

# 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.

Agilent MassHunter WalkUp software lets your lab access and administer Agilent OpenLab CDS ChemStation Edition, OpenLab CDS 2.X, and MassHunter-controlled LC and LC/MS (LC/MSD, TOF, and Q-TOF) instruments.

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:

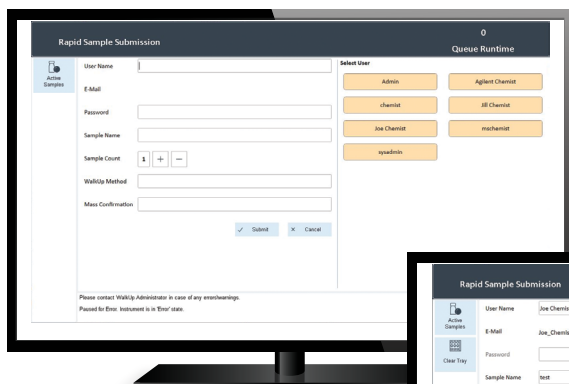
|  | OpenLab CDS 2.X | OpenLab ChemStation Edition | MassHunter |
|--|-----------------|-----------------------------|------------|
| WalkUp 4.0 with target confirmation            | •               | •                           | •          |
| WalkUp 4.0 with purity confirmation            | •               | •                           |            |
| WalkUp 4.0 with mass-based fraction collection |                 | •                           |            |
| WalkUp 4.0 with BioConfirm                     |                 |                             | •          |
| WalkUp 4.0 with ASR file export                |                 | •                           | •          |

# Simple, Convenient Sample Submission

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

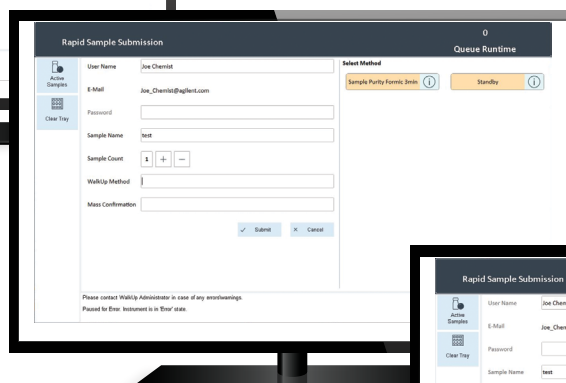
## 1. Log in

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



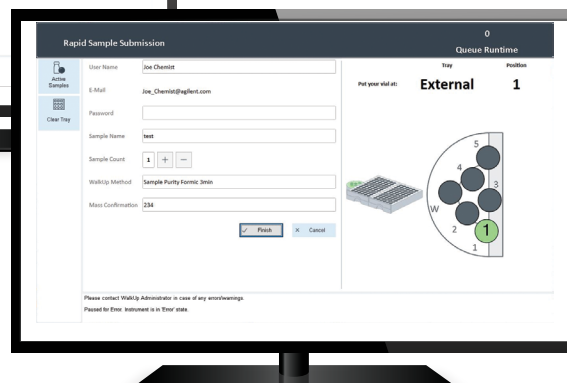
## 2. Select method

Enter sample details and choose from a list of methods.



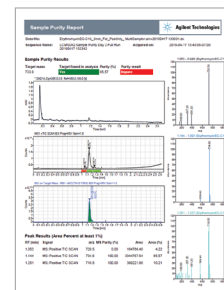
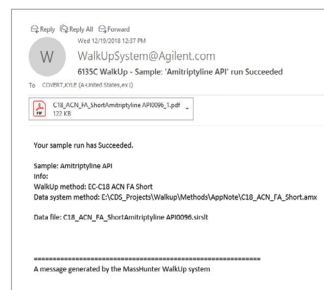
## 3. Load sample

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.

