

MassHunter Walkup System

Quick Start Guide

For fast and intuitive Startup, Sample Submission, and Sample Control

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What is the Agilent MassHunter MassHunter Walkup System?

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What is the Agilent MassHunter MassHunter Walkup System?

Agilent MassHunter Walkup System (Walkup) provides intuitive, walk-up access to Agilent LC and LC/MS systems without requiring users to have specific experience with the instrumentation and data systems involved in processing the samples. Laboratory users can conveniently and easily submit samples and receive their results by e-mail. System administrators have flexible management of security and user access for the system that may consist of one or many instrument installations.

Walkup is typically deployed in a central analytical facility that is managed by one or more individuals skilled in developing LC/MS methods and interpreting the data. A Walkup system manager creates instrument acquisition methods, sample queuing protocol, and conditions for starting or switching between methods.

Walkup can be used in chemical analysis labs in petrochemical, pharmaceutical, environmental, food, and other industries. In pharmaceutical enterprises, Walkup helps lab managers, analysts, and operators in chromatography labs do drug discovery and drug development under non-regulated conditions.

What's New in Version C.03.01

- OpenLAB CDS A.02.03/A.02.2 and ChemStation edition C.01.08 are supported.
- The Agilent InfinityLab LC/MSD and LC/MSD XT are supported with ChemStation Edition C.01.08.
- Agilent MassHunter Data Acquisition for Q-TOF version B.08.00 SP1 and B.08.01 SP1 are supported.
- Agilent MassHunter BioConfirm B.09.00 is supported.
- Mass-based purification is supported with ChemStation Edition C.01.08.
- The installation is not Browser-based.
- Walkup supports all Multisampler drawer heights (1H, 2H, and 3H).
- Walkup allows organizing data files in department subfolders.
- The Instrument Ready Wait timeout is configurable.
- Injection volumes can be specified for each method in case of multiple methods per sample.
- You can select the type of run results to email (selective data emailing).
- These 1260 Infinity II modules are supported:
 - The G7161A 1260 Infinity II Preparative Binary Pump
 - The G7151A 1260 Infinity II Preparative Autosampler
 - The G7166A 1260 Infinity II Preparative Valve-Based Collector
- These 1290 Infinity II modules are supported with ChemStation Edition:
 - The G7161B 1290 Infinity II Preparative Binary Pump
 - The G7163B 1290 Infinity II Column Valve Module
 - The G7170B 1290 Infinity II Active Splitter

Fraction Collection

- These Fraction Collector models are supported with ChemStation Edition: G7159B, G7166A, G1364A, G1364B, G6134C, G1364D, G1364E and G1364F.
- Details of all collected fractions can be viewed in tabular format.
- Details of all fractions collected on a specific tray/plate can be seen in tabular format.
- You can configure percent of the Fraction tray to be filled before calling it full.

- Different fraction collection orientations are supported.
- Fraction details can be printed.
- Fraction collection can be configured to pause for a specific duration.
- Fraction collector status can be reset manually.
- Fraction collection configuration from Easy Access can be migrated.
- When the Fraction Collector tray configuration is changed, you are asked whether to reset/print fraction details.
- When Walkup is launched, you are asked if existing fraction details should be reset/printed.
- Fractions are not collected in locations marked as Recovery or Forbidden in ChemStation.
- A Fraction Collector button which allows you to clear the Fraction Collector Tray is available in the Tools tab in the Ribbon.

Remote Sample Submission

- The Instrument Workload Dashboard program is available.
- Remote samples can be viewed or deleted from the Remote Samples Dashboard.
- Basic sample login and submission is supported - using manual, import, and custom entry.
- You can manage list of remotely submitted samples.
- The system needs to be restarted when Walkup is uninstalled. (applicable only for "Remote Administration")

Run Groups

- Walkup method can be configured to insert blank samples before the sample for which the method is used.
- Equilibration runs are supported with run groups.
- You can abort runs groups.
- Overlapped samples are supported.
- Overlap is not supported for "no-injection" runs.
- Different queue sorting settings are supported along with **Top of Queue** and **Top of Sections**.
- Events configuration and execution are supported, considering the notion of run groups.

