Agilent

MassHunter Acquisition for LC/(Q)-TOF

Release Notes

Notices

Document Identification

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

Software Revision

This guide is valid for the 12.1 revision or higher of Agilent MassHunter Acquisition, for LC/(Q)-TOF.

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Safety Labels

NOTICE

NOTICE indicates a situation which, if not avoided, results in damage to or destruction of the device or data.

CAUTION

CAUTION indicates a hazardous situation which, if not avoided, could result in minor or moderate injury.

WARNING

WARNING indicates a hazardous situation which, if not avoided, could result in death or serious injury.

DANGER

DANGER indicates a hazardous situation which, if not avoided, will result in death or serious injury.

Table of Contents

1 Introduction

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

Instrument documentation, installation instructions, step by step videos, and more can be found by scanning the 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

Version 12.1

NOTE

MassHunter Acquisition 12.1 for LC/(Q-)TOF uses tighter tolerances and higher statistical thresholds to maximize instrument performance relative to the tuning routine in MassHunter Acquisition 11.0 (and prior). It is possible that a system that tuned successfully with MassHunter Acquisition 11.0 (and prior) may fail to complete a tune with version 12.1. In addition, when a tune is started for the first time with MassHunter Acquisition 12.1, the instrument will automatically perform a special tune that requires approximately 5 hours to complete. This extended tune only needs to be completed once. If your system struggles to tune with MassHunter Acquisition 11.0 (or prior) - it is NOT recommended to upgrade to version 12.1. Contact your Agilent Support representative to discuss options for upgrading to version 12.1.

NOTE

MassHunter Acquisition 12.1 for LC/(Q-)TOF introduces a defect that impacts Mass Profiler, MassHunter Explorer, Lipid Annotator, and Profinder. Data acquired in Centroid-only may fail to load in Mass Profiler and MassHunter Explorer, while data acquired in Profile-only may fail to load in Lipid Annotator and Profinder. As a workaround, acquire all data using the "Both" data storage setting.

NOTE

MassHunter Acquisition 12.1 for LC/(Q-)TOF introduces a defect that prevents some acquisition methods from being migrated and imported into MassHunter Acquisition 12.1 if they were originally created in version 10.1 (or prior) versions of the software. Agilent recommends recreating methods in version 12.1 or not upgrading to this release.

Supported Instruments

- 6545XT, 6546, and Revident LC/Q-TOF systems. No other LC/Q-TOF model is supported with this release of MassHunter Acquisition.

Features

- Intelligent Reflex
  - Carryover detection workflow logic
  - Above calibration range workflow logic
  - Fast screening workflow logic
  - Iterative MS/MS
  - Suspect Screening confirmation

- Worklist flexibility
  - Add, delete, re-order, import from CSV, import from worklist – all while the worklist is running
  - Improved copy/paste functions to/from Excel
  - Faster worklist editing

- Support Infinity III LC system
  - InfinityLab Sample ID Reader

- Support for ECM XT 2.8 server and ECM XT 2.7 for 6545XT, 6546, and Revident LC/Q-TOF systems

- Scheduled tune
  - Scheduled tuning alleviates the burden of routine maintenance, so you know that the mass spectrometer is always at peak performance
  - Schedule tune available for 6546 and Revident LC/Q-TOF systems

- Parallel reaction monitoring (PRM) available for Revident LC/Q-TOF systems

- Early Maintenance Feedback (EMF)
  - Provides an easy-to-read dashboard to help visualize LC/MS instrument health and anticipate upcoming maintenance events

- TCD (Tune, Calibration, Diagnostics)
  - Accessible via the Advanced Tune Option in MassHunter Acquisition
  - Removes complex manual tune/voltage control from most customers into a separate node
  - Ramping of multiple ions
  - Custom tune in addition to pre-defined tunes
  - Saving of manual tunes, accessible in MassHunter Acquisition
  - Execution of Diagnostic Tune for comprehensive troubleshooting

User Interface Changes

Instrument status window

- Eco Standby
- Maintenance (EMF)

DA node

- Molecular feature extraction (MFE) conversion
- Delete profile data after SureMass conversion

- Intelligent reflex
  - Intelligent reflex workflows include automatic reinjection for carryover, saturation, fast screening, suspect screening confirmation, and iterative MS/MS that allow the instrument to continuously acquire data while you focus on the results

System settings pane

- Enable time segments
- For 6545XT and 6546:
  - Slicer settings renamed from High Resolution and High Sensitivity to Resolution and Sensitivity
  - Spectrum mode settings renamed from Extended dynamic range and 4 GHz High Resolution to Dynamic range and High res
  - Slicer and Spectrum mode settings of active instrument mode displayed (read only) in System settings

Timed Events

- Divert LC stream without using time segments
- Post-run divertor valve position- now in alignment with LC/TQ

Acquisition modes

MS

- Default method rates and parameters have been changed for real cases, for example, previous 1Hz vs current 3Hz, summed abundances will be 1/3 of previous default method

All Ions mode

- Setup to match PCDL libraries and recommended DA workflow parameter settings

Q-RAI mode:

- Q-RAI acquisition mode isolates a wide m/z band, applies different collision energies, and reduces noise and interference, enabling easy non-targeted analysis and retrospective fragment confirmation
- 6546 and Revident only

Auto MS/MS mode

m/z Inclusion Range pane

- Moved from m/z Static Exclusion list to m/z Inclusion Range

Auto MS/MS Preferred Exclude Ion List pane

- Import from PCDLs
- Color alternate rows
- Change, RT = 0 is now invalid
- Compound name, CAS#, formula, ion species
- Change, Insert row now copies the previous rows parameters