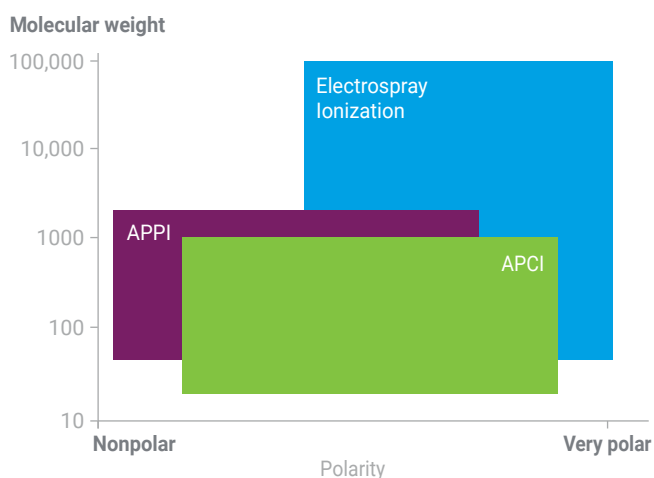


# See More Compounds in Your Sample

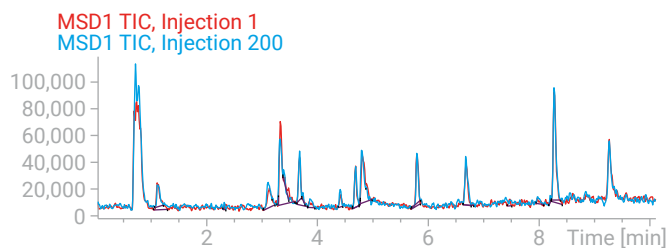
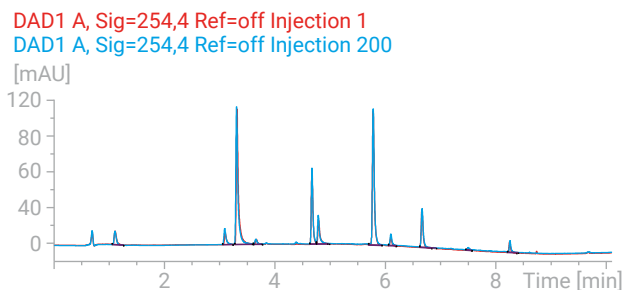


## Our LC/MS portfolio gives you unprecedented flexibility for analyte-agnostic workflows

- 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?



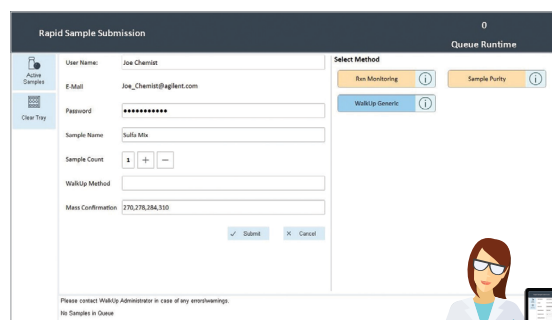
## The MassHunter WalkUp environment simplifies sample submission and gives every analyst—regardless of experience—hands-on access to LC/MS capabilities

Now, even nonexperts can:

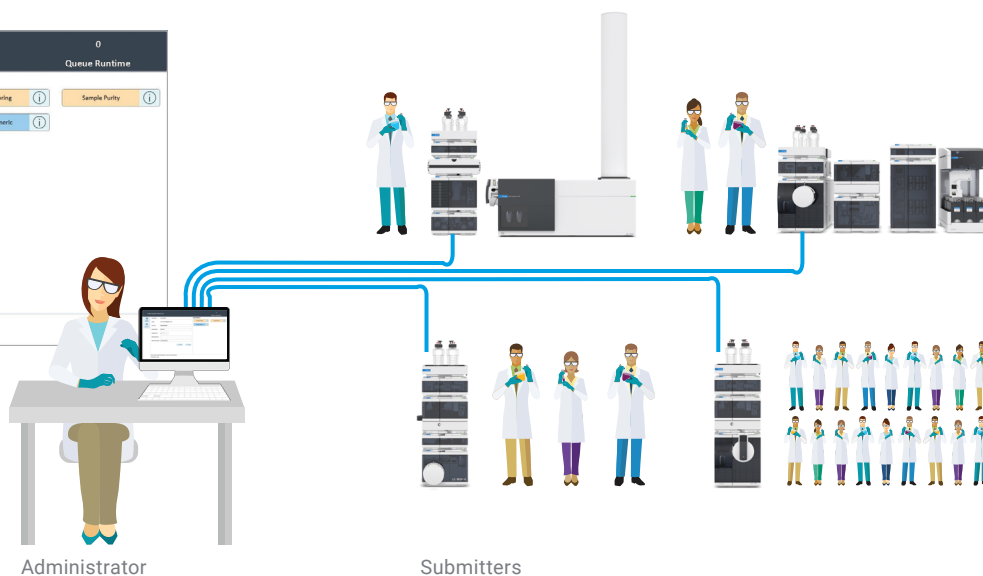
- Control sample preparation, treatment, and storage.
- Access a broad range of applications:
  - Sample purity
  - Compound verification
  - Clone selection
  - Formulation optimization
  - Covalent inhibitor studies
  - Mass-based fraction collection
- Accept protein sequences and drug-linker mass 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.



