



ChemVista Library Manager
Release Notes

Notices

Document Identification

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Software Revision

This Guide is valid for the ChemVista Library Manager 1.1 revision or higher until superseded.

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CAUTION

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1 Introduction

For our Regulated Customers

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Introduction

Introduction

This document provides a listing of the major feature modifications made in each release of actively supported ChemVista Library Manager 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 1.1

ChemVista Library Manager 1.1 provides advanced library management capabilities including:

- Intuitive library management
- Compound-centric data structure
- Workflow-driven list management
- Enhanced cheminformatics
- Flexible imports and exports

This release includes extensive, high-quality curated spectral libraries and compound databases, enabling immediate use upon installation. These integrated resources support confident identification workflows across a wide range of applications, associated with the chosen library product selection: LC applied market or Metlin Library, or the GC/Q-TOF library.

Supported Instruments

- Agilent LC/Q-TOF
- Agilent LC/TOF
- Agilent GC/Q-TOF

Supported Software

NOTE

During installation, select the PCDL library file format (.cdb or .cdbx) that is compatible with the software platform and data files intended for use.

MassHunter Platform - PCDL (.cdb) Library Format

Supported with the legacy .cdb library format:

- MassHunter Qualitative Analysis 13 and earlier

Version History

Version 1.1

- MassHunter Acquisition 12.1 and later
- MassHunter Explorer 1.0 and later
- MassHunter Quantitative Analysis 12.1 and earlier
- MassHunter BioConfirm 12.1 and earlier
- MassHunter VistaFlux 1.0
- MassHunter Mass Profiler 10.0.2
- Mass Profiler Professional (MPP) 15.1
- MassHunter PCDL Manager B.800 SP1 and earlier

OpenLab CDS Platform - PCDL (.cdbx) Library Format

Supported with the newer .cdbx library format:

- BioConfirm 14.0 (also accepts .d file format)
- MassHunter Qualitative Analysis 14.0

NOTE

Qualitative Analysis and BioConfirm support processing of .d data files, with BioConfirm requiring the .cdbx library format.

Features

- **PCDL Format Support:**
 - Supports legacy PCDL (.cdb) library files, compatible with the MassHunter acquisition environment.
 - Supports redesigned PCDL (.cdbx) library files, which reduce database size, improve security, and are compatible with OpenLab CDS 3.0, MassHunter Qualitative Analysis 14, and BioConfirm 14.0.
 - Users select the appropriate PCDL format during installation based on compatibility with their acquisition software environment.
 - A standalone PCDL Converter tool enables batch conversion of .cdb files for users transitioning from MassHunter platforms to the OpenLab CDS 3.0 platform.

Version History

Version 1.1

- **Glycan Visualization:**
 - Glycan visualization is included and works with both BioConfirm 12.1 and BioConfirm 14.0.

Version 1.0

- **Integrated, curated libraries:** ChemVista includes extensive, curated spectral libraries and databases, enabling immediate startup in your lab.
- **LC/Q-TOF coverage:** Library contains over 6,000 compounds with spectra and another 8,000 without spectra, improving unknowns identification in food, environmental, forensic toxicology, and extractables & leachables analyses by mass spectrometry.
- **Application domains & classes:** Food & environmental compounds (pesticides, herbicides, fungicides, mycotoxins, veterinary drugs, PFAS, PPCPs, polar metabolites, cyanotoxins); E&L (stabilizers, accelerators, inks, antioxidants, dyes, residual monomers); forensic toxicology compounds (antidepressants, antiepileptics, hypnotics, stimulants, hallucinogens, designer drugs, etc.).
- **Intuitive library manager:** Organize, edit, or create spectra with an easy-to-use interface, improving workflow efficiency and reducing training needs.
- **Flexible imports:** Import mass spectra and metadata from MassBank EU, MassBank of North America (MoNA), U.S. EPA CompTox Chemicals Dashboard, CSV files, and Agilent Personal Compound Database and Library (PCDL) files for maximum flexibility.
- **Compound-centric structure:** Seamlessly integrates compound details, multiple retention times, and spectra from numerous sources to support confident identification within Agilent MassHunter data analysis.
- **Enhanced cheminformatics:** Generates structures and identifiers, eliminates duplicates, and supports downstream workflows for maximum confidence in matches.
- **List-driven workflows:** Lists act as organizational tools per analysis; a compound can exist in multiple lists with desired analytical conditions (RT, analyzer type, polarity, etc.) to further enhance identification accuracy.
- **Easy curation:** Newly created spectra can be added to the library to expand the scope of unknowns identification.
- **Open science:** Export spectra to open-access databases to enrich the scientific community.



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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 ChemVista Library Manager software at the time of release see the Software Status Bulletins (SSB), which can be found online at:

<http://www.agilent.com/cs/library/support/Patches/SSBs/SLD.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/>

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