

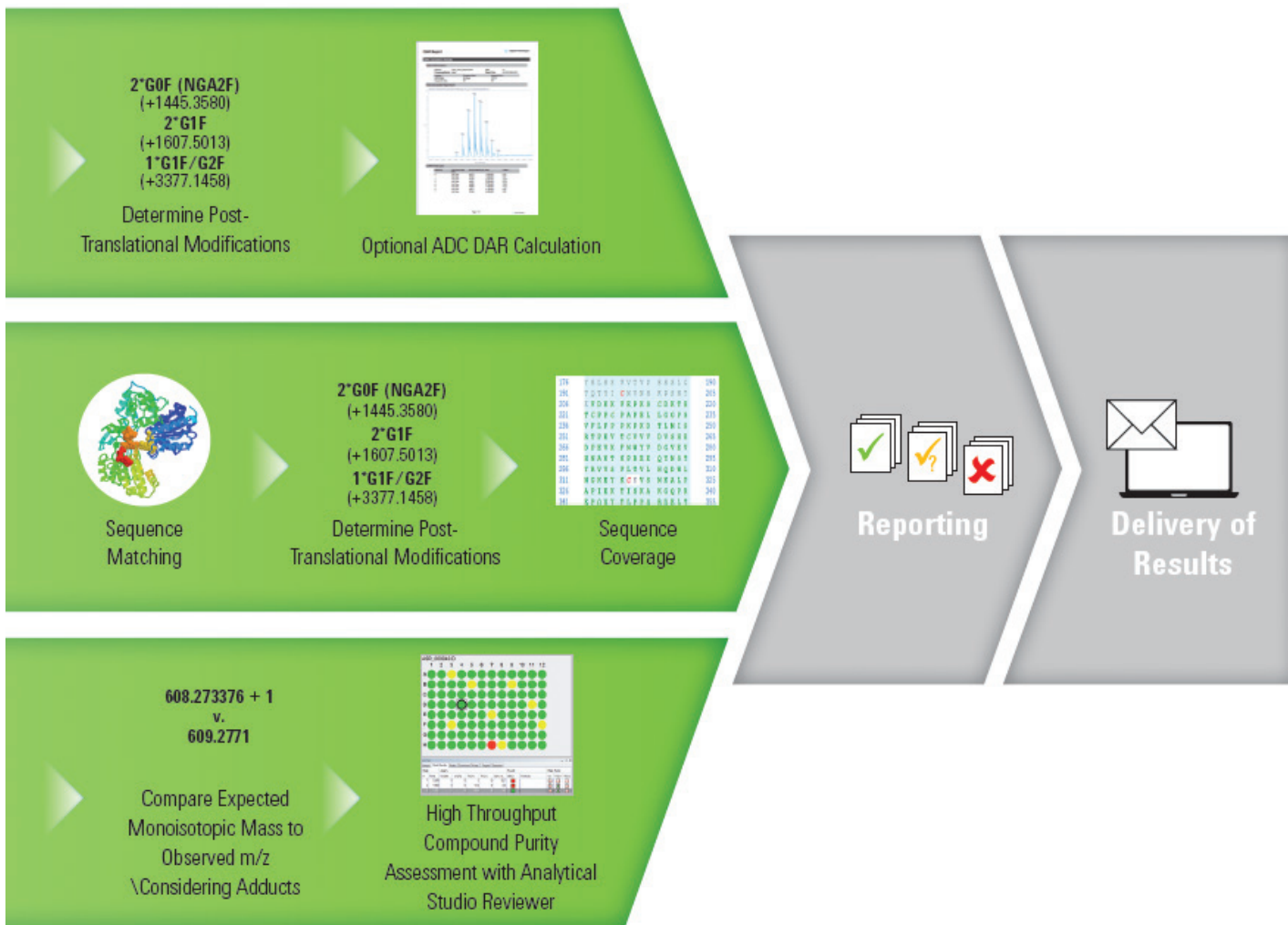
The LC/MS Walkup Solution from Agilent

Agilent MassHunter Walkup software—making drug development decisions faster, with higher confidence

Introduction

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 Walkup software provides a simplified user interface for the Liquid Chromatograph/Mass Selective Detector (LC/MSD) 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.

