

Poster Reprint

**ASMS 2019**

ThP349

# Making Mass Spectrometry Analysis Easy and Automated by using MassHunter WalkUp Open Access Software

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Synthesis of an active pharmaceutical ingredient (API) requires many monitored reaction steps. Each step must be tested for overall purity and yield to ensure a reliable and cost-efficient synthetic pathway is established. Obtaining fast results is key to determining appropriate decisions for the next step. The same can be said for drug discovery, process development, and quality control, where rapid access to analytical results leads to faster decisions in addition to saving time and money. The best way to meet these needs is with an open-access analytical instrument that is easy to use while providing fast, high quality results. The Agilent InfinityLab LC/MSD iQ with MassHunter WalkUp software provide such a solution.

In an open access system, there are two user types: the administrator and the submitter. The administrator is the expert who manages the system. They create the methods that the submitters utilize to analyze their samples. The system can be “secured” so that the submitter interacts only with the sample submission screens (Figure 1).

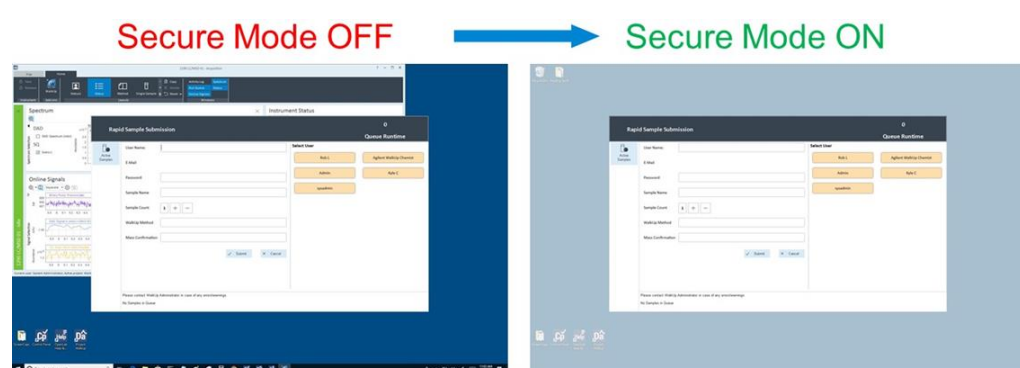


Figure 1. Secure Mode feature of WalkUp

- With *Secure Mode* off, a submitter can access OpenLab CDS and other programs on the computer.
- With *Secure Mode* on, the submitter is restricted to only Walkup sample submission. All other programs and operating system commands are locked out.

For the submitter, they do not need any knowledge of Agilent OpenLab CDS or even how to operate the instrument. With WalkUp, a submitter can simply walk up to the instrument, submit a sample, and return to their desk to receive an emailed report with their analytical results (Figure 2). This allows laboratories to reduce training times and improve operational efficiency.

