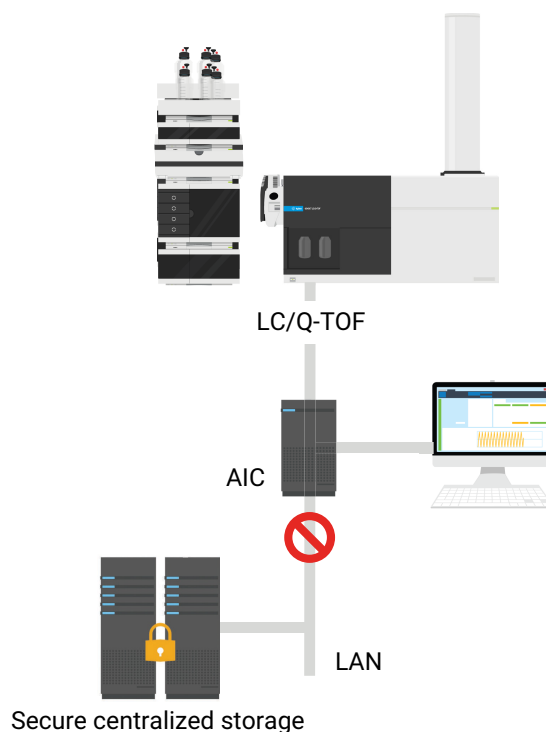


Figure 3. High-level schema of the failover mode (compared to the normal operation as shown in Figure 2).

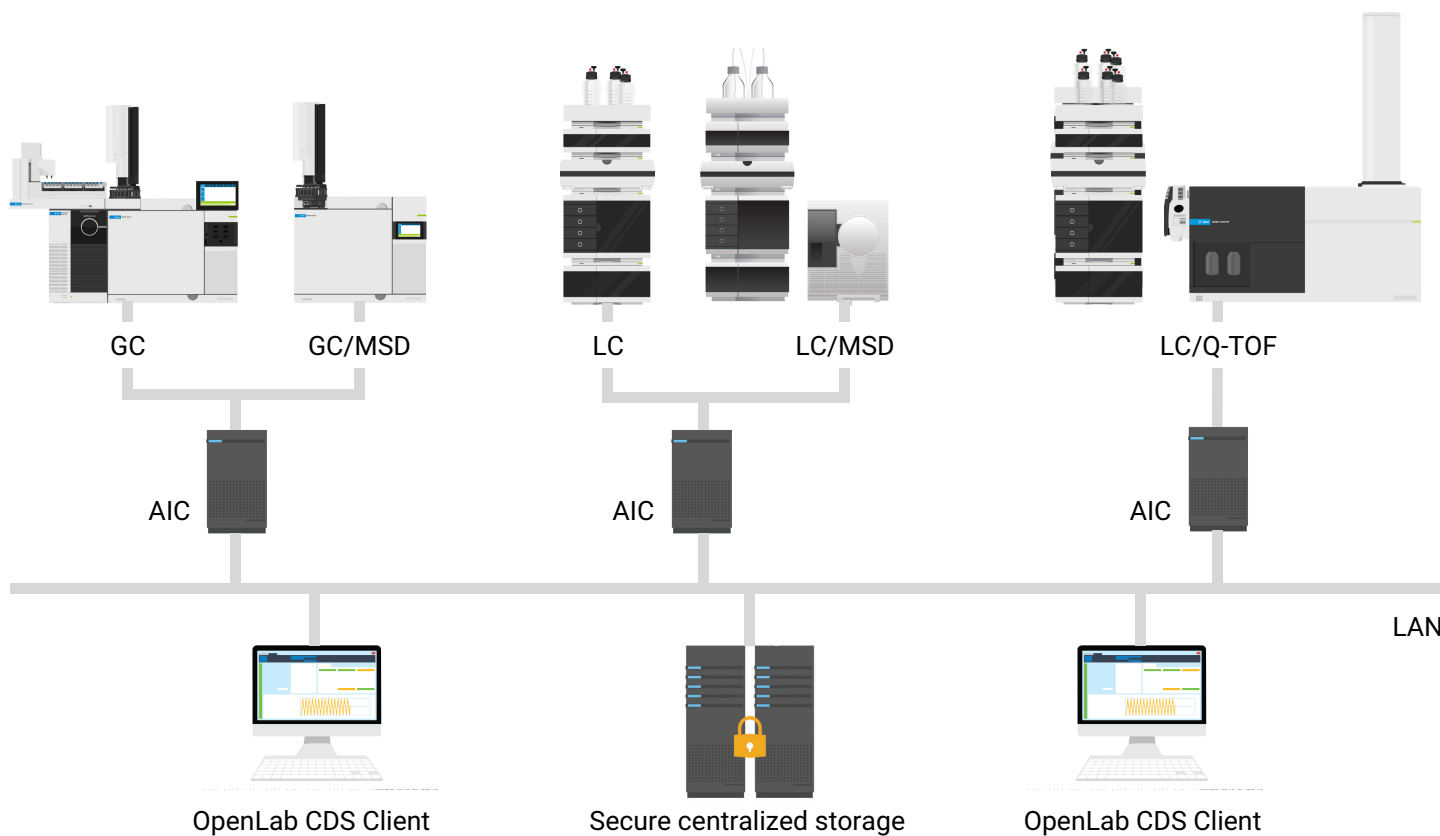


Figure 2. Client-server configuration connecting different instruments across the labs.

Using an LC/(Q-)TOF in OpenLab CDS

Using an LC/(Q-)TOF in OpenLab CDS takes advantage of the current acquisition capabilities, including:

- View instrument status.
- Perform application-based LC/(Q-)TOF tuning and calibration.
- Edit instrument acquisition parameters.
- Submit samples for analysis.
- Automatically process data with MassHunter Qualitative Analysis, MassHunter BioConfirm (optional), or MAM for OpenLab CDS (optional).

In Figure 4, you can see the LC/(Q-)TOF as part of the overall system, including status information, the real time chromatogram (signals) and spectral displays, and the instrument run queue.