Easy Open Access facility administration in a multi-user, multi-instrument environment.

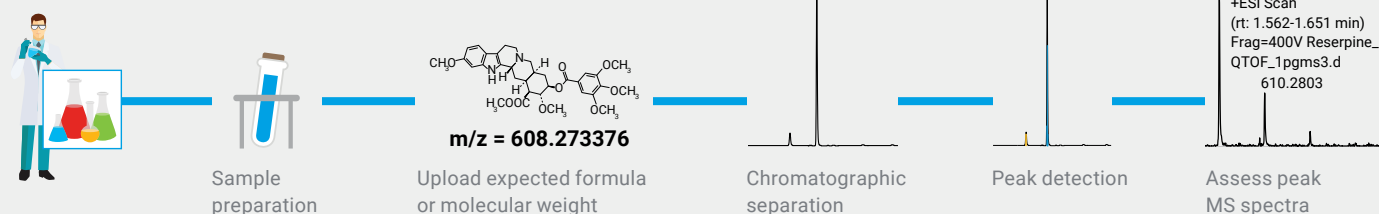


# Many Applications, One Centralized Solution

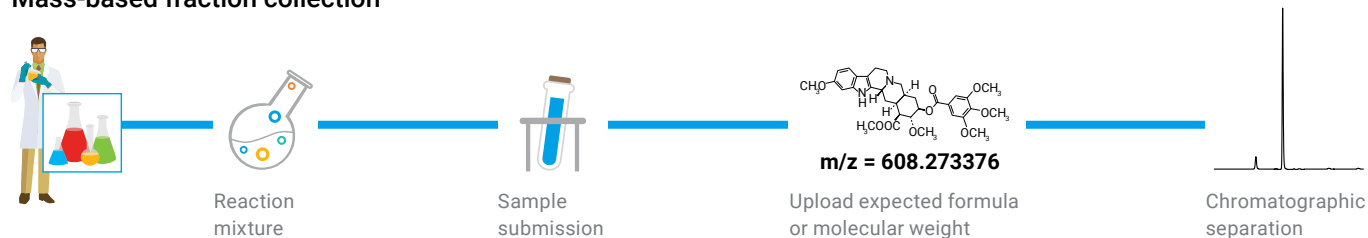


Using MassHunter WalkUp to manage your LC and LC/MS applications increases efficiency, consistency, and throughput with fully automated solutions. You'll also minimize errors associated with maintaining diverse workflows.

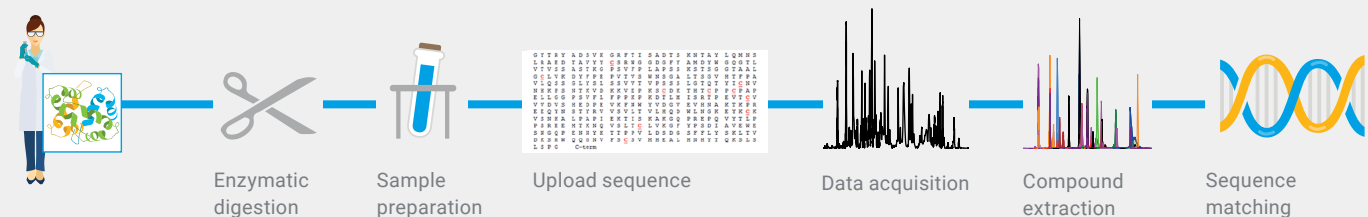
## Compound verification and purity assessment



