



MassHunter Qualitative Analysis Software

Release Notes

Notices

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Agilent Technologies, Inc.
5301 Stevens Creek Blvd.
Santa Clara,
CA
95051
www.agilent.com

Software Revision

This Guide is valid for the 14.0 revision or higher of Agilent MassHunter Qualitative Analysis 14.0 until superseded.

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CAUTION

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Introduction

For our Regulated Customers

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This document provides a listing of the major feature modifications made in each release of actively supported MassHunter Qualitative Analysis software including selected add-ons.



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

For our Regulated Customers

When any change is made to Agilent software, the validation status of the software needs to be re-established by the user/customer.

Whenever software is changed, a validation analysis should be conducted not just for the validation of an individual change, but also to determine the extent and impact of that change on the entire software system.



2 **Version History**

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Version 14.0

MassHunter Qualitative Analysis 14.0 software (Qualitative Analysis) introduces support for OpenLab CDS 3.0 TOF/Q-TOF data in .sirsl format and includes compliance features and tools to help meet 21 CFR Part 11 requirements.

NOTE

Qualitative Analysis licensing is enforced. A valid license file (.lic) is required and must be registered to fully enable the software.

Supported Operating System

Qualitative Analysis 14.0 is supported on Windows Server 2022 and Windows Server 2025 only when deployed as part of an OpenLab CDS Client configuration.

Support for Windows Server operating systems is limited to environments in which OpenLab CDS is installed first and provides the acquisition framework. In this configuration, the software operates as data analysis components within an OpenLab CDS Client/Server deployment.

Windows Server 2022 and Windows Server 2025 are not supported for Qualitative Analysis in a MassHunter Acquisition-only (non-CDS) environment. For standalone or non-CDS MassHunter Acquisition workflows, supported desktop operating systems must be used.

Features:

- **OpenLab ECM Support:** Support for OpenLab ECM 3.6 (Unit Mass data only) and ECM XT 2.8 Feature Pack 1 and later.

- **Integration with OpenLab CDS 3.0 Acquisition Platform**, including support for:
 - Single Sample Results data file (.sirslt) format.
 - Allows .d and .sirslt files to be opened in the same instance.
 - Provides a new conversion option to export .sirslt data as .d files for use with third-party applications.
 - Qualitative Analysis processing method file format (.qlpmx).
 - Distributed (Client/Server) environments.
 - Centralized printing.
 - Cloud and virtualized environments.
 - OpenLab Reprocessor for automatic batch processing, including custom column support for .sirslt data.
- **PCDL (.cdbx) Format**: A redesigned PCDL format that reduces database and library size and addresses obsolete dependancies.
 - A standalone PCDL Converter tool allows batch conversion of .cdb-format PCDL files.
- **Acquisition Report Functionality**: Enables users to view and print Tune and Instrument Configuration Reports directly from the user interface.
- **.CSV Export for Acquisition Compound Information**: Allows users to view the LC/MS/MS precursor ions triggered during acquisition, helping streamline method development.
- **Support for VWD UV Spectra from Stopped Flow Cell**: Adds support for viewing UV spectra acquired using a stopped flow cell.
- **Backward Compatibility**: Qualitative Analysis 14.0 opens and displays results generated by earlier versions without modification. These results remain unchanged unless workflows or manual actions are re-executed. If any workflows are rerun in Version 14.0, the updated algorithms may produce different results from those generated in previous releases.

NOTE

- **Algorithm Updates:**

Improvements made to these algorithms enhanced feature identification quality. As a result, reprocessing data in Qualitative Analysis 14.0 may produce different compound results compared to earlier versions.

- Find by Molecular Feature
- Molecular Formula Generation

- **Ribbon UI Updates:**

- Home > Print includes Tune Report and Instrument Configuration Report.
- View tab includes a Sample Audit Trail window (visible with .sirslr data) and Bar Code Reader fields in the Sample Table.
- Processing > Actions: Find by tools (except Molecular Feature) include a dropdown for Entire Chromatogram or Over Selected Range.
- Tools > Export includes Acq Compound Info CSV and .d Conversion (conversion shown only with .sirslr data).

- **Method Editor Updates:**

- Method Automation > Report > Templates includes a Refresh button.
- Export is now "Exports and Conversions", with separate Exports and Conversions tabs (Conversions requires .sirslr data).

- **Global File Format Update:**

- All PCDL file references now use the .cdbx format.

- **Data and Method Format Compatibility:**

- Supports both MassHunter (.d) and OpenLab CDS (.sirslr) data files. While these formats differ in structure and metadata, the underlying chromatographic and spectral data are equivalent.
- The application continues to support the traditional .m method format and introduces a new CDS native format, .qlpmx, which is fully interchangeable within the application.

