



Pharmaceutical Workflow Solutions

# WALKUP LC/MS FOR PHARMACEUTICAL R&D

Chemists, Peptide/Protein Chemists,  
Biologists, and Beyond



# MASSHUNTER WALKUP

## A Single User Interface for Robust and Reliable LC/MS Implementation

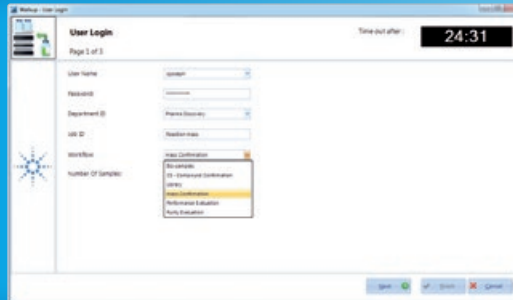
The latest in the evolution of open access software for LC and LC/MS users, Agilent MassHunter Walkup centralizes access to and administration of OpenLAB and MassHunter controlled LC and LC/MS (SQ, TOF and Q-TOF) instruments for a wide variety of applications:

- Small molecules and peptides – determine sample purity, verify compounds, check chemical reaction outcomes, generate or confirm empirical molecular formulas, perform high-resolution accurate mass identification.
- Peptides and large molecule therapeutics – analyze intact proteins, peptides, ADCs, and others; confirm molecular weight and sequence coverage; and calculate ADC drug-to-antibody ratio.

# GET DEEP WORKFLOW CONTROL WITHOUT HAVING TO BUILD DEEP EXPERTISE

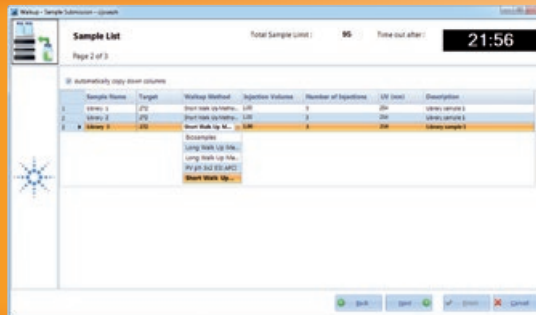
## 1. Login

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



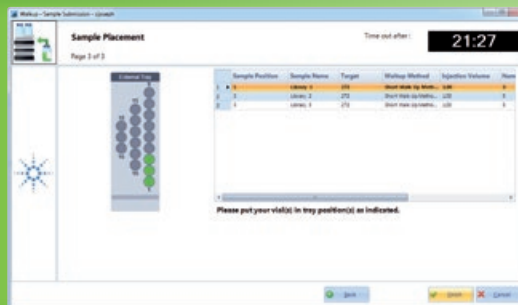
## 2. Choose method

Enter sample information and select from a list of available methods.



## 3. Place sample

Place sample in the position as directed by the software.



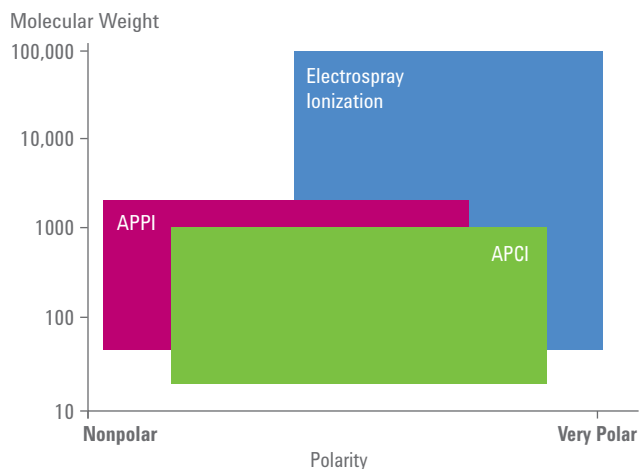
## 4. Receive report



# SEE MORE COMPOUNDS IN YOUR SAMPLE

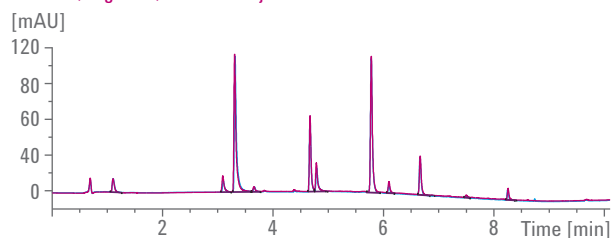
## Our LC/MS portfolio enables unprecedented flexibility for analyte-agnostic workflows.

