# The LC/MS Walk-Up Solution from Agilent

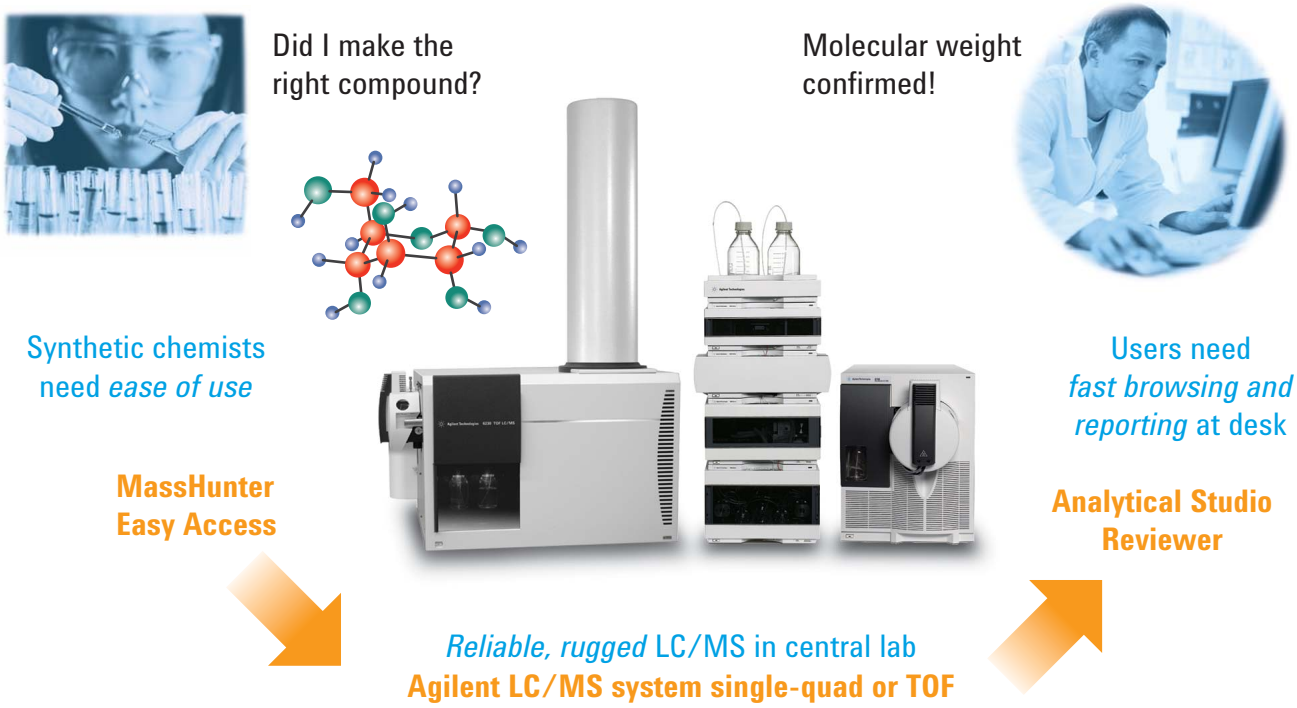
## MassHunter Easy Access software—*making drug development decisions faster with higher confidence*

## Application Note

The rapid and accurate analysis of synthesis products is a crucial activity in early drug discovery. Synthetic and medicinal chemists need easy-to-use walk-up liquid chromatography/mass spectrometry (LC/MS) systems and immediate access to results in a concise, easy-to-read format. Agilent MassHunter Easy Access software provides a simplified user interface for the LC/MS single-quadrupole and time-of-flight (TOF) analyses required for either compound confirmation or purification of small molecules or proteins. For scientists who work with large data sets, the Agilent Analytical Studio Reviewer (ASR) provides fast, flexible and accurate review and reporting of LC/MS data for small compound characterization, to further expedite the development process.

This application note describes MassHunter Easy Access, while another note (Agilent publication 5990-6094EN) discusses Analytical Studio Reviewer. The combination of these two software packages—along with Agilent's rugged LC and MS systems—provides a flexible and powerful solution to the ever present need for faster, high quality data.