- You can select whether or not to prevent copying of data files for samples without an injection.

Walkup Administration Improvements


- You can save partially configured systems.
- An administrator may configure an administrator session timeout.
- The administrator can clone a user.
- The Sample Import Path defined at a group level offers the administrator an option to apply this path to all the users in the group.
- A job summary report is emailed to the submitter.
- The job summary report contains information about individual sample execution status.
- The administrator can configure whether to allow multiple injections from a sample.
- The Status Description for a sample is available in the tray/plate control tooltip.
- The administrator can assign custom names to data files for events.
- The Events view warns the user to limit the length of custom names.
- The **Save** and **Cancel** buttons are moved to the top right.

Where to Find More Information

You can access more information about MassHunter Walkup System as follows.

Online Help

Press F1 To get more information about a pane, window, or dialog box, place the cursor on the pane, window, or dialog box of interest and press F1.

Help Menu Click **View Help**  in the Walkup ribbon for in-depth information about how to administer, configure, and use the MassHunter Walkup System.

Setup Guide

The *MassHunter Walkup System Setup Guide* describes how to install the MassHunter Walkup System.

Agilent Web Site

To view support information for Walkup and other Agilent products, see:

<http://www.agilent.com>

Software Status Bulletin

A list of known problems and issues for MassHunter Walkup System, with possible solutions, is described in the Software Status Bulletin. You can find the Software Status Bulletin and the Software Release Bulletin in the support folder on the setup disk.

Getting Started

Before you begin, install and configure the MassHunter Walkup System as described in the *Walkup System Setup Guide*.

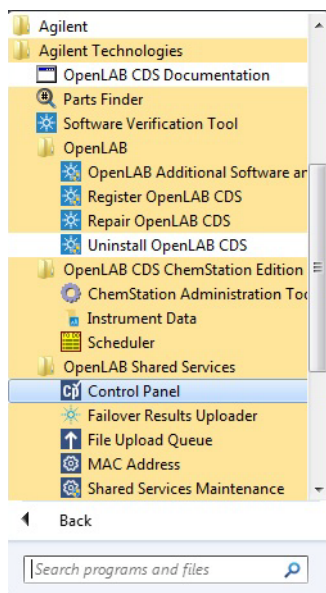
The appropriate Walkup privilege is required to start the Walkup program. If you do not have the privilege to start Walkup, see your Walkup System Administrator.

To start Walkup (OpenLAB CDS ChemStation Edition)

- 1 Double-click the **OpenLAB Control Panel** icon  on your desktop to open the OpenLAB Control Panel

In Windows 7, you can instead click **Start > All Programs > Agilent Technologies > OpenLAB > OpenLAB Control Panel**.

For Windows 10, you can instead click the Windows icon, and then click **All Apps > Agilent Technologies > Control Panel**.