- Choice of ionization sources: ESI, APCI, APPI, or Multi mode (APCI+ESI) (see figure)
- Fast pos/neg switching for narrow UHPLC peaks
- Sensitive detection for low-level components
- Divert valve for reduced contamination
- External tray for sample submission
- Automatic discard of used vials

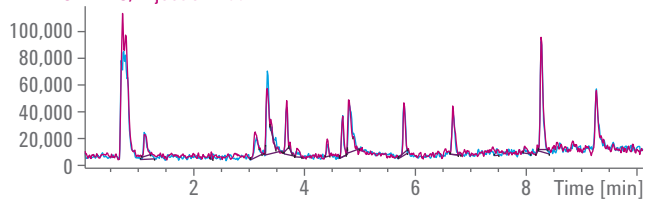


Select from multiple ionization techniques for all analyte types with our LC/MS portfolio.

DAD1 A, Sig=254,4 Ref=off Injection 1  
DAD1 A, Sig=254,4 Ref=off Injection 200



MSD1 TIC, Injection 1  
MSD1 TIC, Injection 200



Our LC/MS instruments deliver superior reproducibility of retention time, peak area, peak resolution and mass accuracy. Data for repeat injections on an LC/MS Single Quadrupole system are shown.

# HOW MASSHUNTER WALKUP BENEFITS SAMPLE SUBMITTERS

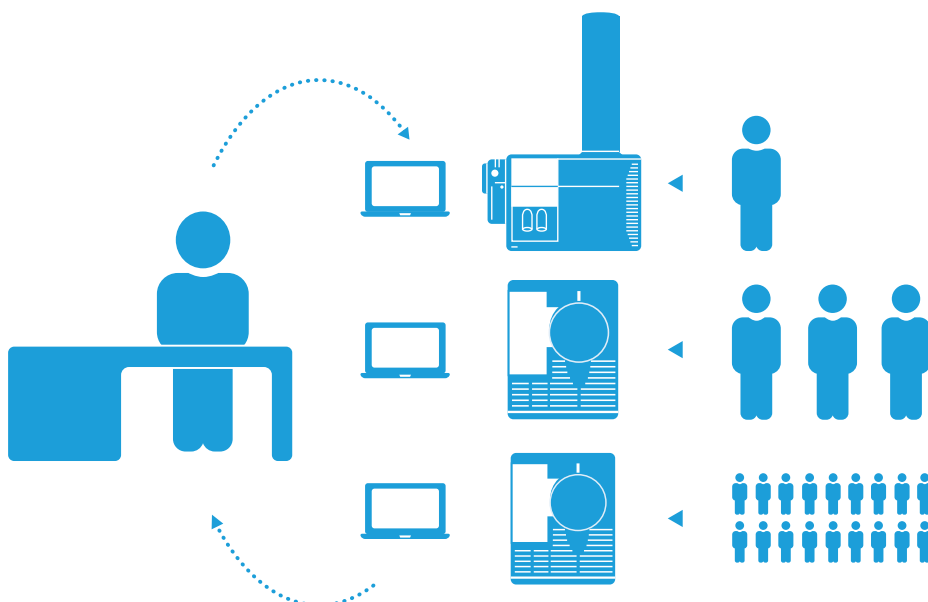
**The MassHunter Walkup environment provides sample submitters with hands-on access to expert LC/MS capabilities – without requiring them to be LC/MS experts.**

- Control sample preparation, treatment, and storage
- Access a broad range of applications:
  - Sample purity
  - Compound verification
  - Clone selection
  - Formulation optimization
  - Covalent inhibitor studies
- Accept protein sequences and drug-linker mass by the end user at the time of sample submission.
- Get consistent data analysis and spectral deconvolution (e.g., pseudo first-order rate constants), for greater confidence during comparative studies.

## Overcome Common Open Access LC/MS Implementation Challenges for Biomolecules

Take full advantage of high resolution TOF and Q-TOF measurement with the Integration of MassHunter Walkup and MassHunter BioConfirm offering biologists an open-access type environment previously only available for small molecule analysis.

- Eliminate risk
- Increase efficiency
- Automate interpretation and delivery of results

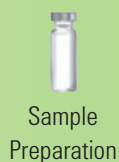


Easy open access facility administration in a multi-user, multi-instrument environment

# MANY WORKFLOWS – ONE CENTRALIZED SOLUTION

By adopting MassHunter Walkup software to manage your LC/MS applications, you'll increase efficiency, consistency, and throughput and minimize the errors associated with maintaining multiple diverse workflows.