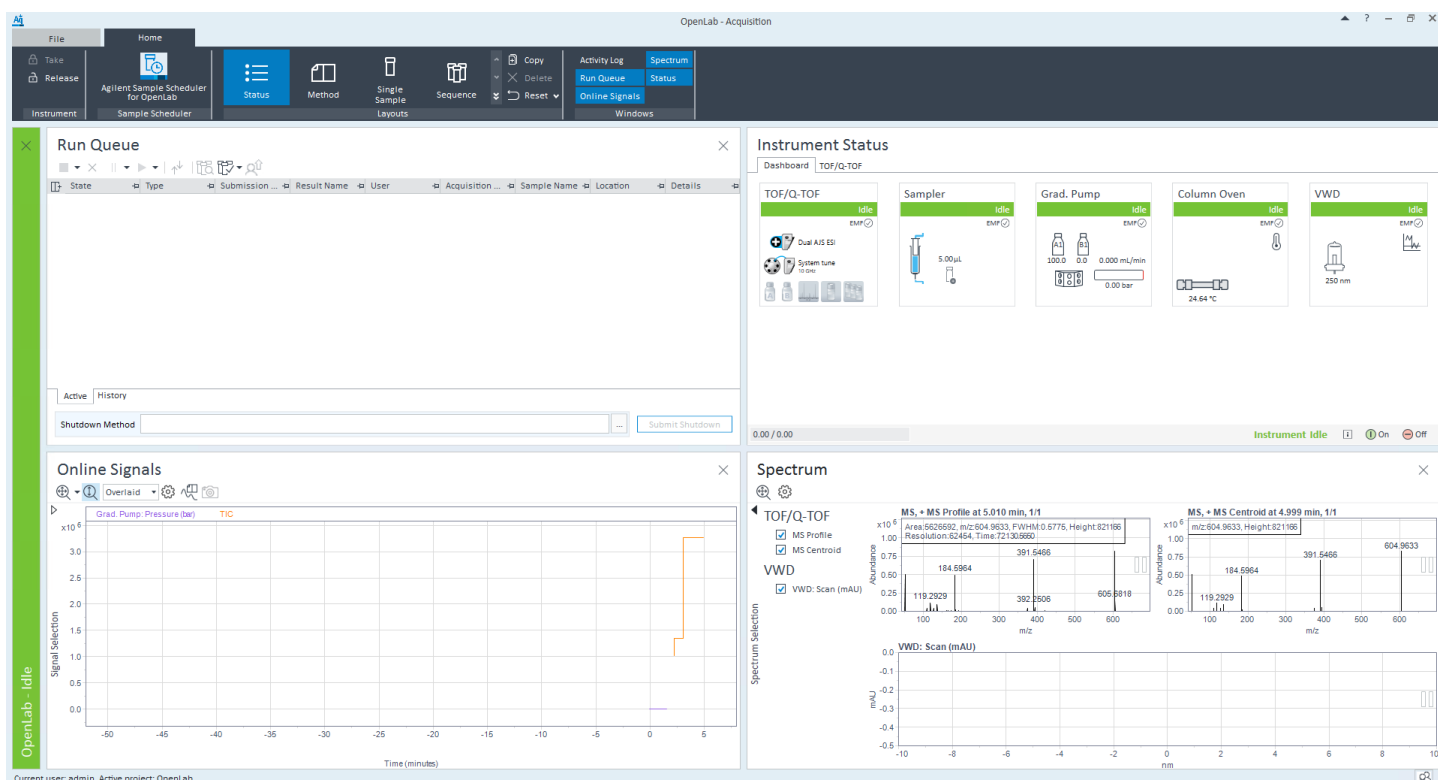


Figure 4. LC/Q-TOF in OpenLab CDS - the status layout.

LC/(Q-)TOF status

In OpenLab CDS, the LC/(Q-)TOF provides comprehensive instrument status visibility and enables direct control of selected functions, such as switching the instrument to eco standby and managing calibrant flow (Figure 5).

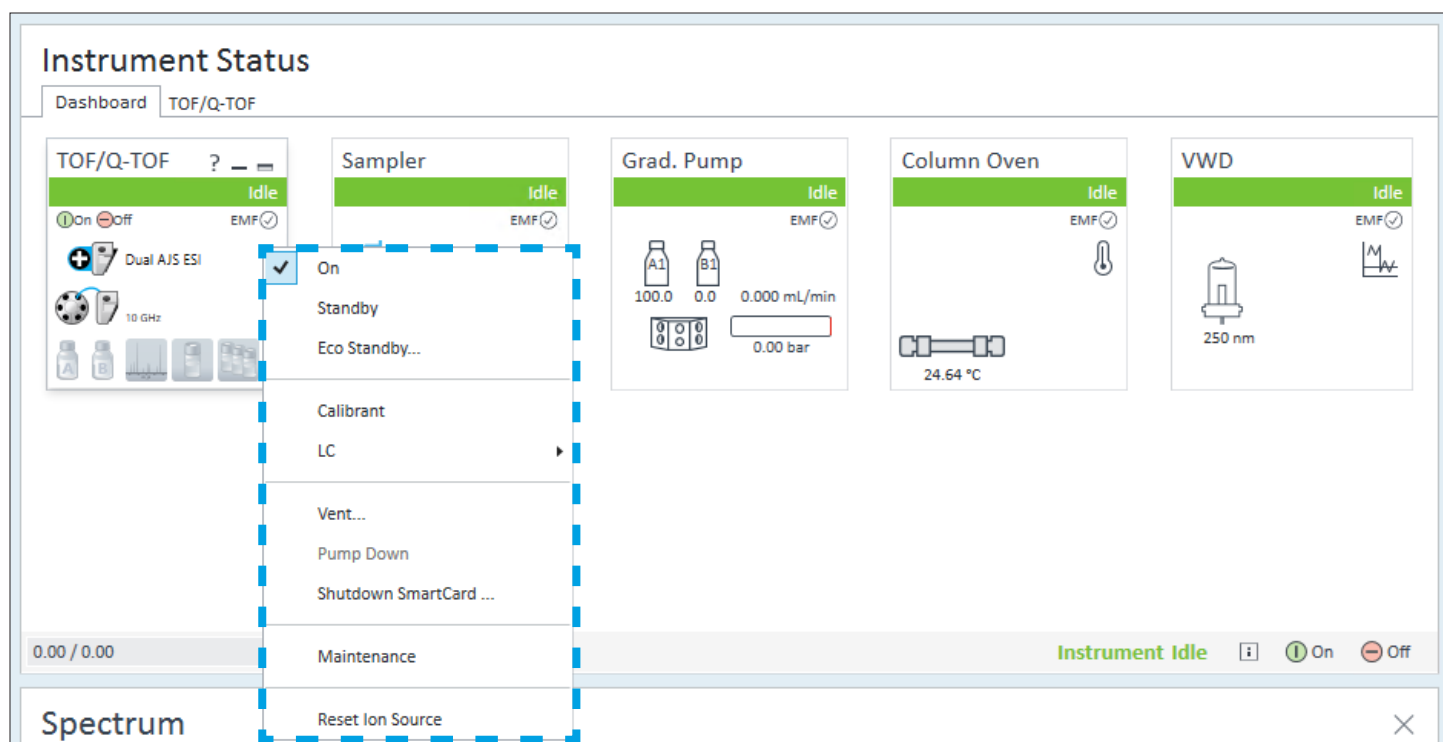


Figure 5. OpenLab CDS instrument status window showing an LC/(Q-)TOF instrument.