This Technical Overview describes MassHunter Walkup software, and 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 for faster, high-quality data.



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



Accurate mass compound confirmation with the InfinityLab 1290 UHPLC and 6230 LC/TOF.



Mass based fraction collection with InfinityLab II Preparative Pump and Fraction Collector with a LC/MSD XT.

Simple and convenient sample submission

MassHunter Walkup 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
- Return to their labs and wait for an e-mail of the results

Key benefits of MassHunter Walkup software include:

- Simple sample submission and status checking
- Convenient sample submission from remote computer
- Rapid confirmation of molecular weight and target ion presence
- A single user interface for Agilent single-quadrupole (LC/MSD) and time-of-flight (TOF) MS systems
- Automatic equilibration when methods and solvents change
- Automated e-mailing of data and reports, including reports from Agilent Analytical Studio Reviewer

MassHunter Walkup software 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 Agilent 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
- Rugged Agilent 6100 Series Single Quadrupole LC/MS Systems, InfinityLab LC/MSD Series Systems, Agilent 6200 Series Accurate-Mass TOF LC/MS systems, and Agilent 6500 Series Q-TOF LC/MS Systems
- Agilent's InfinityLab 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:

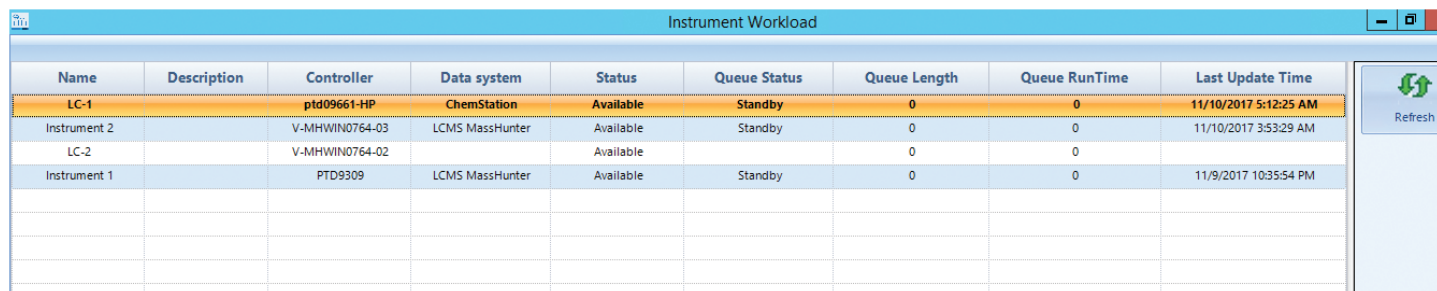
- Flexible administrative tools to set user access, track queues, and manage projects

- Networking of multiple instruments to share databases, eliminating the need to manage redundant configurations, reducing administrative tasks
- Remote monitoring and management of all instruments managed by the OpenLab Shared Services (OLSS) server

A simplified workflow lets chemists focus on syntheses

Synthetic organic chemists who prepare new compounds often have minimal experience in mass spectrometry. They want to submit a few samples for purification or analysis and receive notification when the analyses are complete. They want to retrieve the fractions 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 locate an instrument available for the analysis. With MassHunter Walkup software, a user can see instrument status from any location on the network (Figure 1), and choose the appropriate instrument.