Agilent Technologies




*Synthetic and medicinal chemists in modern discovery labs need an analytical workflow that is easy to use and delivers rapid results.*

### Simple and convenient sample submission

Agilent MassHunter Easy Access software allows users to simply "walk up" with their samples, input simple sample information, choose from a list of methods, position the samples as directed by the system, and then return to their labs and wait for an e-mail of the results. Key benefits of MassHunter Easy Access include:

- Very simple sample submission and status checking
- Rapid confirmation of molecular weight and target ion presence
- Single user interface for both Agilent single-quadrupole and time-of-flight (TOF) MS systems
- Automatic pre-equilibration on change of method
- Automated e-mailing of data and reports, including reports from Agilent Analytical Studio Reviewer

MassHunter Easy Access is designed to take advantage of the latest high-throughput hardware for LC/MS. It is compatible with:

- Agilent Rapid Resolution LC and ultra high performance LC systems—including the 1290 Infinity LC Injector HTS/HTC—for fastest LC analyses with uncompromising performance
- Additional samplers supported include: CTC Analytics HTS PAL and HTC PAL injection systems and Agilent automatic liquid samplers
- Agilent's rugged 6100 Series Single Quadrupole LC/MS Systems and 6200 Series Accurate-Mass TOF LC/MS Systems
- Up to three Agilent 1200 Series fraction collectors

A single system administrator can set up the system for use by multiple synthetic or medicinal chemists. For easy configuration, the software features:

- Flexible administrative tools to set user access, queue tracking, and manage projects
- Networking of multiple instruments so they can share databases, which eliminates the need to manage redundant configurations and reduces administrative tasks

## Simplified workflow lets chemists focus on syntheses

Synthetic organic chemists who prepare new compounds often have little or no experience in mass spectrometry. They simply want to submit a few samples for purification and/or analysis and to receive notification when the analyses are complete. In most cases, they want to retrieve the fractions and/or results as soon as possible, to make appropriate decisions for the next step in target compound development. They need to confirm that they made the correct compound and get an approximate purity or yield.

Many organizations have multiple LC/MS systems that are set up for high-throughput molecular weight confirmation. Medicinal chemists who need results quickly must first locate an instrument that is available for the analysis. With MassHunter Easy Access software, a user can see instrument status from any location on the network (**Figure 1**), and can rapidly choose the most appropriate instrument.

Once the chemist has located an instrument, he simply logs in by supplying a password (optional security), describes the samples, and assigns a method from a list. Then the software shows the locations in the sampler where the samples should be placed. **Figure 2** shows the status screen, which displays the overall status of the system and contains the following key information:

- Current samples and approximate time remaining in the queue
- Current method and name of last submitter
- Status of Easy Access and mass spec system (TOF in this example)

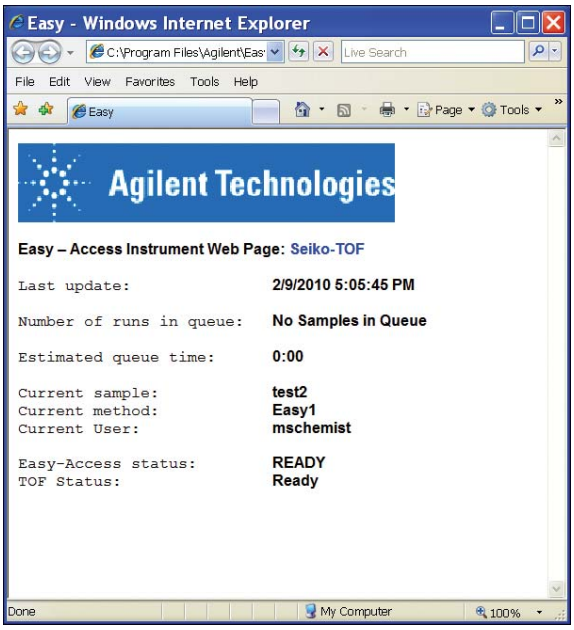



*Figure 1. Users can view the status of any instrument from the convenience of their desks.*