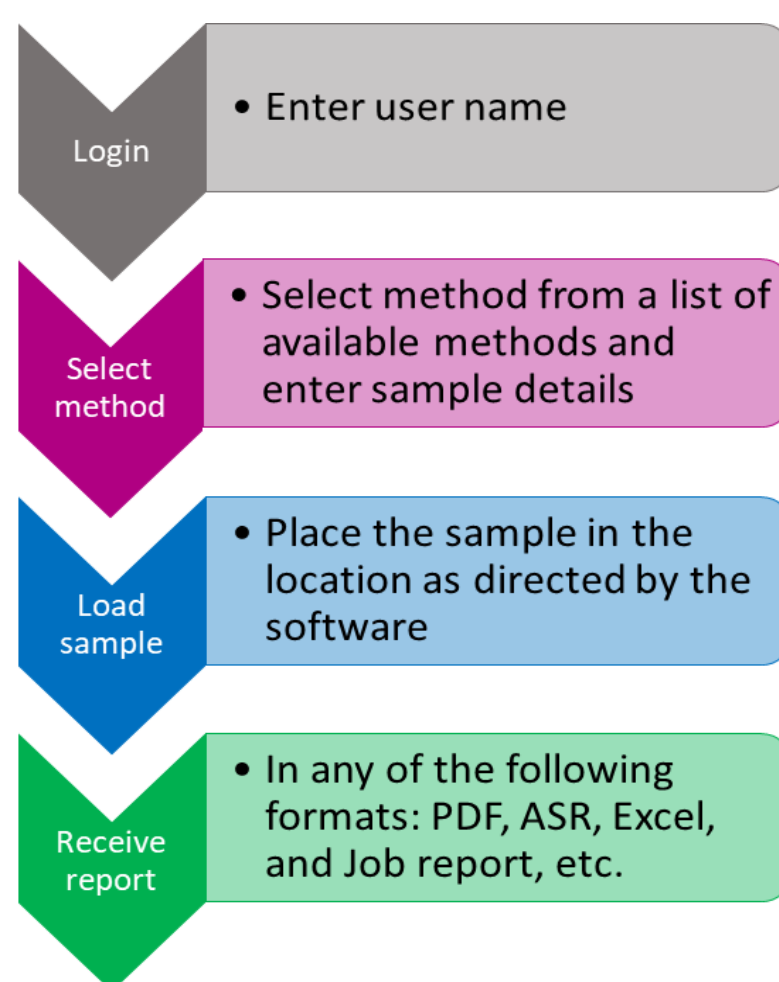


Figure 2. Typical user workflow for the Agilent LC/MSD iQ WalkUp system.

## Experimental

### Typical WalkUp Instrumentation

The Agilent InfinityLab LC/MSD iQ WalkUp system consists of the following modules:

- Agilent 1290 Infinity II High-Speed Pump (G7120A)
- Agilent 1290 Infinity II Multisampler (G7167B) or Agilent 1290 Infinity II Vialsampler (G7129B)
- Agilent 1290 Infinity II Multicolumn Thermostat (G7116B)
- Agilent 1290 Infinity II Diode Array Detector (G7117B)
- Agilent LC/MSD iQ (G6160AA)

Figure 3. Agilent's LC/MSD iQ with an InfinityLab II Prime HPLC stack

## Easy sample submission for users from any background

There are two ways to submit samples depending on the lab's intended use of the WalkUp system. *Rapid Sample Submission* is specifically designed for use with a *Sample Purity* or *Target Mass Confirmation* workflow (Figure 4). Alternatively, *Classic Sample Submission* is used for more complex workflows requiring multiple methods, or for mass-based fraction collection (Figure 5). Both sample submission workflows require the same steps for submitters to follow:

- Identify themselves to the WalkUp system and enter an optional password
- Input simple sample information
- Choose from a list of analytical methods
- Input target masses (optional)
- Load the sample into the sampler, as directed by the system
- Receive the results report via email

Figure 4. Rapid Sample Submission: all inputs are made from this single screen. The right side shows the methods available for submitters and “buttons” for method selection are provided for touch screen use.

Sample Name	User Name	Sample Position	Completion Time	WalkUp Method	Target Masses	Injection Volume	Number of Injections
1 Resepine	Agilent Wal...	D1F-A1	10:48 AM	Sample Purity	600	1	1
1.1 Resepine	Agilent Wal...	D1F-A1	10:48 AM	Sample Purity	600	1	1
2 Sulfix Mix	Agilent Wal...	D1F-A2	10:51 AM	WalkUp Ge...	270,278,284,310	1	1
3 Pharma Mix	Agilent Wal...	D1F-A3	10:53 AM	WalkUp Ge...	385,371,277,3...	1	1

Figure 5. Classic Sample Submission: Multiple samples can be submitted at once with specific methods for each sample. An active sample queue shows which sample is currently analyzed.