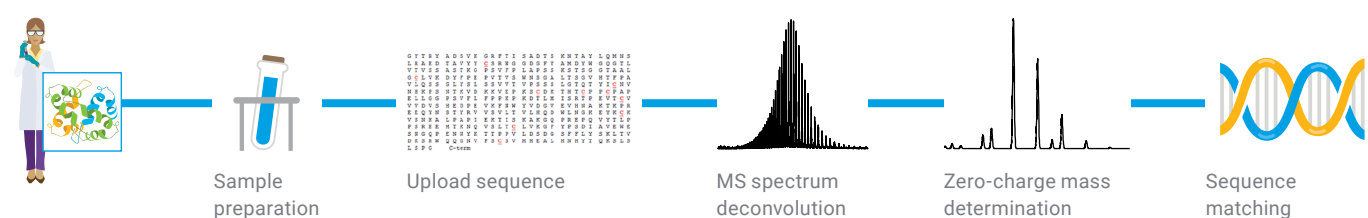
## Mass-based fraction collection



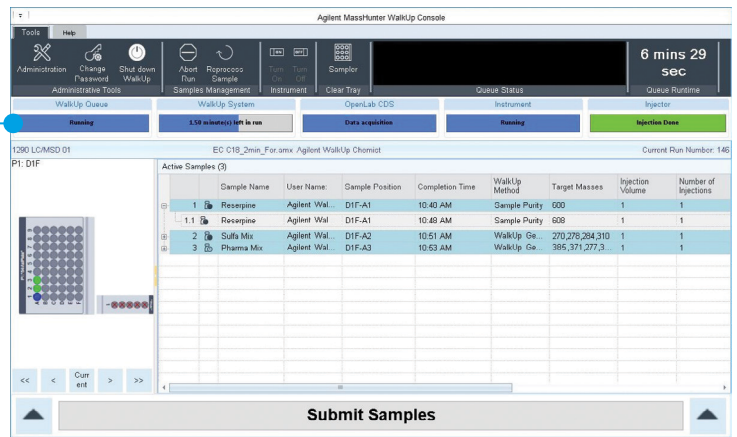
## Peptide mapping



## Intact protein analysis



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

|     |   |   |   |   |   |   |   |   |   |   |   |     |
|-----|---|---|---|---|---|---|---|---|---|---|---|-----|
| 176 | T | L | S | S | T | T | P | S | S | I | G | 150 |
| 191 | G | I | L | L | G | D | S | R | F | P | S | 205 |
| 206 | V | D | K | V | D | R | K | L | C | A | K | 220 |
| 221 | C | P | P | C | A | P | E | L | L | G | O | 235 |
| 236 | V | F | L | P | P | K | P | K | D | L | M | 250 |
| 251 | K | T | P | P | T | C | V | V | D | T | S | 265 |
| 266 | D | R | V | T | F | R | V | V | D | V | V | 280 |
| 281 | H | N | A | K | T | K | P | E | S | O | T | 295 |
| 296 | F | V | V | S | L | T | V | L | R | D | L | 310 |
| 311 | R | G | R | E | T | C | T | V | S | H | A | 325 |
| 326 | R | T | E | R | T | S | T | R | K | A | R | 340 |
| 341 | R | P | V | V | T | L | P | P | R | R | L | 355 |

Sequence coverage

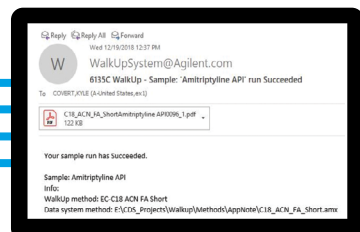
2\*G0F (NGA2F)  
(+1445.3580)  
2\*G1F  
(+1607.5013)  
1\*G1F/G2F  
(+3377.1458)