Real-time data viewing

In a client-server setup, multiple clients can independently view, zoom, and adjust live HRMS spectra without impacting acquisition performance in the spectrum window. Clients can also view other instrument signals such as total ion chromatogram (TIC) and pump pressure in the online signals window. Two users viewing the same analytical run from different client windows have independent control over HRMS spectral displays (Figure 6).

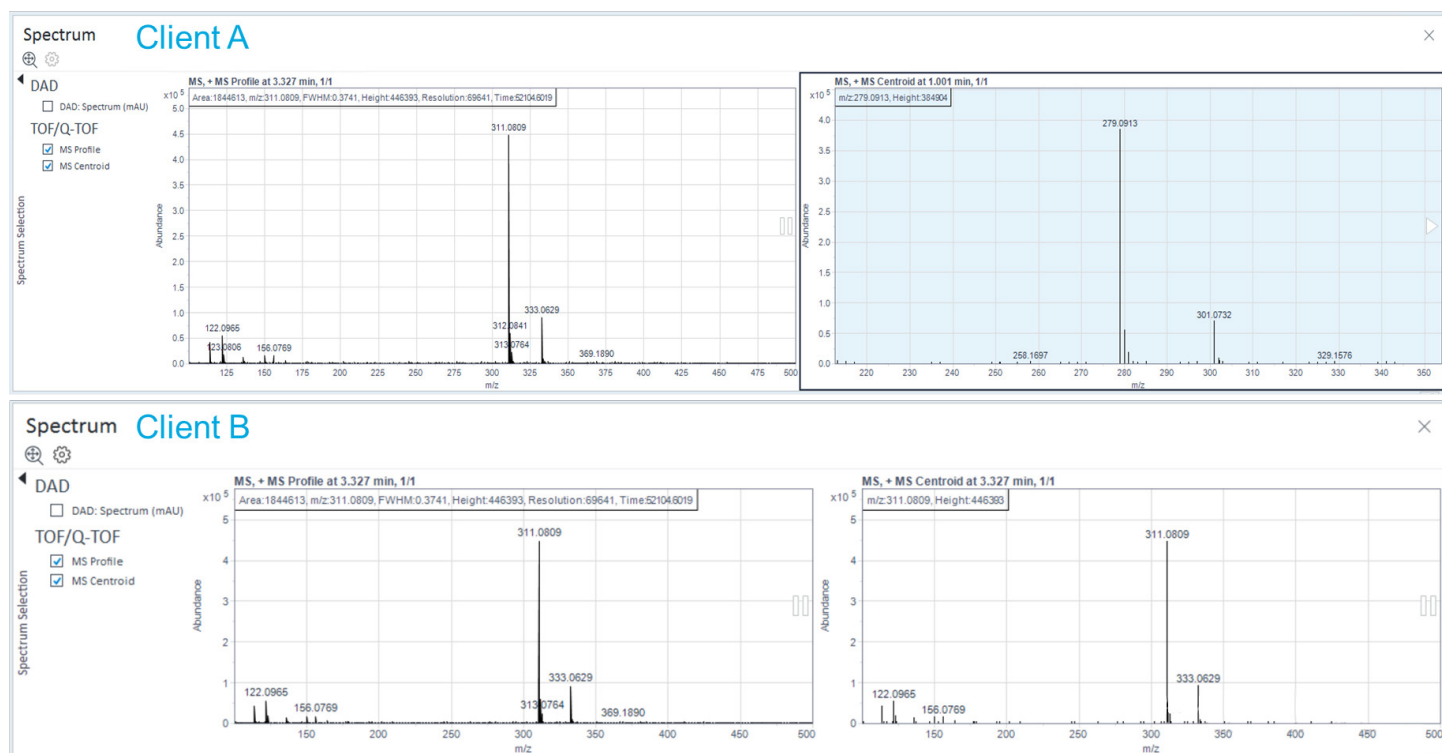


Figure 6. Real-time mass spectra of a running sample captured at the same time from client A (top) and client B (bottom). Client A has paused and zoomed in on the centroid spectrum, whereas client B is still viewing the entire spectrum in real time.

Optimized application-based instrument tuning

LC/Q-TOF instruments require precise tuning for optimal performance, particularly after installation, maintenance, pump-down, or restart. OpenLab CDS provides multiple tuning options in the acquisition software, including:

- Autotune for fully automated optimization.
- Mass calibration to ensure rapid and accurate mass assignments.
- Configure tune for selecting application-specific settings such as polarity (positive/negative) and m/z range.
- Advanced tune for expert-level performance adjustments.
- Diagnostic tune for troubleshooting and performance verification.

Preconfigured application-based tunes, combined with scheduling capabilities (available with the Agilent Revident LC/Q-TOF), allow laboratories to optimize performance with minimal downtime while maintaining consistency across users, as shown in Figure 7. They also allow the lab manager to properly configure the instrument for all users with different levels of permission.