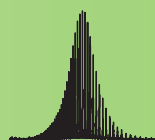
## Intact Protein Analysis



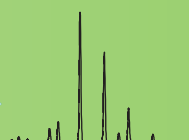
Sample Preparation



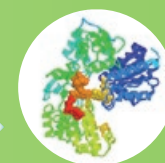
Upload Sequence



MS Spectrum Deconvolution



Zero-charge Mass Determination



Sequence Matching

## Peptide Mapping



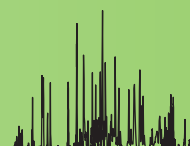
Enzymatic Digestion



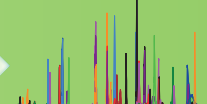
Sample Preparation



Upload Sequence



Data Acquisition

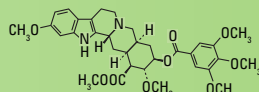


Compound Extraction

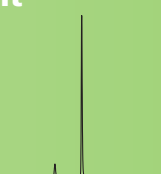
## Compound Verification and Purity Assessment



Sample Preparation



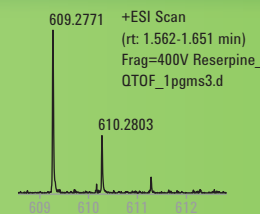
Upload Expected Formula or Molecular Weight



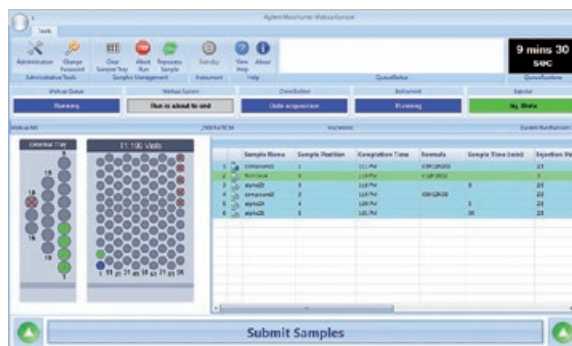
Chromatographic Separation



Peak Detection



Assess Peak MS Spectra



With the new MassHunter Walkup user interface, users always know what is happening in the instrument's queue.

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

Determine Post-Translational Modifications

Optional ADC DAR Calculation

Sequence Matching

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

Determine Post-Translational Modifications

Sequence Coverage

608.273376 + 1  
 v.  
 609.2771

Compare Expected Monoisotopic Mass to Observed m/z \Considering Adducts

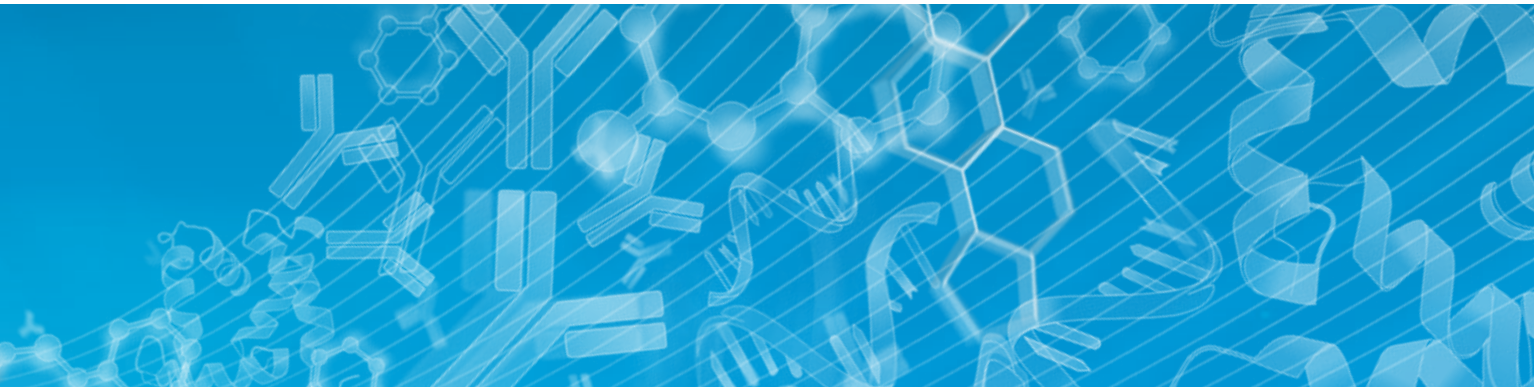
High Throughput Compound Purity Assessment with Analytical Studio Reviewer