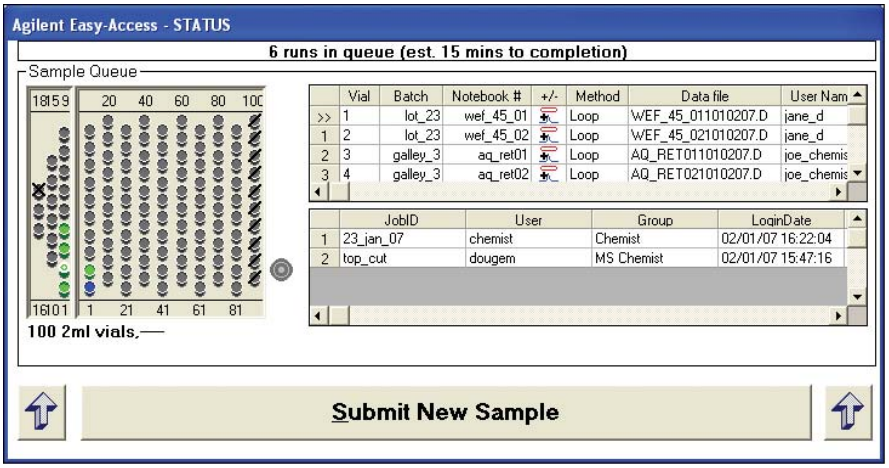



*Figure 2. The software shows the current sample in blue, and provides an approximate completion time for all samples in the queue.*

After submitting the sample, the chemist can return to his desk or lab, and wait for e-mail notification that the sample analysis is complete.

## Easy system administration

To help the system administrator manage the MassHunter Easy Access system, the software provides these key capabilities:

- User and group administration, including optional passwords, method access, and ChemStation or MassHunter availability
- Sample queue management, including moving priority samples to the front of the queue
- Method management, which defines the methods available to the users

**Figure 3** shows the main configuration screen for MassHunter Easy Access software. For security, the system administrator can require a password for specific users or groups and can limit access to specific methods. Note also that the mouse can be restricted to the user panels, preventing access to anything but MassHunter Easy Access. Finally, this screen is also where the system administrator sets up e-mailing of results to users.