Minimum Supported Software

- MassHunter Acquisition for LC/MS TOF/QTOF 13.0

- OpenLab CDS 3.0
- MassHunter Acquisition for LC/MS TQ 13.0
- GC/MS MassHunter Acquisition 14.0
- MassHunter BioConfirm 14.0
- MassHunter Quantitative Analysis 13.0
- MassHunter Profinder
- Mass Profiler Professional
- MassHunter Mass Profiler
- ChemVista 1.1
- MassHunter Explorer 2.0

Configurations

The software was released in three deployment configurations:

- Workstation
- Networked Workstation (MassHunter only)
- Client/Server (OpenLab CDS only)

These configurations include features for regulatory-compliant environments and participate in the OpenLab Shared Services ecosystem. The latter configurations are designed for integration with OpenLab ECM XT and OpenLab ECM 3.x (unit mass instrument only) to enable centralized data storage, electronic signatures, and role-based access control.

In the Workstation configuration:

- All data is stored on the local file system without content management. There is no option to change this in the Control Panel.
- Turn Authentication Mode on or off in CDS Control Panel and set to internal or Domain. Users must log in to perform any action.

In the Networked Workstation configuration:

- MassHunter Qualitative Analysis is connected to an ECM XT 2.8 Feature Pack 1 server or an ECM 3.6 server (unit mass data only), requires OpenLab Shared Services Server.
- All data is stored by the Enterprise Content Management system.
- Authentication Mode is always on.
- Import existing data files, methods, libraries/databases, and report templates into a project within Enterprise Content Management.
- E-signatures for data analysis results are supported (ECM XT only).

In Client/Server Configuration:

- MassHunter Qualitative Analysis is connected to an ECM XT 2.8 Feature Pack 1 server.
- All data is stored by the Enterprise Content Management system.
- Authentication Mode is always on.
- Import existing data files, methods, libraries/databases, and report templates into a project within Enterprise Content Management.
- E-signatures for data analysis results are supported.

Version 13

Features

- **OpenLab ECM Support:** Support for OpenLab ECM 3.6 (Unit Mass data only) and ECM XT 2.7 and later.
- **Integration with OpenLab Control Panel:** Centralized management of instruments, projects, as well as Privileges for Users, Groups, and Roles.
- **E-signature:** Enables the capture and display of the signer's full name, date, time, and the purpose of the signature (e.g., review, approval, responsibility, authorship).
- **InfinityLab Sample ID Reader:** Supported functionality for the identification of sample positions that need to be measured in a given sequence.
- **GC/MS Barcode Reader:** Updated functionality for data acquired with GC/MS MassHunter Acquisition 13.1.
- **Reporting:** Cross Sample reporting example template included in the shipping media for Report Builder.
- **Snapshot Review:** Updated View Data functionality for data currently being acquired on the acquisition PC.
- **Algorithm Updates:**
 - Find by Molecular Feature
 - Find by Formula
 - Find by Fragments
 - Find by Chromatogram Deconvolution
 - Agile 2 Integrator
 - ChemStation Integrator
- **User Interface Changes:** The modernized interface maintains a consistent look and feel with other Agilent software packages, enhancing the user experience through improved functionality and layout selection.

The following features or functionality have been removed:

- ASR Export
- Excel reporting support
- Algorithm Configuration functionality
- Excel-based templates

Version 12

Features

- **Compound Mining and Identification Workflow:** View and edit workflow parameters in either Compounds View or Navigator View.
- **Compound List Window:** Reorganize columns using the new custom Categories functionality.
- **Algorithm Updates:** Updated Find by Molecular Feature algorithm.
- **Spectral Curation Workflow (Send to PCDL):** Added RT/RI support.
 - Send RTs from all accurate mass data.
 - Send RIs from all GC/MS accurate data.
- **LC/MS/MS Library Search:** Improved support for Agilent and third party public libraries.
 - Restrict library search to the sample spectrum m/z range.
 - Add a minimum m/z for matching to reduce common ion bias.
- **Export Formats:**
 - Support for mzXML and mzML export formats.
 - Improved MGF export to support GNPS workflows.
- **Spectrum Identification**
 - Support for UniProt ID when manually identifying a spectrum.
 - Support for MS/MS isolation width in MS spectrum headers.

- **Parallel Reaction Monitoring (PRM) Acquisition Mode for 6575 LC/Q-TOF**
 - Similar to Targeted MS/MS acquisition mode, but without interleaved MS level spectra to increase duty cycle.
 - Reference mass information acquired at the beginning of a sample run and applied throughout the acquisition.
 - Supported by Find by Targeted MS/MS and Identify by Library Search algorithms, and interactive manual data analysis in Navigator View.
 - Not supported by algorithms requiring an MS level spectrum, such as:
 - Find by Molecular Feature Extraction
 - Find by Auto MS/MS
 - Find by Formula, including Sample Purity workflow
 - Find by Integration
 - Identify by Database Search
 - Identify by Formula Generation



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Overview

For a list of defects fixed with this release, please see the Software Release Bulletin (SRB) included in the \Support\SSB and SRB\ folder.

For known issues and workarounds in the MassHunter Qualitative Analysis at the time of release see the Software Status Bulletins (SSB), which can be found online at:

<https://www.agilent.com/cs/library/support/Patches/SSBs/MHQual.html>

Agilent Community

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