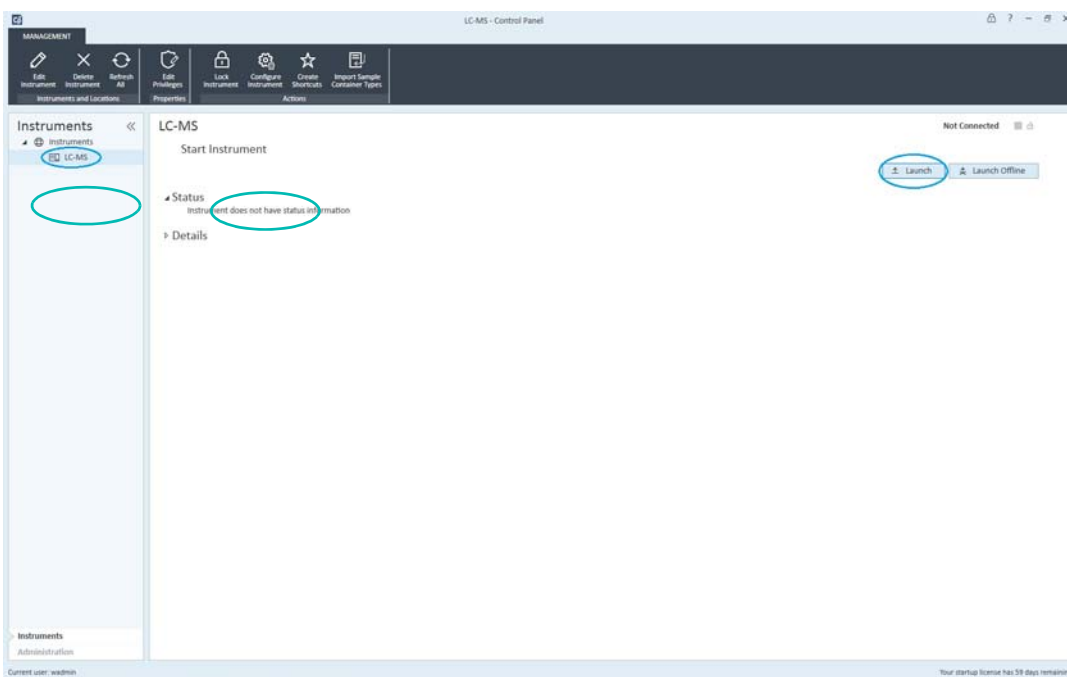
Getting Started

To start Walkup (OpenLAB CDS ChemStation Edition)

2 Type your **Login** and **Password**.



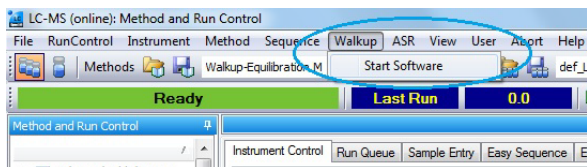
3 Select an instrument in the Navigation pane.



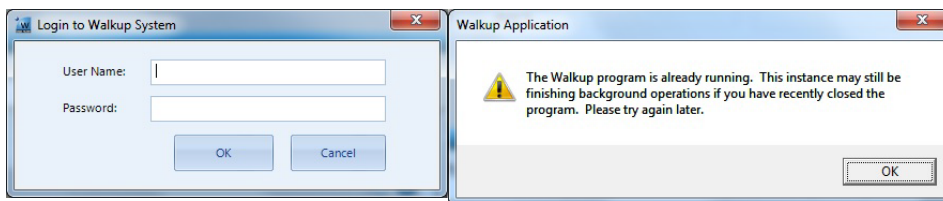
4 Click the **Launch**  button.

5 Start the Walkup program.

a Click **Walkup > Start Software** in the ChemStation console.



- b Type a **User Name** and **Password** in the **Login to Walkup System** dialog box. This user needs permission to launch Walkup. By default, the administrator has this permission. If Walkup is already running, the **Walkup Application** dialog box is displayed.



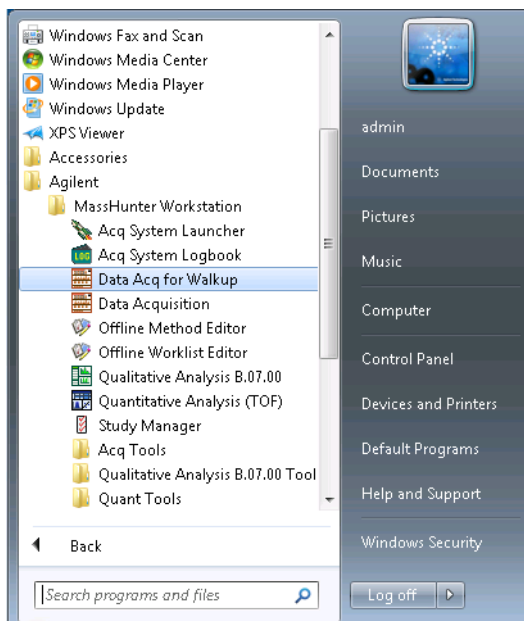
- c Click **OK**.

To start Walkup (MassHunter Data Acquisition)

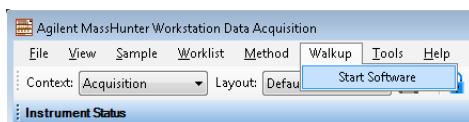
- 1 Double-click the **Data Acq for Walkup** icon  on your desktop to start the MassHunter Data Acquisition program.