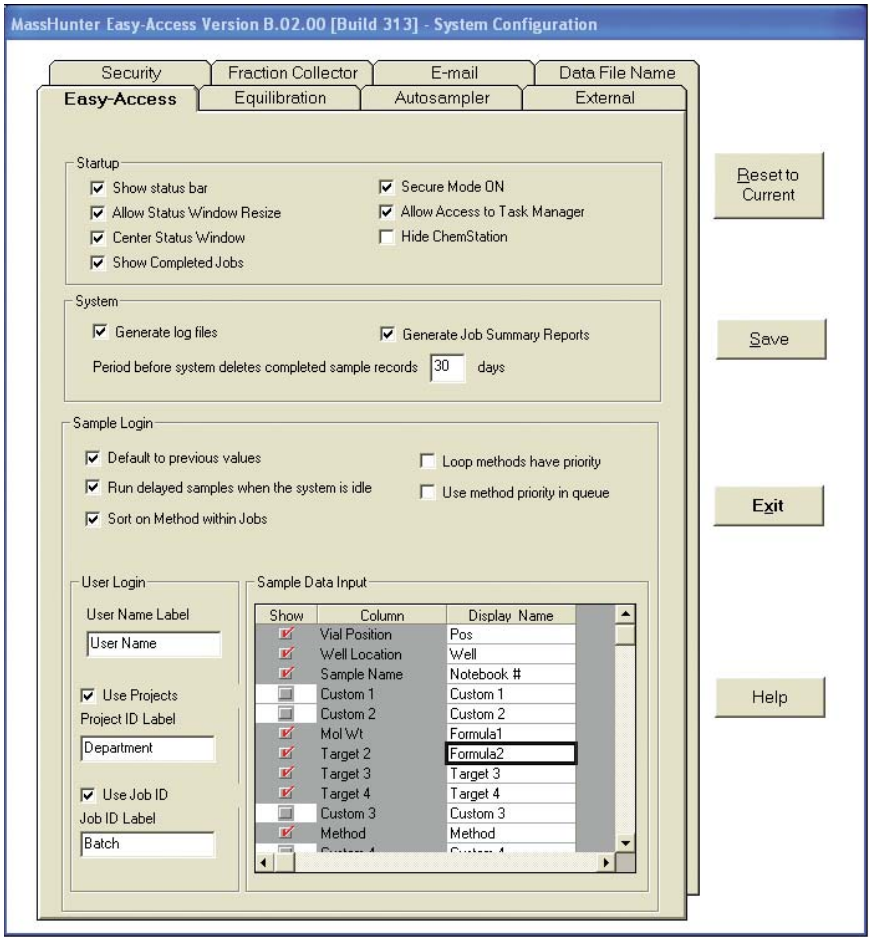



*Figure 3. The MassHunter Easy Access configuration screen sets user access and establishes e-mail capabilities. The laboratory can choose its own labels for most fields (for example, change Project ID to Department or Job ID to Batch), and can decide which labels to show.*

## Results sent by e-mail

The system can be directed to send the results of the analysis to selected users by e-mail. It can e-mail ChemStation or MassHunter reports, raw data, and Analytical Studio Reviewer files. **Figure 4** is an example of an e-mail that contains a report in Adobe® PDF format, and **Figure 5** shows one of the pages from an e-mailed report—in this case a TOF accurate mass report. The sample submitter has provided the molecular formula, which appears in the report. The system calculates the expected monoisotopic mass, obtains an extracted ion chromatogram that includes specified adducts, displays a zoomed spectrum that includes the adduct range, and shows the calculated mass error and calculated purity based on MS, UV, or data from other detectors.