Determine post-translational modifications



Optional ADC DAR calculation

Delivery of results



Reporting

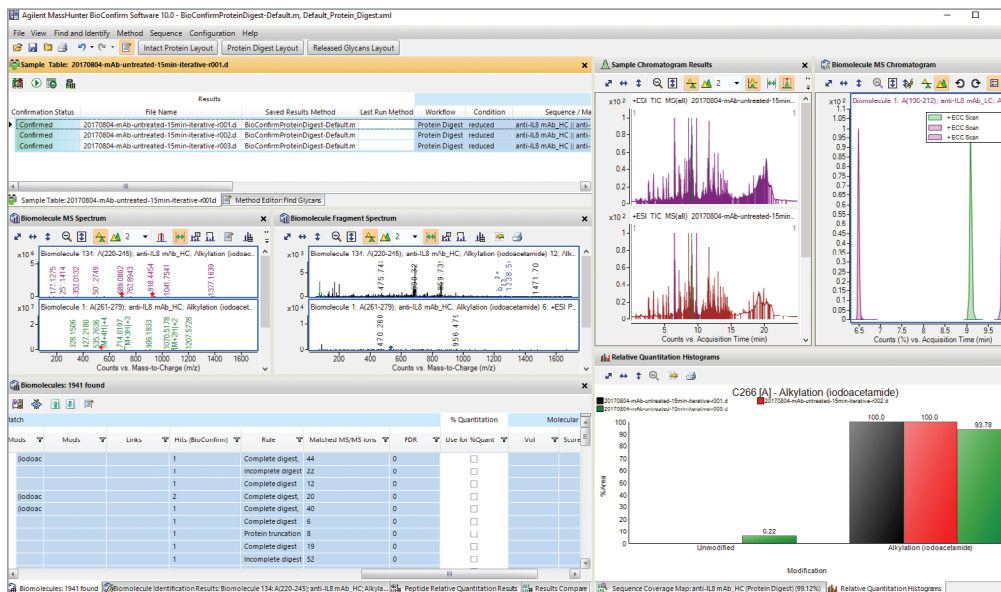


# Simplified LC/MS for Everyone



## 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.

# How Does MassHunter WalkUp Benefit Administrators?



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:

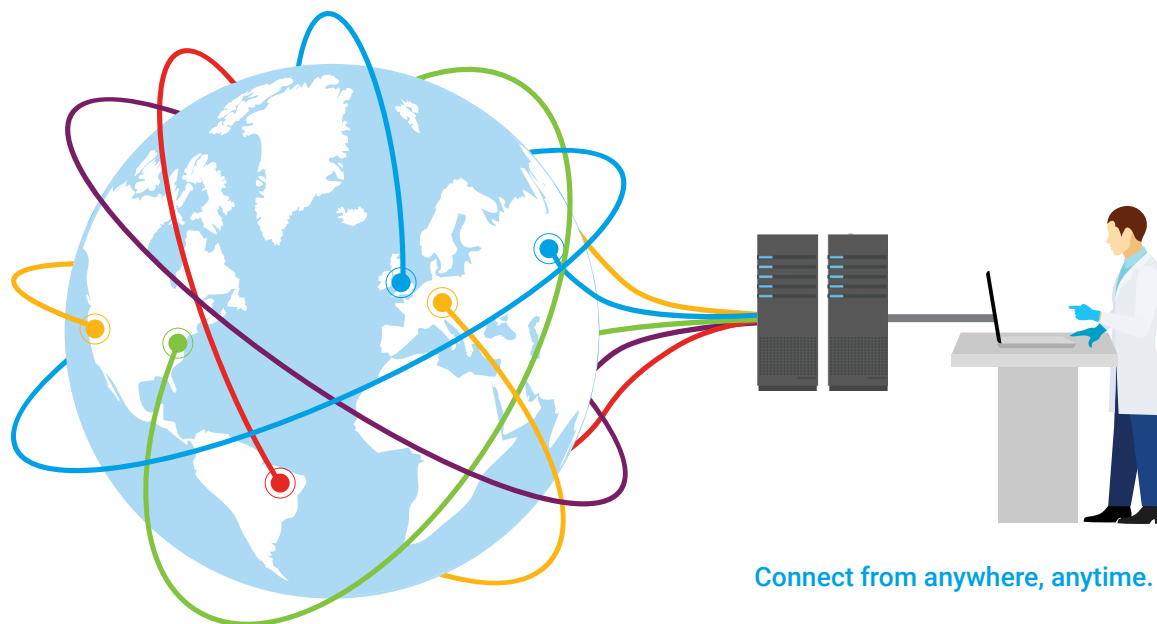
- Easily manage many systems and workflows.
- Customize sample submission screens on a system-by-system basis.
- View instrument status remotely.
- Add, modify, or delete user profiles and methods.
- Receive system error notifications by text message or email.

