



MassHunter Explorer
Release Notes

Notices

Document Identification

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Software Revision

This guide is valid for revision 2.0 or higher of Agilent MassHunter Explorer.

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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.

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Introduction

This document provides a listing of the major feature modifications made in each release of actively supported MassHunter Explorer 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.



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Version History

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Version 2.0

MassHunter Explorer 2.0 introduces a significantly enhanced non-targeted analysis workflow for LC/Q-TOF and LC/TOF data, as well as IM data collected in Q-TOF mode only. This release extends the unified platform to support non-targeted MS/MS workflows—streamlining project set up, feature finding and alignment, MS/MS extraction, statistical analysis, and MS/MS identification.

With this release:

Support of MS/MS Profiling Workflow

- Introduced support for MS/MS profiling workflows, including deisotoping to enhance fragment ion clarity and compound identification.

Improved Processing Speed

- Optimized spectral processing algorithms, resulting in faster MS/MS extraction and overall workflow performance.

Improved Spectral Matching & ID Confidence

- Enhanced scoring combines accurate mass, isotope pattern, retention time, and MS/MS spectral matching.

Integration with SIRIUS and NIST

- Enables direct export of compound data to tools such as SIRIUS CSI:FingerID and NIST MS Search for advanced structural identification.

Supported Instruments

- Agilent LC/TOF
- Agilent LC/Q-TOF
- IM-Q-TOF (operating in Q-TOF mode only)

Minimum Supported Software

- MassHunter Acquisition for LC/MS TOF/Q-TOF 12.0
- MassHunter Qualitative Analysis 12.0
- MassHunter Quantitative Analysis 12.0
- ChemVista 1.0
- SIRIUS 6.3.0
- NIST MS Search 3.0

NOTE

SIRIUS must be installed using the .msi installation package to enable integration with MassHunter Explorer. If any errors occur after installation, contact support@bright-giant.com.

Features

Support of Non-targeted MS/MS mass profiling workflow

- Seamless integration of MS1 non-targeted data with iterative AutoMS/MS fragmentation within a single interface.

Streamlined Identification Pipeline

- Combines setup, alignment, normalization, filtering, statistical analysis, and feature identification in six defined steps—all in one application interface.

Advanced Spectral Matching & Scoring

- Compound identification leverages high mass accuracy, isotope pattern matching, retention time, and MS/MS spectra.

High-Quality Visual Output

- Interactive figures—such as isotope overlays and mirror plots—exportable as publication-ready images.

Version 1.0

Features

Broad Statistical Capability

- Supports hierarchical cluster analysis, volcano plots, PCA, one- and two-way ANOVA, fold-change analyses, and unique-feature comparisons with all with integrated visualizations.

Project-Based Workflows

- Enable easy method setup and seamless transferability between users and instruments.

Integrated Navigation

- Streamlined procedures simplify movement between linked results within a single environment.

Guided Parameter Selection

- Supports optimization of various analytical processes with intuitive guidance.

Flexible Statistical Tools

- Includes t-tests, fold-change analyses, volcano plots, one- and two-way ANOVA, and hierarchical cluster analysis (HCA) to support multiple data evaluation strategies.

Comprehensive Data Visualization

- Chromatographic, spectral, statistical, and compound ID data are displayed together, enabling faster decision-making.

Accelerated Processing

- Enhanced speed improves compound discovery throughput in your laboratory.

Interoperable Results

- Exported data can be used with other common software platforms for additional analysis and reporting.



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 Explorer 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/MSDMPNG.html>

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