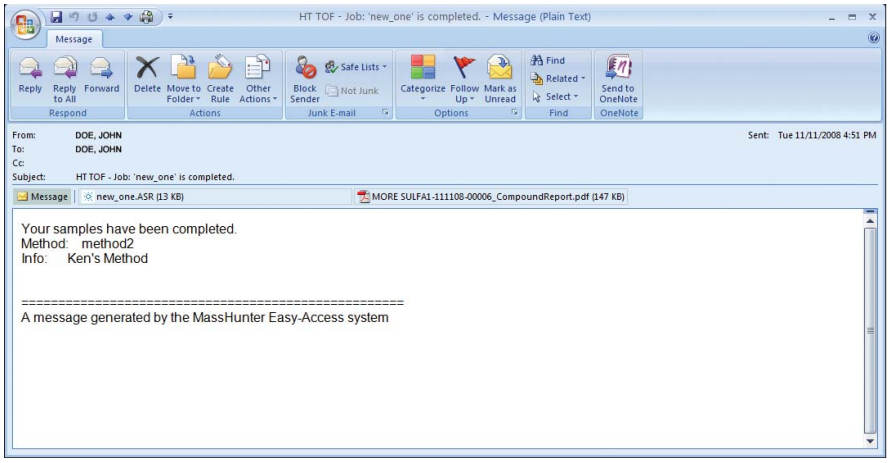



*Figure 4. An e-mail that contains a MassHunter Easy Access PDF report.*

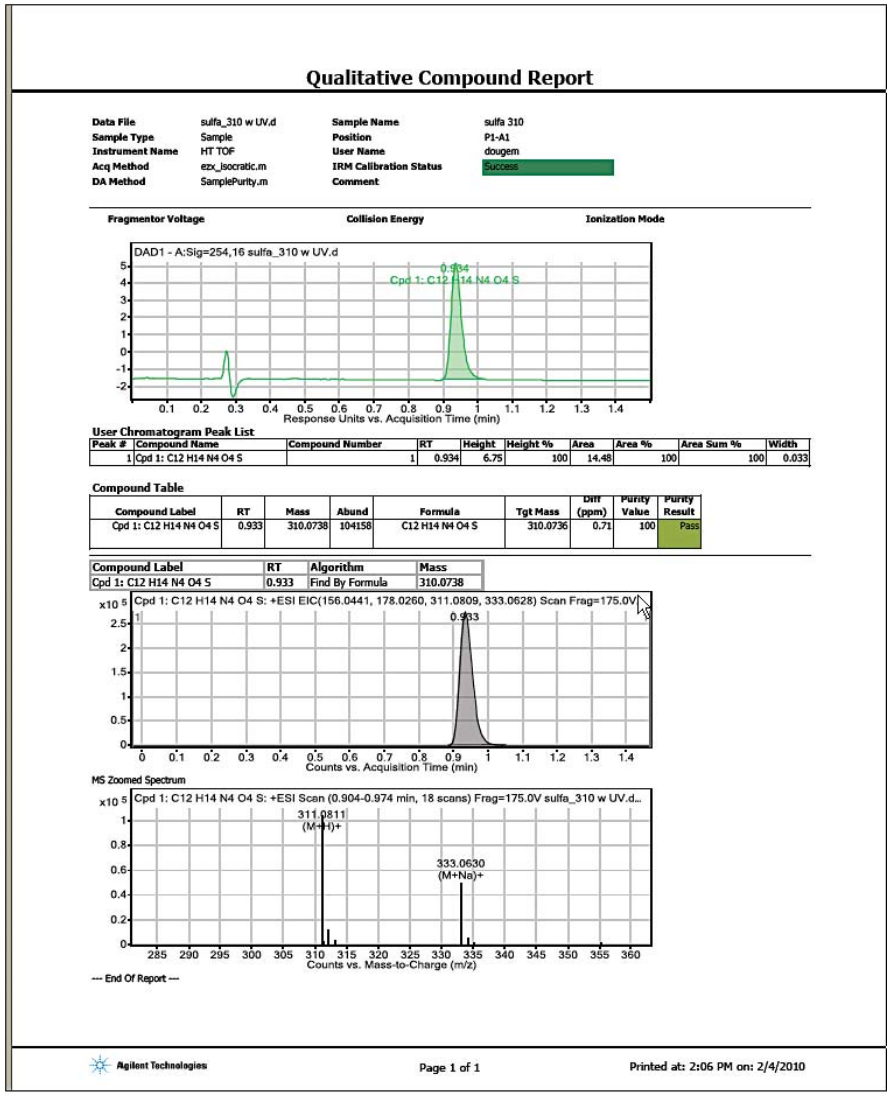



*Figure 5. A TOF accurate mass report sent by e-mail.*

## High throughput with large-capacity samplers

Agilent MassHunter Easy Access supports large-capacity samplers like CTC Analytics HTS PAL and HTC PAL injection systems. These high-throughput samplers enable very rapid injections, allow scientists to load up to 24 microplates, and enable combinations of plates and vials. The MassHunter Easy Access user interface changes to show the plate or tray where the current sample is located (**Figure 6**). After logging in, the user selects whether he has vials or well plates and the software displays the appropriate stack tray or external tray.