## Advantages and benefits for Lab Managers

For the administrator of the system, some of the key benefits of WalkUp are:

- Touch screen capability using Rapid Sample Submission
- Control of group and user privileges (Fig. 6)
- Ability to import defined worklists with Classic Sample Submission
- External sample tray for uninterrupted sample submissions
- Real-time sample queue and instrument status in small or large labs
- Management of multiple systems using OpenLab CDS shared services in large laboratory configuration
- Verification of system configuration after changes have been made
- Email or SMS alerts when a problem occurs with the system

Privilege	Agilent
1 WalkUp: Allow to manage Walk...	<input checked="" type="checkbox"/>
2 WalkUp: Allow to manage System...	<input checked="" type="checkbox"/>
3 WalkUp: Allow to manage Users...	<input checked="" type="checkbox"/>
4 WalkUp: Allow to manage Depart...	<input checked="" type="checkbox"/>
5 WalkUp: Allow to shutdown Wal...	<input checked="" type="checkbox"/>
6 WalkUp: Allow to show/hide Dat...	<input checked="" type="checkbox"/>
7 WalkUp: Allow to start/stop Sac...	<input checked="" type="checkbox"/>
8 WalkUp: Allow to manage Active...	<input checked="" type="checkbox"/>
9 WalkUp: Allow to manage Comp...	<input checked="" type="checkbox"/>
10 WalkUp: Allow to manage Incom...	<input checked="" type="checkbox"/>
11 WalkUp: Allow to clear Sampler...	<input checked="" type="checkbox"/>
12 WalkUp: Allow to clear error...	<input checked="" type="checkbox"/>
13 WalkUp: Allow to start WalkUp...	<input checked="" type="checkbox"/>
14 WalkUp: Allow to run events ma...	<input checked="" type="checkbox"/>
15 WalkUp: Allow to abort executi...	<input checked="" type="checkbox"/>

Figure 6. The group permissions tab contains a list of all the groups and their users. Each group can be given a set of privileges and methods they can use.

Column Type	Column Display Name	Mandatory	Custom Values
1 Mass Confirmation	Precursor Mass	<input checked="" type="checkbox"/>	Target 1
2 Mass Confirmation	Product Mass	<input checked="" type="checkbox"/>	Target 2

Figure 7. A workflow for reaction monitoring. Two columns are added to the sample submission screen for a precursor target mass and product target masses.



## Automatic scheduling of important system events

Key events can be scheduled on a time basis (e.g., every day, week, work day) or sample submission basis (e.g., after a plate is complete, after N runs) (Figure 8). Any number of WalkUp methods can be selected. Sample vials can be stored in reference positions, which are not utilized by the sample queue. Some examples of events that can be made are:

- Running reference standards throughout the work day
- Calibration standards to ensure that reported amounts are on target
- System suitability check for instrument and column stability
- Blank runs to check for carry over or contamination
- Scheduled Autotune or Checktune available with the LC/MSD iQ.

Event Name	Frequency	Time/Event	Action	WalkUp Method	Load Duration	100 Vials Tray	40 2mL Half Tray	15 6mL Half Tray	2 Well Plus 10 Vials Tray	Multi Sampler Tray
SystemSut	Every N Runs	20	RUN	WalkUp.Generic	0	No-inje...	No-injec...	No-inje...	No-injection	3

Figure 8. OL CDS data acquisition screen.

## Reports and data emailed right to the submitter's inbox

The acquired data is automatically processed by the data analysis method which creates the data analysis report. The administrator then configures what is sent to the submitter (Figure 9). The submitter receives the report created by the administrator right to their inbox (Figure 10).

Figure 9. Data files, data analysis reports, and ASR files can be emailed to submitters.