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.



Connect from anywhere, anytime.



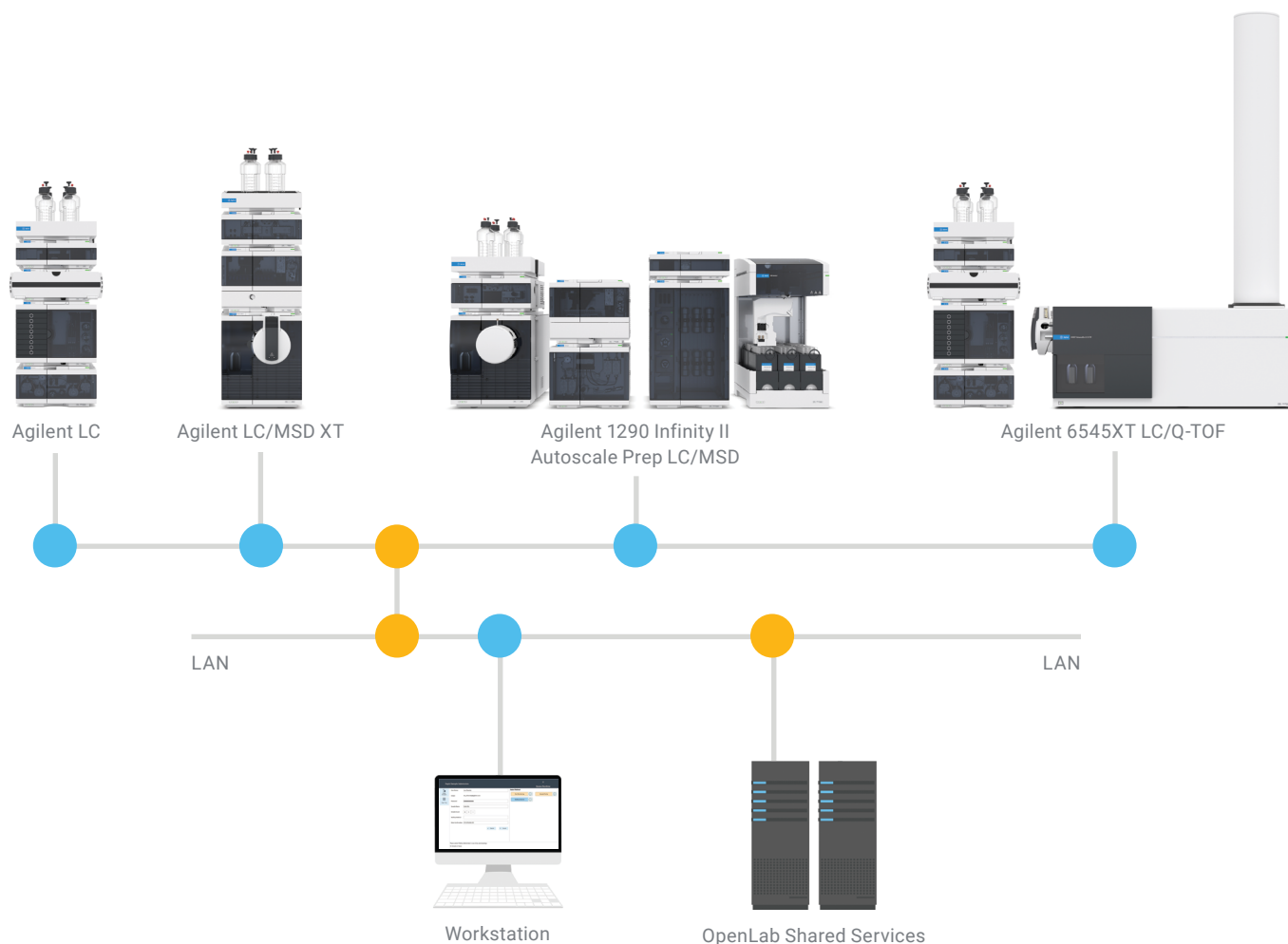
# Manage MassHunter and OpenLab Controlled Instruments



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.



## Agilent CrossLab services

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

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