The screenshot shows a window titled "Instrument Workload" with a table of instrument status. The table has columns for Name, Description, Controller, Data system, Status, Queue Status, Queue Length, Queue RunTime, and Last Update Time. There are three rows of data, each representing an instrument. A "Refresh" button is visible on the right side of the table.

| Name | Description | Controller | Data system | Status | Queue Status | Queue Length | Queue RunTime | Last Update Time |
|--------------|-------------|----------------|-----------------|-----------|--------------|--------------|---------------|-----------------------|
| LC-1 | | ptd09661-HP | ChemStation | Available | Standby | 0 | 0 | 11/10/2017 5:12:25 AM |
| Instrument 2 | | V-MHWIN0764-03 | LCMS MassHunter | Available | Standby | 0 | 0 | 11/10/2017 3:53:29 AM |
| LC-2 | | V-MHWIN0764-02 | | Available | | 0 | 0 | |
| Instrument 1 | | PTD9309 | LCMS MassHunter | Available | Standby | 0 | 0 | 11/9/2017 10:35:54 PM |
| | | | | | | | | |
| | | | | | | | | |
| | | | | | | | | |

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

Once the chemist has located an instrument, he or she logs in by supplying a password (optional security), describes the samples, and selects a method from a list. 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 Walkup and mass spectrometry system (TOF in this example)

After submitting the sample, the chemist can return to other tasks, and wait for e-mail notification that the sample analysis is complete.

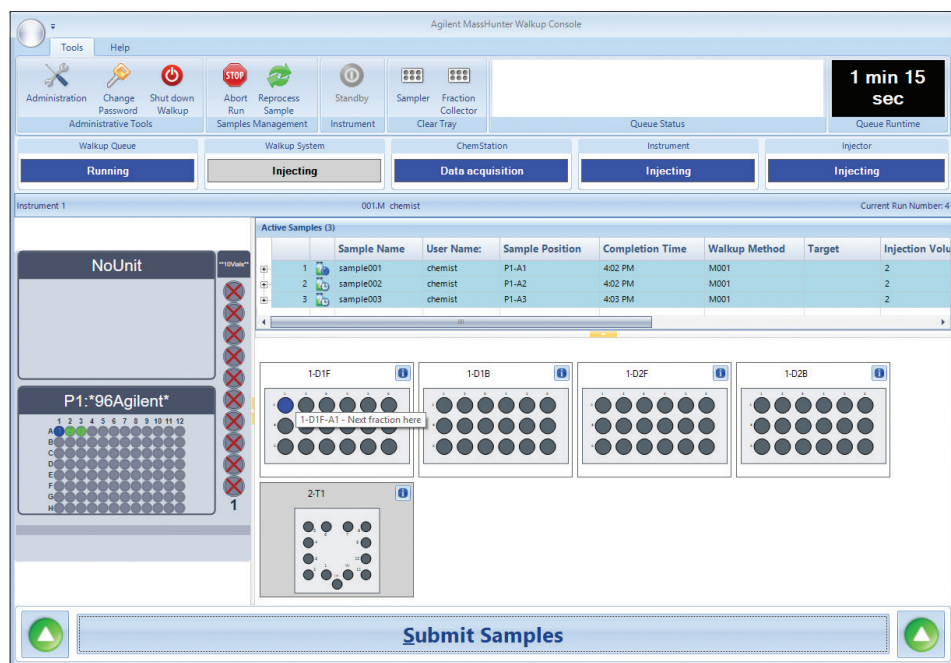


Figure 2. The software shows the current sample in blue, and provides an approximate completion time for all samples in the queue.

Easy system administration

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

- User and group administration, including optional passwords, method access, and Agilent 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 users

Figure 3 shows the Verification Log for the MassHunter Walkup software. When the system administrator makes multiple changes to the system, the software verifies that all changes are valid. Any errors found are highlighted to the administrator. Upon clicking on the error, the administrator is taken to the section of the software where the fault is present, allowing for fast resolution of problems.