Directed MS/MS mode

- New Acquisition mode identical to Auto MS/MS with “preferred list only” checkbox enabled. Similar to Targeted MS/MS but isolates precursors only when they are observed.
- Import from PCDLs
- Color alternate rows
- Change, RT = 0 is now invalid
- Compound name, CAS#, formula, ion species
- Change, Insert row now copies the previous rows parameters
- Preferred ion list is shared between Auto MS/MS and Directed MS/MS

Targeted MS/MS mode

- Import from PCDL's
- Color alternate rows
- Change, RT = 0 is now invalid
- Compound name, CAS#, formula, ion species

- Change, Insert row now copies the previous rows parameters

Concurrent MS/MS spectra pane

- Understanding the density of the targets across the chromatogram. Analogous to dMRM viewer on LC/TQs

PRM mode

For Revident only

- Time segments disabled with PRM

FPS mode

- Autodetection of capillary type (only displayed when resistive capillary installed, if dielectric capillary installed will not be visible)
- Time segments disabled with FPS

Source node

- Auto detection of ion source. In offline method editor there is a drop down
- Copy source parameters to all time segments
- To prevent mismatched parameters when using time segments

Reference Mass node (under Source node)

- Reference Mass Solution notes, saved on a per method basis
- Revident Reference Solution flow rate and pressure

Change in behavior

- Only up to two masses can be selected.
- Displaying both Positive and Negative reference mass ions

- Detection window was 100 ppm and is now 20 ppm

Chromatograms

- New icons

Tune nodes

- Removal of Tune context and Tune parameters moved into Tune nodes under Q-TOF method editor tab
- Manual tune has moved to Advanced Tune TCD
- Moved Quad amu out of tune into Advanced section of Method node
- Application based tune architecture
- Diagnostic tune
- Simplified UI for routine users
- Scheduled tune (for 6546 and Revident)
- Editable description for application tunes
- EMF
- Improved View tune report UI
- Select and run multiple tunes at a time
- Estimation of time to run multiple tunes

Version 12.0

- The only supported instrument is Revident. All changes from 11.0 are covered in **"Version 12.1"** on page 6.

Version 11.0

Supported Instruments

- The following Agilent Q-TOF mass spectrometers are supported:
  - 6560A, 6560B, 6550 iFunnel, 6546, 6545XT AdvanceBio, 6545B, 6545A, 6540B, 6540A, 6538A, 6530C, 6530B, 6530A, and 6520B
  - The Agilent 6230B, 6230A, and 6224A Accurate-Mass TOF mass spectrometers are supported in this release
  - Agilent Control Panel is supported

Configurations

- Data Acquisition now has two configurations:
  - MassHunter Data Acquisition Workstation
  - MassHunter Data Acquisition Networked Workstation
- Data Acquisition Networked Workstation includes features for the regulatory compliant environments.
- In Workstation configuration:
  - Data storage is always local, with no content management. You do not have an option to change this in the Control Panel
  - Authentication Mode can be turned on or off in the Control Panel Authentication Mode means that you have to log in to perform any action. You can set authentication to internal or Domain
- In Networked Workstation configuration:
  - Data is always stored and managed in the Content Management component of OpenLab Server or ECM XT
  - Authentication Mode is always on
  - You can import existing Data Files, Methods, and Worklists into a project in the Content Management component

Additional Information

- Data Acquisition has different user roles and privileges in this release. You may not be able to use some features if you do not have the correct role
- All changes in the method are recorded in the Audit Trail except parameters in the Chromatogram tab (which are not data related parameters) and parameters in the 2D-LC File Splitter section in the DA > Data Conversions tab
- You can review changes shown in the Audit Trail window and add a reason for any changes that have not been reviewed
- 2D-LC acquisition is supported in content management mode, but only without file splitting
- The Tune file is saved in the SmartCard hard drive
- Electron-Capture Dissociation (ECD) (third party hardware controlled by eMSion software and firmware add-on) is supported. Agilent software shares Polarity, Scan type (MS1, ,MS2), Scan Time (the next spectrum scan time), and collision energy. (CE)
- Optional SLIM hardware which is controlled by MOBILion software and firmware addon is supported. SLIM stands for Structures for Lossless Ion Manipulation.
- RapidFire software is supported
- The AP-MALDI ion source is supported
- Third party high resolution demultiplexing is supported in addition to the Agilent Demultiplexing tool
- The Q-TOF driver can down-sample from 10 GHz to 4 GHz for the G6546A
- The MS data file supports a new header schema which includes isolation windows width
- Sure Mass optimization is supported for the 6546, the 6545, and the 6545XT AdvanceBio instruments
- The 6546 Q-TOF supports using the PC for MS/MS decisions
- Iterative MS/MS is introduced for classic MS/MS decisions
- The Ribbon replaces the menu and the toolbar in the Data Acquisition program

Version 10.1

Supported Instruments

- The Agilent 6545XT AdvanceBio Q-TOF mass spectrometer is supported
- The Agilent 6550 iFunnel, 6546, 6545B, 6545A, 6540B, 6540A, 6538A, 6530C, 6530B, 6530A, and 6520B Q-TOF mass spectrometers are supported in this release
- The Agilent 6230B, 6230A, and 6224A Accurate-Mass TOF mass spectrometers are supported in this release

Additional Information

- You can select the Data Independent mode for Q-TOF instruments that have Q-RAI enabled Quad drivers installed. Only 6546A support Q-RAI for this release.
- SureMass is available as an alternative way to find peaks

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 can be found online at:

https://www.agilent.com/cs/library/support/Patches/SSBs/MHAcqLCQTOF.html

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