Reporting

Delivery of Results



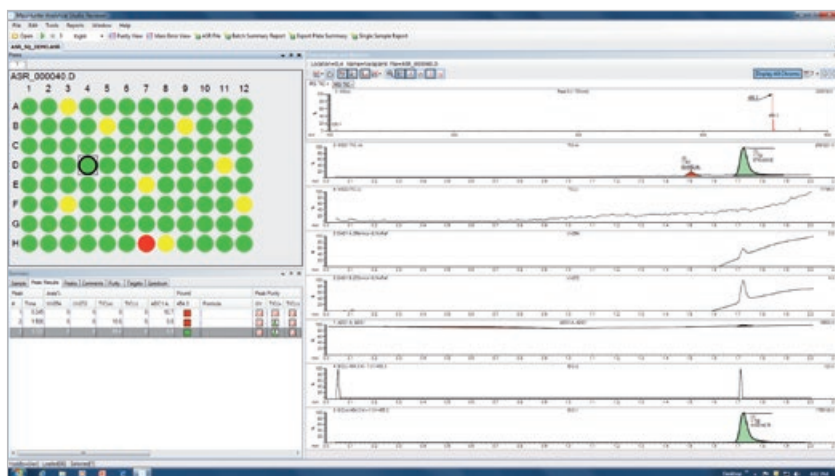




## Analytical Studio Reviewer

Analytical Studio Reviewer enables quick visualization of results and selective data review. Results files can be emailed to users; these files open up into a viewer allowing the user to interactively browse the results and quickly navigate to problem samples. This is particularly useful when users submit larger sample sets, like whole plates.

By eliminating the need for chemists to have data analysis software installed at their desks, Analytical Studio Reviewer can bring significant cost savings to large installation environments.



Quickly visualize and review data using Analytical Studio Reviewer.

## HOW MASSHUNTER WALKUP BENEFITS ADMINISTRATORS

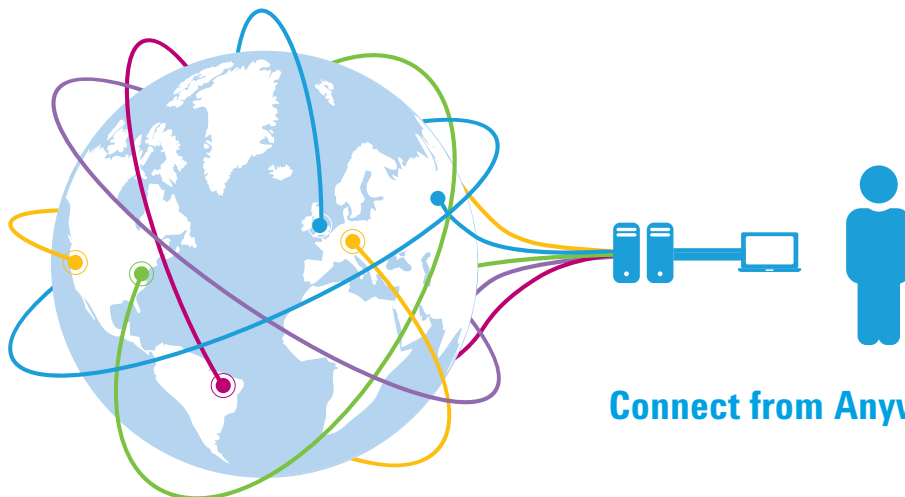
**MassHunter Walkup is designed to provide powerful yet straightforward system administration to meet the needs of even the most diverse user base.**

### **Maximize uptime, minimize training costs**

With MassHunter Walkup, a single administrator can easily manage many systems and applications. Instrument status can be viewed remotely, and user profiles and methods can be added, altered, or modified. Notification of system errors by SMS text message or email to your smartphone.

You can even remotely take an instrument offline – useful for accommodating scheduled preventative maintenance – with minimal negative impact to the sample submitters. The sample queue finishes and the screen locks so that no new samples can be submitted.

*MassHunter Walkup makes our instruments “easy to use and hard to break”, says an Open Access Lab Administrator at a major pharmaceutical company, where medicinal chemists use MassHunter Walkup for LC/MS analyses of small molecules during drug discovery in a large open-access environment. “MassHunter’s ease of use helps us bring complex assays done by experts to a Walkup method.”*

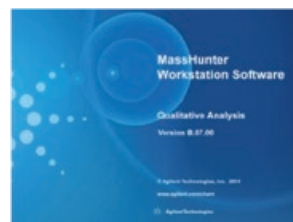
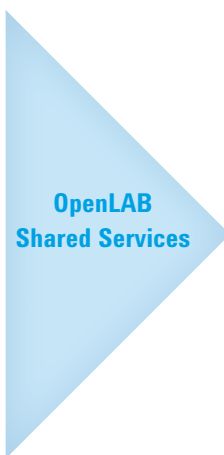


**Connect from Anywhere. Anytime.**

# OPENLAB SHARED SERVICES

## Manage MassHunter and OpenLAB-controlled instruments

With OpenLAB Shared Services, MassHunter Walkup can manage the lab from anywhere on the network. There is no requirement for an instrument to be attached; the data system (OpenLAB CDS ChemStation edition or MassHunter) and the updates are implemented immediately because the settings are hosted on a central server that has OpenLAB Shared Services on it.



Agilent  
**OpenLAB**





Agilent CrossLab combines the innovative laboratory services, software, and consumables competencies of Agilent Technologies and provides a direct connection to a global team of experts who deliver vital, actionable insights at every level of the lab environment. Our insights drive improved economic, operational, and scientific outcomes.

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