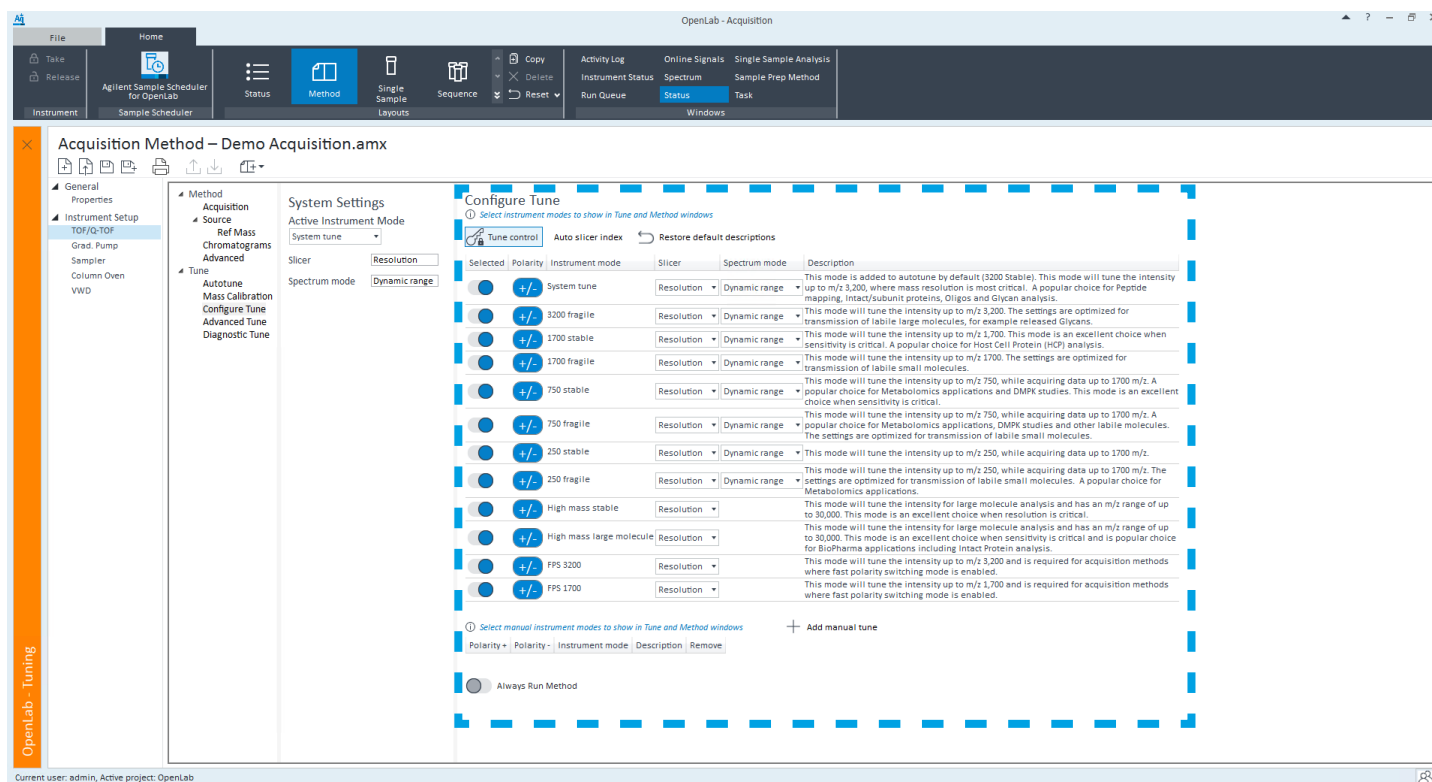


Figure 7. Tuning options for an Agilent LC/Q-TOF instrument.

Supported acquisition modes

The LC/(Q-)TOF in OpenLab CDS supports seven acquisition modes tailored for diverse analytical workflows:

- **MS:** Full-spectrum acquisition without ion isolation
- **Fast polarity switching:** Available with a resistive capillary for rapid alternation between polarities

LC/Q-TOF only:

- **All ions:** Collection of all fragment ions at defined collision energies without quadrupole isolation
- **Quadrupole-resolved all ions (Q-RAI):** Isolates wide *m/z* bands, enabling retrospective analysis and reducing noise from coeluting fragments (hardware-dependent)

- **Auto MS/MS:** Data-dependent acquisition alternating between MS and MS/MS, dynamically selecting precursor ions
- **Directed MS/MS:** Data-dependent, limited to a preferred ion list
- **Targeted MS/MS:** User-defined, reproducible isolation and fragmentation of specific ions

These accommodate both exploratory and highly targeted applications, giving analysts the flexibility to adapt to changing project requirements. All modes are shown in Figure 9 except the fast polarity switching mode. Fast polarity switching mode is only available when a resistive capillary is installed in the ion source.

