



MassHunter Qualitative Analysis  
**Release Notes**

# Notices

## Document Identification

D0131336 A.00

May 2025

## Copyright

© Agilent Technologies, Inc. 2024

No part of this manual may be reproduced in any form or by any means (including electronic storage and retrieval or translation into a foreign language) without prior agreement and written consent from Agilent Technologies, Inc. as governed by United States and international copyright laws.

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

## Software Revision

This guide is valid for the 13.0 revision or higher of Agilent MassHunter Qualitative Analysis 13.0 Release Notes.

## Warranty

The material contained in this document is provided "as is," and is subject to being changed, without notice, in future editions. Further, to the maximum extent permitted by applicable law, Agilent disclaims all warranties, either express or implied, with regard to this manual and any information contained herein, including but not limited to the implied warranties of merchantability and fitness for a particular purpose. Agilent shall not be liable for errors or for incidental or consequential damages in connection with the furnishing, use, or performance of this document or of any information contained herein. Should Agilent and the user have a separate written agreement with warranty terms covering the material in this document that conflict with these terms, the warranty terms in the separate agreement shall control.

## Technology Licenses

The hardware and/or software described in this document are furnished under a license and may be used or copied only in accordance with the terms of such license.

## Restricted Rights Legend

U.S. Government Restricted Rights. Software and technical data rights granted to the federal government include only those rights customarily provided to end user customers. Agilent provides this customary commercial license in Software and technical data pursuant to FAR 12.211 (Technical Data) and 12.212 (Computer Software) and, for the Department of Defense, DFARS 252.227-7015 (Technical Data - Commercial Items) and DFARS 227.7202-3 (Rights in Commercial Computer Software or Computer Software Documentation).

## Safety Notices

### CAUTION

A **CAUTION** notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in damage to the product or loss of important data. Do not proceed beyond a **CAUTION** notice until the indicated conditions are fully understood and met.

### WARNING

A **WARNING** notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in personal injury or death. Do not proceed beyond a **WARNING** notice until the indicated conditions are fully understood and met.

# Table of Contents

<b>1</b>	<b>Introduction</b>	<b>4</b>
	For our Regulated Customers	4
<b>2</b>	<b>Version History</b>	<b>5</b>
	<b>Version 13.0</b>	<b>6</b>
	With this release:	6
	Configurations:	7
	Minimum Supported Software	8
	Features	8
	User Interface Changes	10
	<b>Version 12.0</b>	<b>11</b>
	Features	11
<b>3</b>	<b>Important Support Information</b>	<b>13</b>

# 1

## Introduction

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.



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

### 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

### **Version 13.0 6**

With this release: **6**

Configurations: **7**

Minimum Supported Software **8**

Features **8**

User Interface Changes **10**

### **Version 12.0 11**

Features **11**

## Version 13.0

MassHunter Qualitative Analysis 13.0 introduces a new software interface and compliance features and tools to help meet 21CFR Part 11 requirements.

### **With this release:**

- Configure user roles and privileges in OpenLab CDS to control access and functionality, if required. System access is limited to authorized persons where each user is identified by a unique ID and password combination.
- Audit Trail functionality records who was logged in, when changes are made, and displays the version of the file in which the change was saved.
- Two additional Audit Trail windows are available, Results and Method Audit Trail, which allows users to review changes and add reasons for changes.

## Configurations:

The software is available in two configurations: Workstation and Networked Workstation. These configurations include features for regulatory compliant environments and participate in the OpenLab Shared Services ecosystem.

### 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 2.7 server or an ECM 3.6 server (unit mass data only).
- 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.

**NOTE**

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

## Version History

### Minimum Supported Software

## Minimum Supported Software

- MassHunter Acquisition for LC/MS TOF/QTOF 12.2
- MassHunter Acquisition for LC/MS TQ 12.3
- MassHunter BioConfirm 12.1
- MassHunter Quantitative Analysis 12.1 Update 3
- MassHunter Profinder
- Mass Profiler Professional
- MassHunter Mass Profiler
- ChemVista
- MassHunter Personal Compound Database and Library Manager (PCDL)
- MassHunter Explorer

## 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).

## Version History

### Features

#### 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

#### The following features or functionality have been removed

- ASR Export
- Excel reporting support
- Algorithm Configuration functionality

## Version History

### User Interface Changes

- Excel-based templates

## 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.

## Version 12.0

### 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 3rd 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

## 3 Important Support Information

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 OpenLab software at the time of release see the Software Status Bulletins (SSB), which is found online at:

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

### 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/>

### Agilent on the web

Visit Agilent's website

<https://www.agilent.com/en/product/software-informatics/mass-spectrometry-software/data-acquisition/acquisition-for-lc-ms> for up-to-date information on Data Acquisition for LC/MS for up-to-date issue information on Agilent's Analytical Software suite.

[www.agilent.com](http://www.agilent.com)

© Agilent Technologies, Inc. 2025

D0131336

May 2025

