Reliable LC/MS for Medicinal Chemists, Peptide/Protein Chemists, Biologists, and Beyond

Open Access LC and LC/MS using Agilent MassHunter WalkUp software
Enable Robust Open Access LC or LC/MS Analysis with a Single User Interface

Announcing the latest evolution of Open Access software for LC and LC/MS users, based on years of feedback from Agilent customers.


These capabilities open new doors for applications such as:

- Determining sample purity, verifying compounds, checking chemical reaction outcomes, generating or confirming molecular formulas, and performing high-resolution accurate mass identification of small molecules or peptides.
- Characterizing peptides and large molecule therapeutics. That includes analyzing intact proteins, peptides, and antibody drug conjugates (ADCs); performing relative quantitation of peptides/ADCs/intact proteins; confirming molecular weight and sequence coverage; and calculating ADC drug-to-antibody ratios (DAR).
- Collecting fractions based on UV and/or mass-based signals.

MassHunter WalkUp is now supported with:

<table>
<thead>
<tr>
<th>MassHunter WalkUp</th>
<th>OpenLab CDS 2.X</th>
<th>OpenLab ChemStation Edition</th>
<th>MassHunter</th>
</tr>
</thead>
<tbody>
<tr>
<td>WalkUp 4.0 with target confirmation</td>
<td>●</td>
<td>●</td>
<td>●</td>
</tr>
<tr>
<td>WalkUp 4.0 with purity confirmation</td>
<td>●</td>
<td>●</td>
<td>●</td>
</tr>
<tr>
<td>WalkUp 4.0 with mass-based fraction collection</td>
<td>●</td>
<td></td>
<td></td>
</tr>
<tr>
<td>WalkUp 4.0 with BioConfirm</td>
<td>●</td>
<td></td>
<td></td>
</tr>
<tr>
<td>WalkUp 4.0 with ASR file export</td>
<td>●</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Simple, Convenient Sample Submission

With MassHunter WalkUp software, chemists and biologists can submit their samples in four easy steps:

1. Log in
Enter username, password (optional), workflow, and number of samples.

2. Select method
Enter sample details and choose from a list of methods.

3. Load sample
Place the sample in the location indicated.

4. Receive report
Choose from formats such as PDF, ASR, and Excel.

Classic Open Access screens are still available, and can be configured on a system-by-system basis.
Our LC/MS portfolio gives you unprecedented flexibility for analyte-agnostic workflows

- Choice of ionization sources: ESI, APCI, APPI, or Multimode (APCI+ESI)
- Fast positive/negative switching for narrow UHPLC peaks
- Sensitive detection for low-level components
- Divert valve for reduced contamination
- External tray for sample submission and automatic discard of used vials
- Mass-based fraction collection
- Localized sample submission screens in Chinese and Japanese

Select from multiple ionization techniques for all analyte types.

Our LC/MS instruments deliver superior reproducibility of retention time, peak area, peak resolution, and mass accuracy. Here we show data for repeat injections on an LC/MS single quadrupole system.
How Does MassHunter WalkUp Benefit Analysts?

The MassHunter WalkUp environment simplifies sample submission and gives every analyst—regardless of experience—hands-on access to LC/MS capabilities

Now, even nonexperts can:
- Control sample preparation, treatment, and storage.
- Access a broad range of applications:
  - Sample purity
  - Compound verification
  - Clone selection
  - Formulation optimization
  - Covalent inhibitor studies
  - Mass-based fraction collection
- Accept protein sequences and drug-linker mass at the time of sample submission.
- Consistently analyze data and perform spectral deconvolution (such as pseudo first-order rate constants) for more confident comparative studies.

Overcome Open Access LC/MS implementation challenges for biomolecules

Take full advantage of high-resolution TOF and Q-TOF measurements by integrating MassHunter WalkUp and MassHunter BioConfirm. This combination gives biologists an Open Access environment previously available only for small molecule analysis, which eliminates risk, increases efficiency, and automates the interpretation of results.
Many Applications, One Centralized Solution

Using MassHunter WalkUp to manage your LC and LC/MS applications increases efficiency, consistency, and throughput with fully automated solutions. You’ll also minimize errors associated with maintaining diverse workflows.