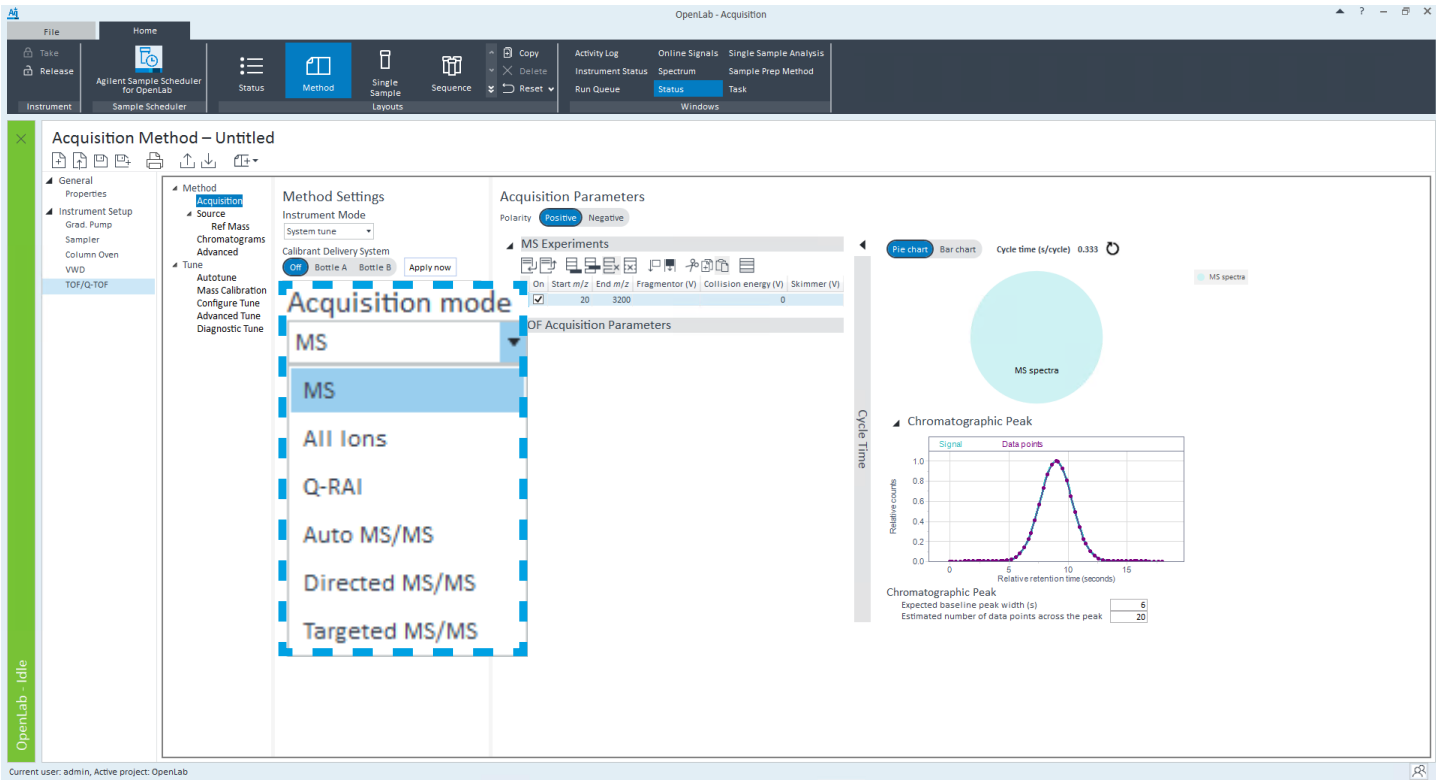


Figure 8. Acquisition modes for an Agilent LC/Q-TOF instrument.

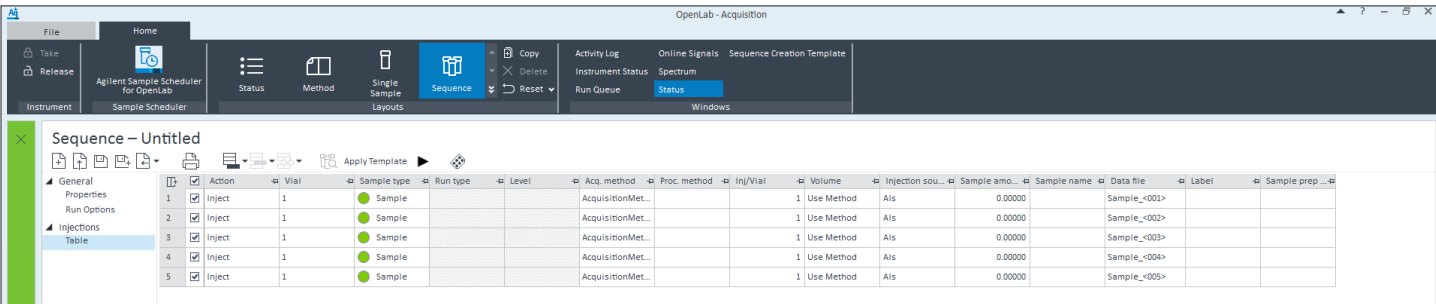


Figure 9. OpenLab CDS sequence table.

Acquiring data

OpenLab CDS provides a single user interface, to control Agilent LC, GC, single quadrupole LC/MSD, and GC/MSD instrument, along with the LC/(Q-)TOF. The OpenLab CDS sequence table (Figure 9) allows a user to:

- **Define actions:** Inject a sample, wait, task, or iterative MS/MS
- **Input sample information:** Vial number, sample type, and replicates (Inj/Vial)
- **Specify:** Acquisition method and data processing method
- **Enter additional sample custom parameters:** Sample custom parameters for MassHunter Qualitative Analysis and BioConfirm

Enhanced sequence management

To support LC/(Q-)TOF workflows, OpenLab CDS has the following enhanced sequence capabilities:

- **Wait action:** Holds and resumes the sequence manually or automatically (after or until a defined time) between runs.
- **Task action:** Executes predefined instrument tasks such as calibration or shutdown mid-sequence.

- **Iterative MS/MS (LC/Q-TOF Only):** An advanced MS/MS workflow used to improve sample characterization.⁵
- **Shutdown method:** Defines the shutdown actions to be done when all samples have been completed.

The wait action allows users to add a defined waiting period between the runs in the sequence. There are four ways to configure the Wait action (as shown in Figure 10).

The task action provides users with the capability to define and run instrument tasks at any point in the sequence; tasks such as mass axis calibration or instrument power on/off can be added to the sequence table, as illustrated in Figure 10.

The iterative MS/MS workflow (Figure 10) boosts identification by iteratively excluding higher abundant precursors while allowing low level precursors to be acquired.⁶

The shutdown method can be submitted to the run queue and is placed as the final run. If a shutdown method is added in the run queue, it will automatically shut down your LC instrument after all other runs in the run queue are complete, for example, by setting the pump to standby mode and turning off the oven and UV lamp.

The screenshot displays the OpenLab - Acquisition software interface. The top menu bar includes File, Home, and various tool icons. The main window is titled 'Sequence - Untitled' and contains a table with columns for Action, Vial, Sample type, Acq. method, TOF/Q-TOF: It..., Inj/Vial, Volume, Injection so..., Level, Run type, Sample am..., Proc. method, and Data file. The table lists several actions: Task, Inject, Wait, Iterative MS/MS, and Task. The 'Wait' action is highlighted in blue. Below the table, there are configuration options for the 'Wait' and 'Task' actions. The 'Wait' action configuration includes options for 'Wait until manually resumed', 'Automatically resume after', and 'Automatically resume at'. The 'Task' action configuration includes a dropdown menu for 'Task' with 'EcoStandby.tmx' selected. At the bottom, there are fields for 'Result path', 'Result name', and 'Save result as', along with 'Validate' and 'Run' buttons.

Action	Vial	Sample type	Acq. method	TOF/Q-TOF: It...	Inj/Vial	Volume	Injection so...	Level	Run type	Sample am...	Proc. method	Data file
Task												
Inject	1	Sample	Demo Acquisition.amx			1	Use Method	Als		0.00000		
Wait												
Iterative MS/MS	1	Sample	IterativeMSMS_001.amx	Start/Reset		1	Use Method	Als		0.00000		
Iterative MS/MS	1	Sample	IterativeMSMS_001.amx	Iterate		1	Use Method	Als		0.00000		
Iterative MS/MS	1	Sample	IterativeMSMS_001.amx	Iterate		1	Use Method	Als		0.00000		
Iterative MS/MS	1	Sample	IterativeMSMS_001.amx	Iterate		1	Use Method	Als		0.00000		
Task												

Wait action configuration:

- ☒ Wait until manually resumed
- ☐ Automatically resume after
- ☐ Automatically resume at (UTC-08:00) Pacific Standard Time
- ☐ Automatically resume after or at (UTC-08:00) Pacific Standard Time - whichever occurs first

Task action configuration:

Task:

Result path: Save result as:

Result name:

Buttons: Validate, Run

Figure 10. The sequence table displays samples, task lines, and a wait line, highlighted in the upper region. One sample is shown running with an iterative MS/MS workflow. The lower left and right regions highlight the wait and task actions, respectively

Sequence creation

The sequence creation template is a powerful tool used to define a flexible pattern for generating new sequences and is particularly useful for creating sequences with repeating elements such as QC sample before each set of 10 injections (Figure 11).