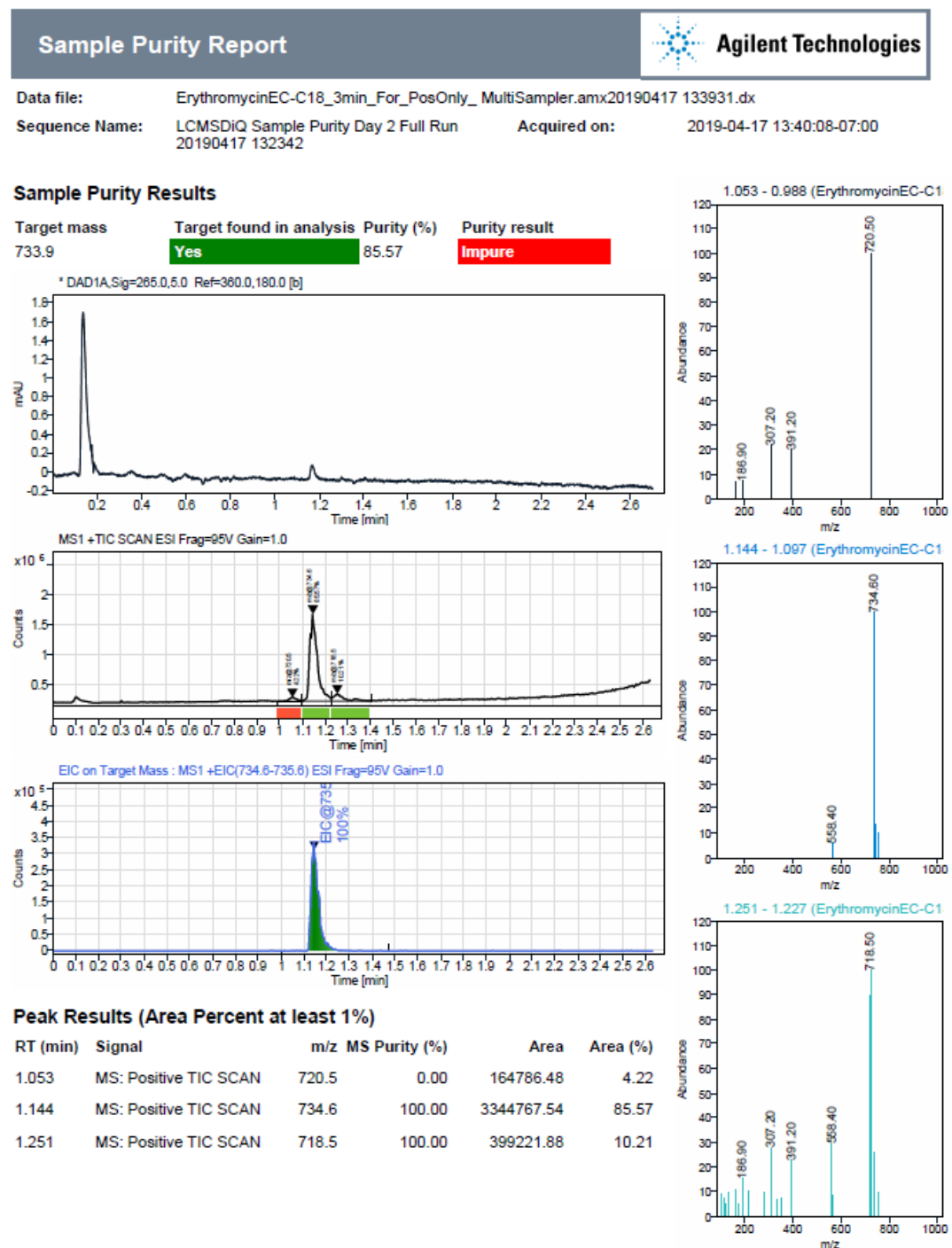


Figure 10. A sample purity WalkUp report emailed to the submitter shows the sample purity of target mass m/z 733.9 (erythromycin) along with the UV chromatogram and MS total ion current. The colored bars below the TIC peaks show whether the MS peak is pure (green) or impure (red).

## Conclusions

- With fast, flexible, and intuitive sample submission capabilities combined with flexible report generation options, MassHunter WalkUp provides an open-access experience that is easy to work with and feature rich for sample submitters and administrators.
- Combined with an InfinityLab LC/MSD iQ, submitters are provided mass information for more definitive identifications.
- Sophisticated administrative tools allow a system administrator to configure workflows that can be executed with virtually no training required.

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