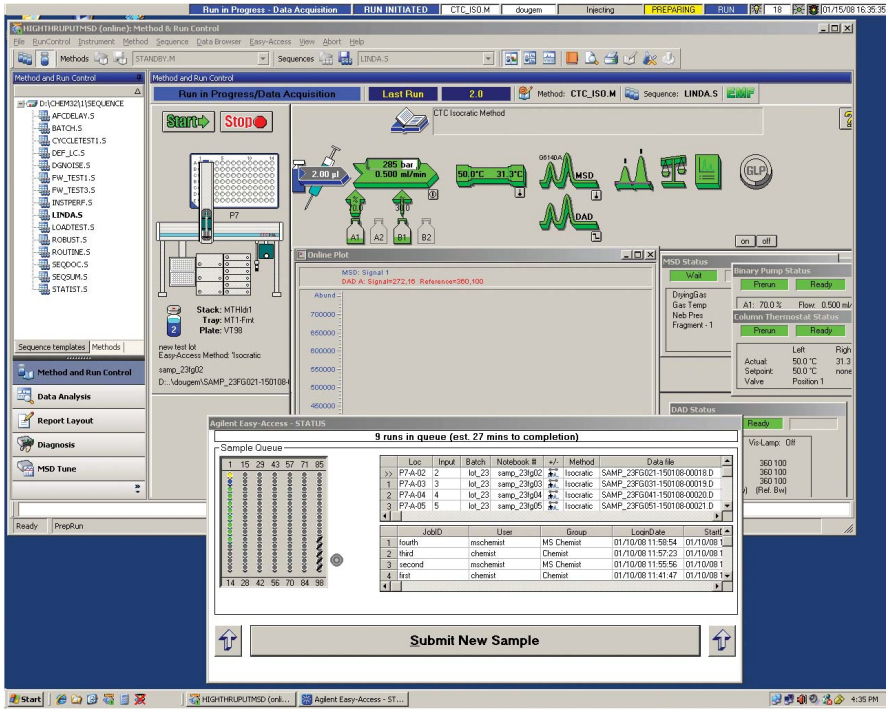



*Figure 6. Status screen showing large open-bed sampler configuration.*

## Efficient management of fraction collection

MassHunter Easy Access is ideal for mass-based fraction collection for high-throughput labs. When the system is doing fraction collection, users may wish to retrieve their fractions while other samples are still in the queue. To maximize lab productivity, MassHunter Easy Access allows users to pick up fractions as soon as possible (**Figure 7**). The system can be set up to pause briefly between each submitter's samples. On systems with multiple fraction collectors, MassHunter Easy Access directs the system to cycle between fraction collectors with each user, which allows chemists to retrieve their fractions immediately upon completion.

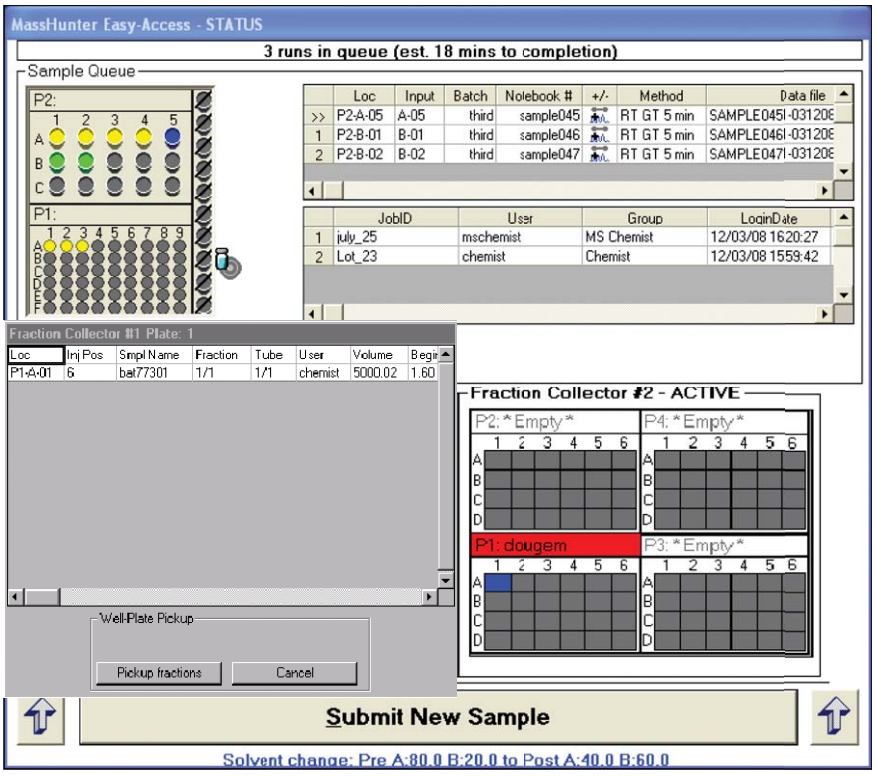



*Figure 7. This status screen shows the user the location of fractions to be retrieved.*

## Summary

With fast, flexible, and intuitive sample submission capabilities, Agilent MassHunter Easy Access software is a perfect complement to the Agilent 6100 Series Single Quadrupole LC/MS Systems and 6200 Series Accurate-Mass TOF LC/MS Systems. The powerful compound identification and purity assessment capabilities of these solutions enable the user to make the right decisions faster, leading to enhanced drug development efficiency.


## Related information

Agilent offers MassHunter Analytical Studio Reviewer software for rapid data review and reporting of large batches of data, such as from 96-well plates. Please see Agilent publication 5990-6094EN for details.

www.agilent.com/chem/masshunter



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