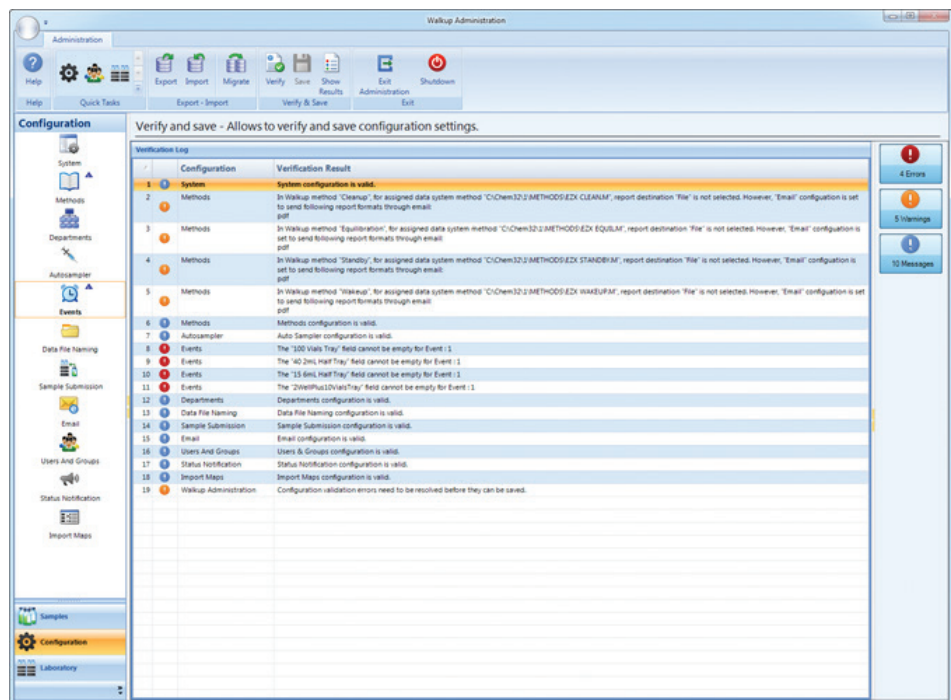


Figure 3. Verification Log for the MassHunter Walkup software.

Results sent by e-mail

The system can be directed to e-mail the results of the analysis to selected users. 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. Figure 5 shows one of the pages, a TOF accurate mass report, from an e-mailed 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
- Shows the calculated mass error and calculated purity based on MS, UV, or data from other detectors

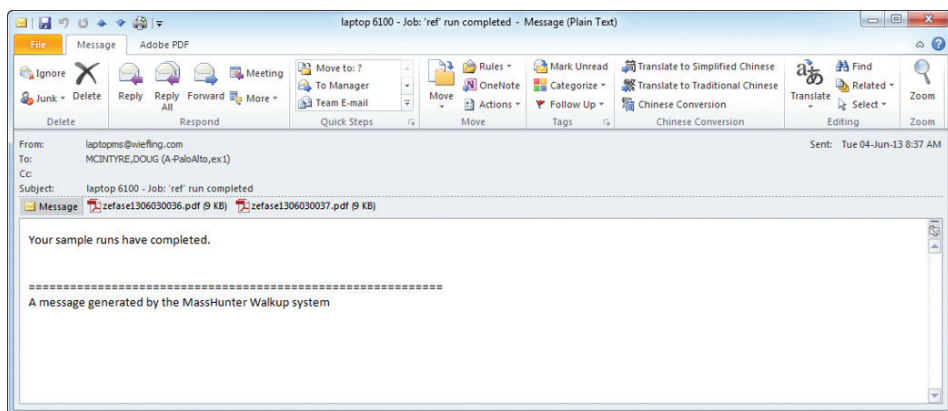


Figure 4. An example e-mail that contains the data analysis reports.