**Compound verification and purity assessment**
- Sample preparation
- Upload expected formula or molecular weight
- Chromatographic separation
- Peak detection
- Assess peak MS spectra

**Mass-based fraction collection**
- Reaction mixture
- Sample submission
- Upload expected formula or molecular weight
- Chromatographic separation

**Peptide mapping**
- Enzymatic digestion
- Sample preparation
- Upload sequence
- Data acquisition
- Compound extraction
- Sequence matching

**Intact protein analysis**
- Sample preparation
- Upload sequence
- MS spectrum deconvolution
- Zero-charge mass determination
- Sequence matching
With the new MassHunter WalkUp interface, users always know what’s happening in the instrument queue.

608.273376 + 1
v. 609.2771
Compare expected monoisotopic mass to observed m/z considering adducts

High throughput compound purity assessment with Analytical Studio Reviewer software

Fraction purity determination
Fraction pooling

2*G0F (NGA2F)
(+1445.3580)
2*G1F
(+1607.5013)
1*G1F/G2F
(+3377.1458)
Determine post-translational modifications

Sequence coverage

2*G0F (NGA2F)
(+1445.3580)
2*G1F
(+1607.5013)
1*G1F/G2F
(+3377.1458)
Determine post-translational modifications

Optional ADC DAR calculation

Delivery of results

Reporting
Optional BioConfirm and ADC DAR Calculator

Make LC/MS accessible to all biologists and chemists. MassHunter WalkUp works seamlessly with BioConfirm and ADC DAR Calculator to enable protein confirmation, ADC DAR calculation, and peptide mapping with PTM identification.

MassHunter BioConfirm streamlines data processing for therapeutic proteins.
Analytical Studio Reviewer

Enable quick visualization of results and selective data review—especially for larger sample sets, like whole plates. With Analytical Studio Reviewer, results files can be emailed to users. These files open into a viewer, allowing users to browse the results and navigate to problem samples quickly.

By eliminating the need for chemists to have data analysis software at their desks, Analytical Studio Reviewer can significantly reduce costs for large installations.

Quickly picture and review data using Analytical Studio Reviewer.
MassHunter WalkUp provides powerful-yet-straightforward system administration to meet the needs of a diverse user base. So your lab can maximize uptime and minimize training costs.

With MassHunter WalkUp, a single administrator can:
- Easily manage many systems and workflows.
- Customize sample submission screens on a system-by-system basis.
- View instrument status remotely.
- Add, modify, or delete user profiles and methods.
- Receive system error notifications by text message or email.

And when it's time for maintenance, you can take instruments offline remotely with minimal impact. The sample queue will finish and the screen will lock, preventing new samples from being submitted.

Here's what one administrator is saying...

“MassHunter WalkUp makes our instruments easy to use and hard to break. Its ease of use helps us bring complex assays done by experts to a WalkUp method.”

— Open Access Administrator at a major pharmaceutical company, where medicinal chemists perform LC/MS analyses of small molecules during drug discovery.
With OpenLab Shared Services, MassHunter WalkUp can manage your lab from anywhere on the network.

Because the settings are hosted on a central server, you can immediately implement the data system (OpenLab CDS ChemStation Edition or MassHunter) and any updates. So there's no need to attach an instrument.

Manage MassHunter and OpenLab Controlled Instruments

Agilent LC
Agilent LC/MSD XT
Agilent 1290 Infinity II Autoscale Prep LC/MSD
Agilent 6546 LC/Q-TOF

LAN
Workstation
OpenLab Shared Services
LAN
Agilent CrossLab services. From insight to outcome.

CrossLab is an Agilent capability that integrates services and consumables to support workflow success and important outcomes like improved productivity and operational efficiency. Through CrossLab, Agilent strives to provide insight in every interaction to help you achieve your goals. CrossLab services include method optimization, flexible service plans, and training for all skill levels. We have many other products and services to help you manage your instruments and your lab for best performance.

Learn more about Agilent CrossLab, and see examples of insight that leads to great outcomes, at www.agilent.com/crosslab

Learn more:

Buy online:
www.agilent.com/chem/store

Find a local Agilent customer center:
www.agilent.com/chem/contactus

U.S. and Canada
1-800-227-9770
agilent_inquiries@agilent.com

Europe
info_agilent@agilent.com

India
lsca-india_agilent@agilent.com

Asia Pacific
inquiry_lsca@agilent.com

For Research Use Only. Not for use in diagnostic procedures.

This information is subject to change without notice.