In OpenLab CDS, tokens can be used to dynamically generate sample or file names based on sample information and other fields such as sample name, injection number, injection date and time.

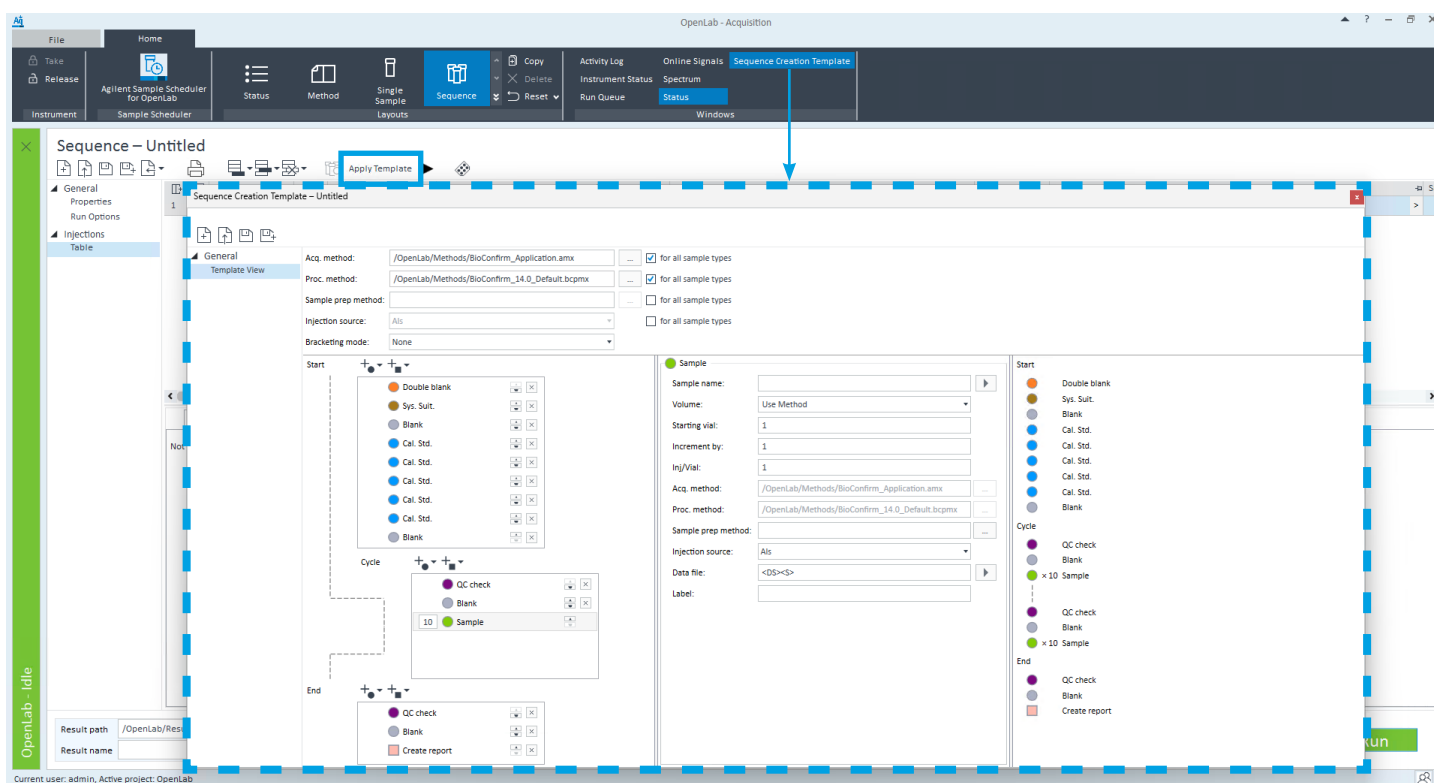


Figure 11. Sequence creation template editor showing a multi-point calibration followed by a repeating QC check with ever 10 samples.

Bridging acquisition and data processing

OpenLab CDS integrates seamlessly with MassHunter Qualitative Analysis and BioConfirm, through:

- Sample custom parameters to define processing parameters at the acquisition stage.
- Unattended data analysis for asynchronized data acquisition and processing.
- Error handling rules to either pause or continue acquisition if processing fails.
- Snapshot view of partially acquired data for early insight.
- Reprocessor for batch reprocessing without manual intervention.

Sample custom parameters provide the ability to modify the parameters of a processing method for a specific sample. In addition to the user-defined parameters, MassHunter Qualitative Analysis and BioConfirm have a predefined set that can be configured in advanced DA options. The laboratory can define which parameters can be used, whether this is mandatory, and how these are viewed in the sequence table. (Figure 12).