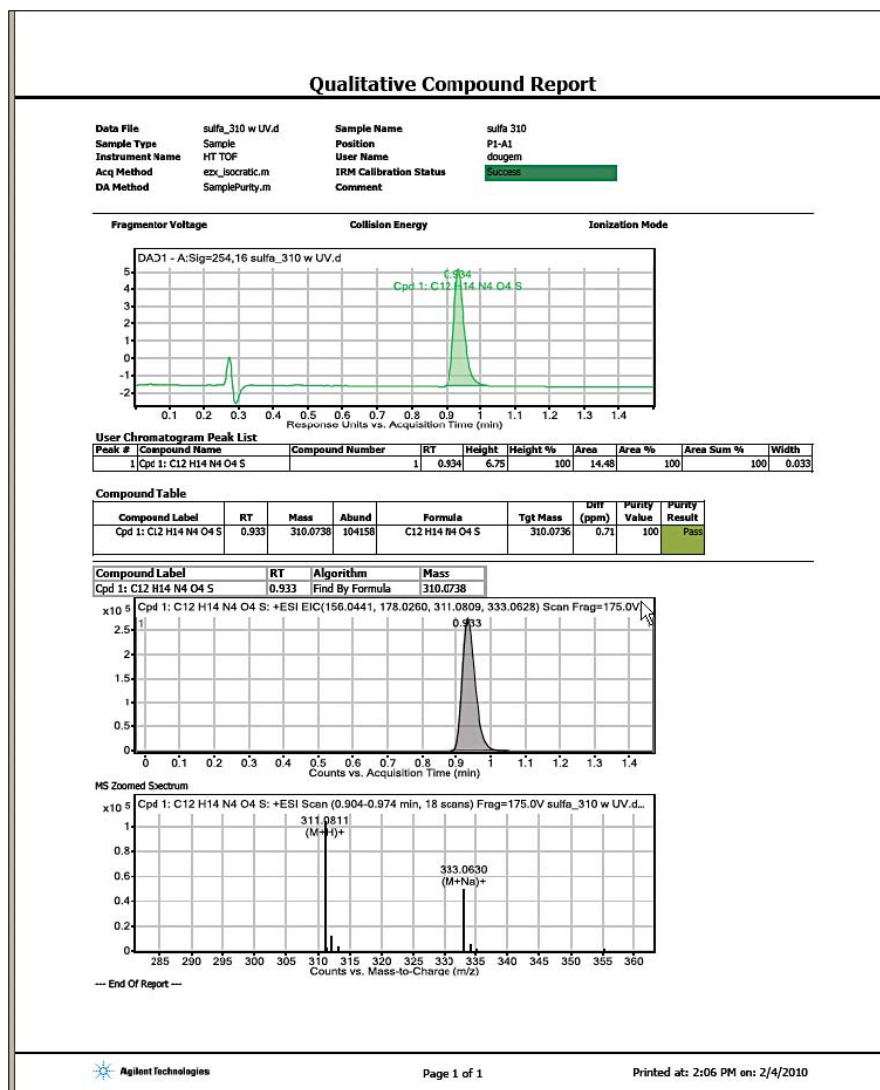


Figure 5. A TOF accurate mass report sent by e-mail.

High throughput with large-capacity samplers

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



Figure 6. Agilent MassHunter Walkup Status screen showing fractions collected with 1290 Infinity II Preparative Open-Bed Fraction Collector and 1260 Infinity II Preparative Valve-Based Collector.

Efficient management of fraction collection

In high-throughput labs, MassHunter Walkup is ideal for mass-based fraction collection. When the system is doing fraction collection, users may retrieve their fractions while other samples are still in the queue. To maximize lab productivity, MassHunter Walkup 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 Walkup directs the system to cycle between fraction collectors with each user. This cycle allows chemists to retrieve their fractions immediately upon completion.

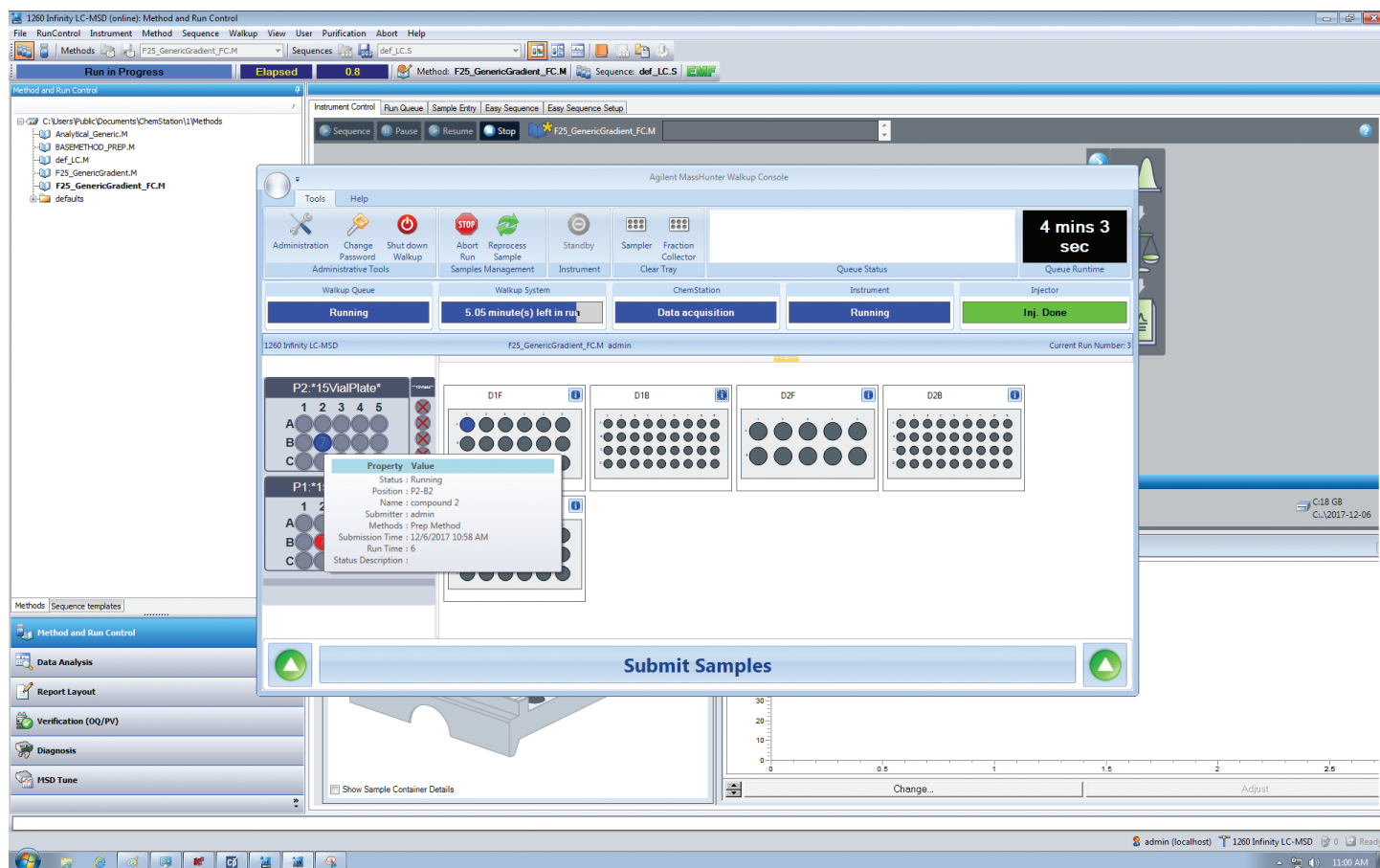


Figure 7. This status screen shows the user the location of fractions to be retrieved.

Conclusions

With fast, flexible, and intuitive sample submission capabilities, Agilent MassHunter Walkup software is a perfect complement to the Agilent InfinityLab LC/MSD Series systems and Agilent 6200 Series accurate-mass time-of-flight LC/MS system. 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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