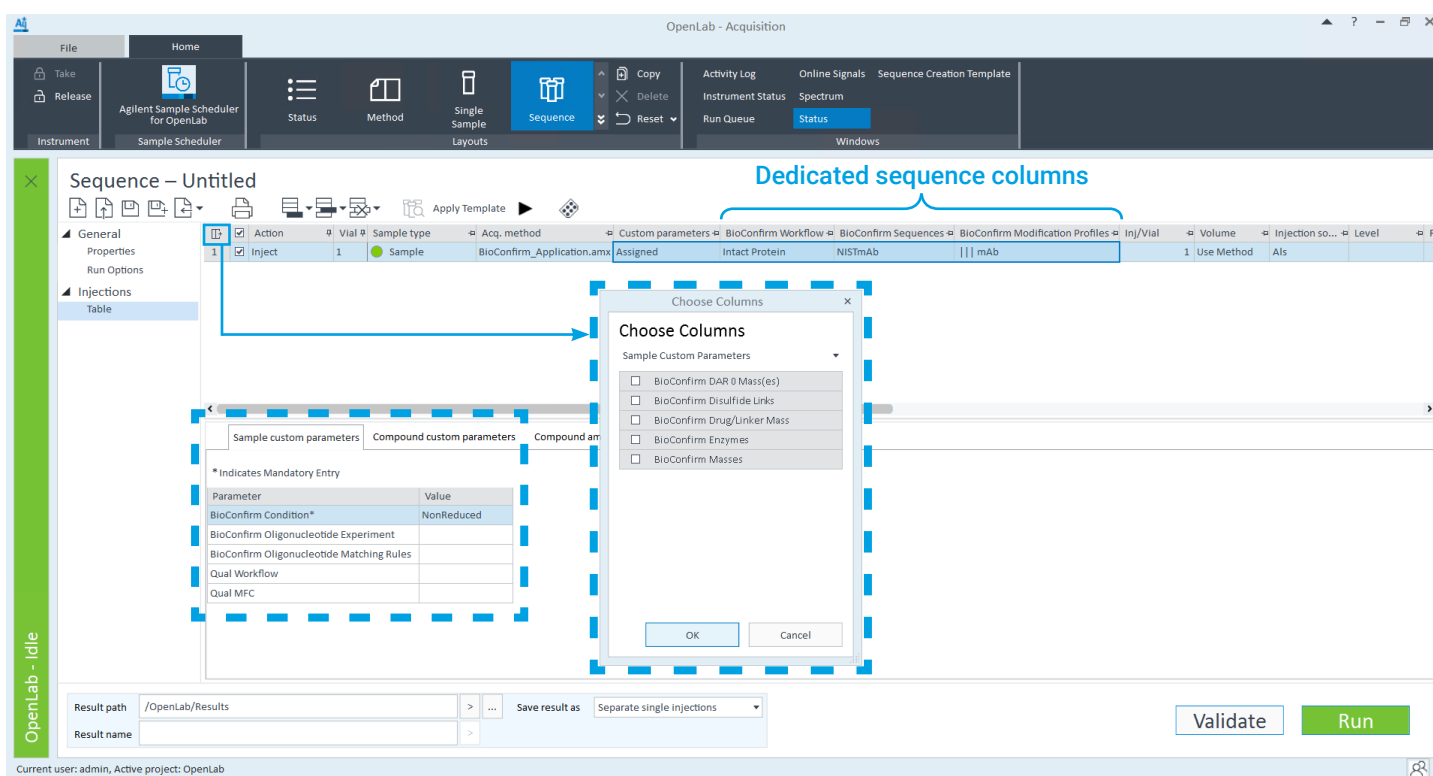


Figure 12. Display options for sample custom parameters in MassHunter Qualitative Analysis and BioConfirm: either within the sample custom parameters column or as a separate sequence column.

Unattended data analysis enables samples in a sequence to be processed immediately after each run is complete using the predefined MassHunter Qualitative Analysis, BioConfirm, or MAM processing methods. (Figure 13).

Note: The user has several options on how to handle possible errors during a sequence, including the ability to select **On error, pause after current injection**.

The snapshot feature (Figure 14) enables the user to extract and view data from an actively acquiring sample using MassHunter Qualitative Analysis software.

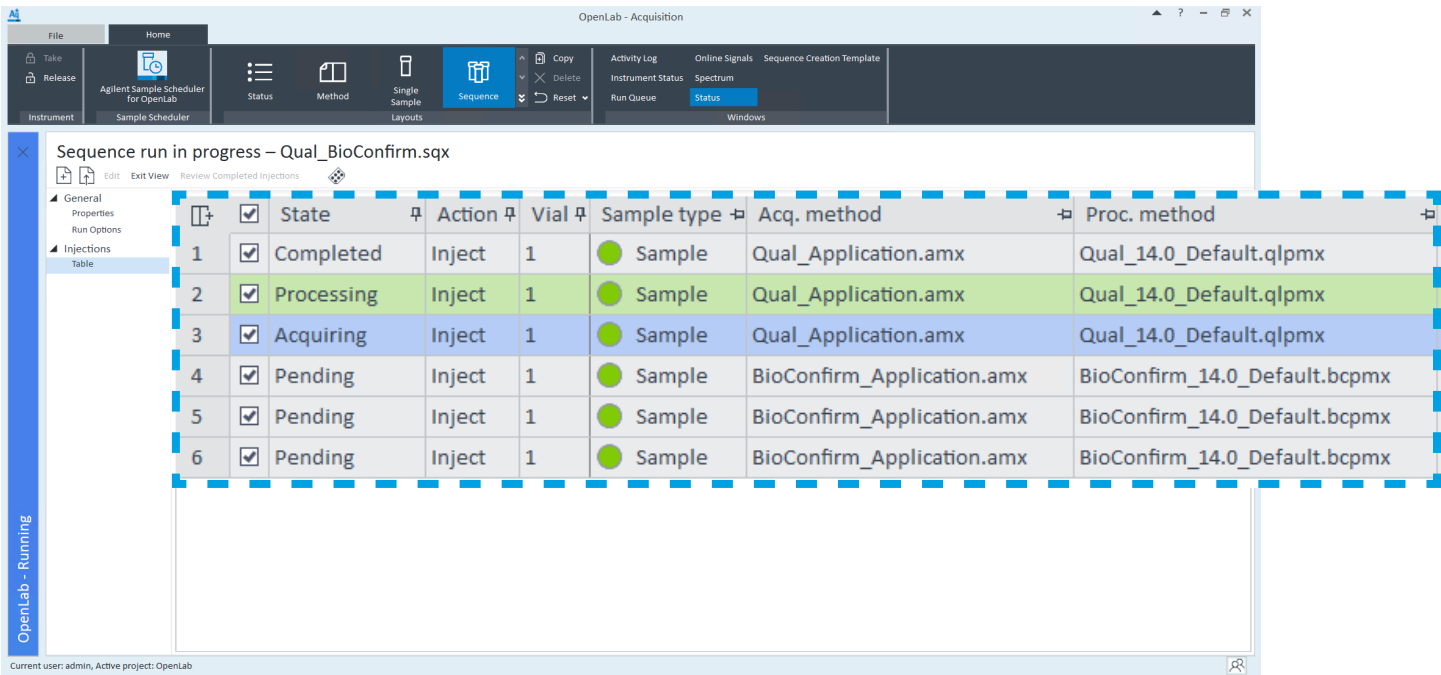


Figure 13. The OpenLab Sequence showing a mixture of MassHunter Qualitative Analysis and BioConfirm processing methods.

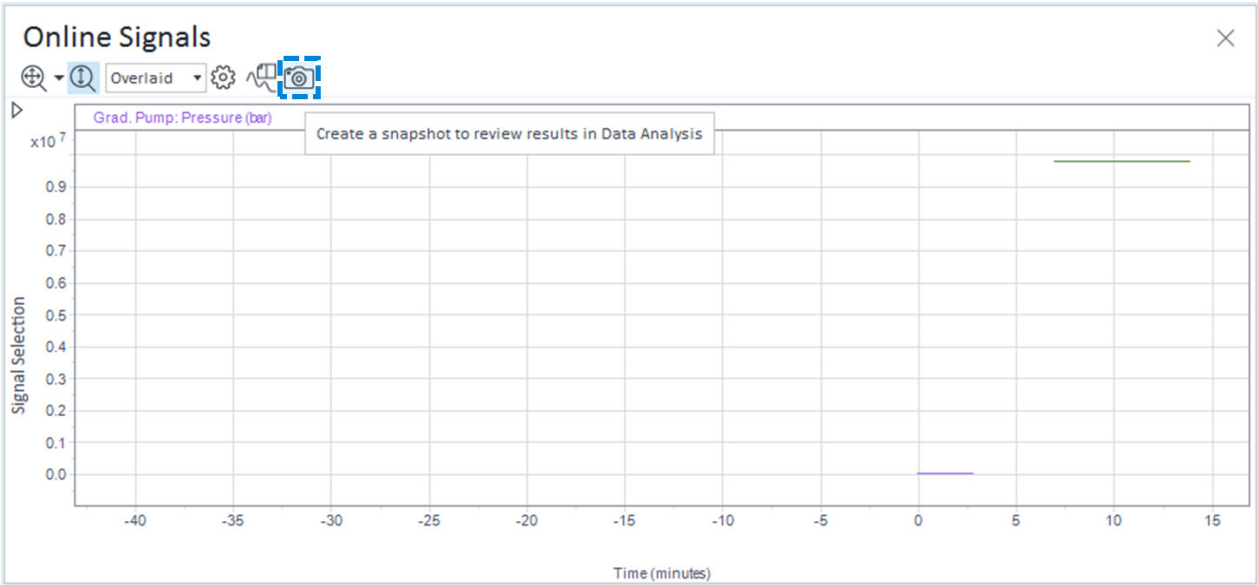


Figure 14. The snapshot button in the online signals window.

The reprocessor enables the user to automatically reprocess multiple single injection data files (.sirslt) without requiring interaction with MassHunter Qualitative Analysis or BioConfirm software (Figure 15). These features reduce manual intervention, accelerate data turnaround, and ensure a consistent, automated pipeline from acquisition to results.

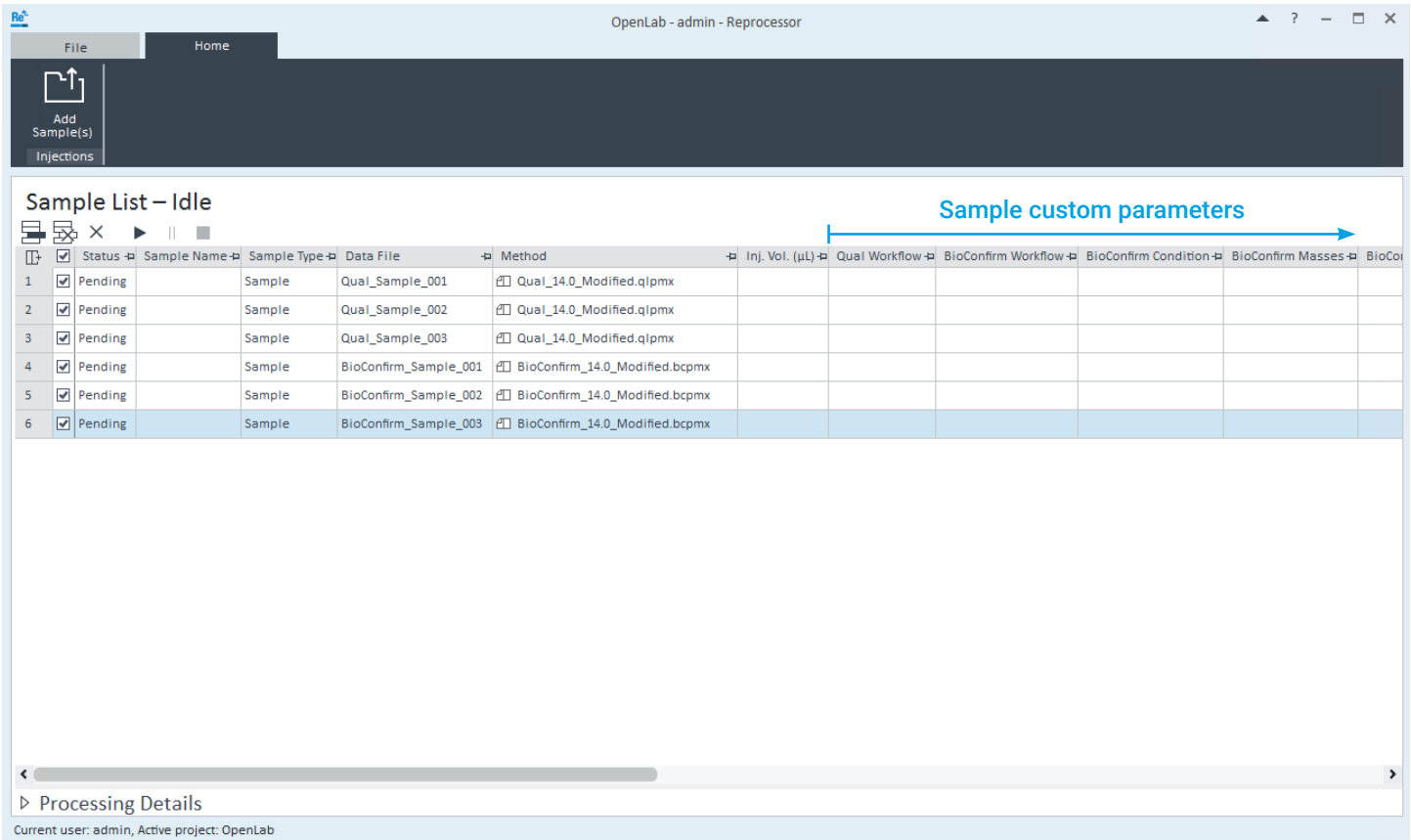


Figure 15. The view of the reprocessor.

Conclusion

The Agilent OpenLab ecosystem expands its capabilities to support LC/TOF and LC/Q-TOF instruments. This new ecosystem delivers:

- A single, consistent platform for chromatography and mass spectrometry.
- Scalable, collaborative connectivity across global laboratory networks.
- Unified data formats for simplified management and compatibility.
- Robust compliance features to meet regulatory requirements.
- Streamlined workflows from acquisition to data analysis and reporting.

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