For Windows 7, you can instead click **Start > All Programs > Agilent > MassHunter Workstation > Data Acq for Walkup**.

For Windows 10, you can instead click the Windows icon, and then click **All Apps > Agilent > Data Acq for Walkup**.

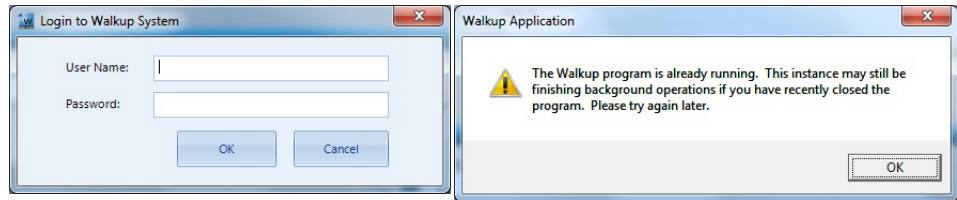


- 2 Start the Walkup program.
 - a Click **Walkup > Start Software** in the MassHunter Data Acquisition program.




- b Type a **User Name** and **Password** in the **Login to Walkup System** dialog box. This user needs permission to launch Walkup. By default, the

administrator has this permission. If Walkup is already running, the **Walkup Application** dialog box is displayed.



c Click OK.

To view Walkup online Help

- Click **View Help**  in the Help tab in the Walkup ribbon or press the **F1** key.

Walkup Console User Interface

The Walkup Console consists of four main parts: (1) the Ribbon, (2) the Status bar, (3) the Main Window, and (4) the Sample bar. The Main Window is divided into two panes, the Plate Tray Diagram and the Sample Queue Table.

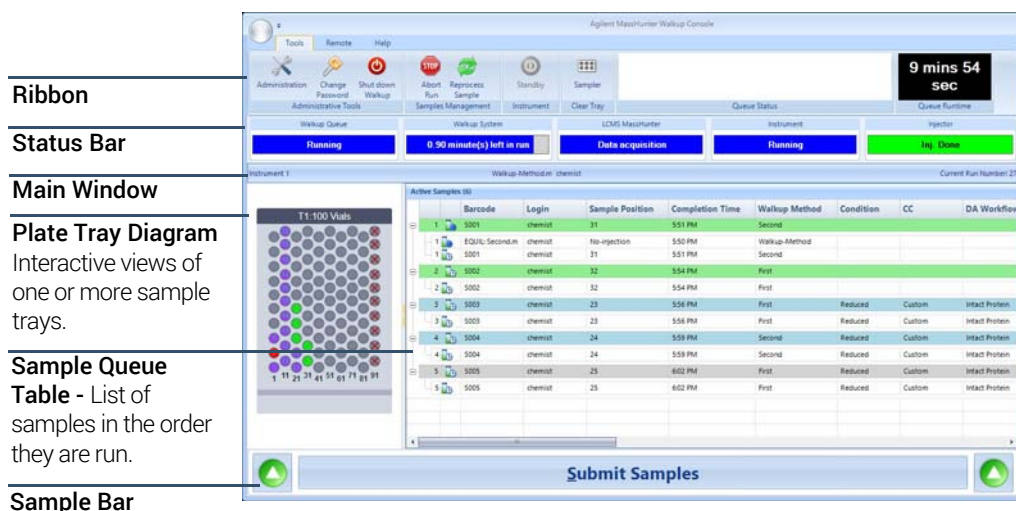


Figure 1 The main functional areas of the Walkup Console user interface. The Main Window and Ribbon can be minimized to show only the system status as shown in **Figure 2** on page 12.



Figure 2 System status view of the Walkup Console user interface.

Ribbon

The ribbon contains access to tools used for Walkup administration, samples management, online Help, and viewing the sample queue.

Tools tab in the Ribbon

Administrative Tools

Administration Change to the Walkup Administration mode.

Change Password Change user passwords.

Shut down Walkup Shut down the Walkup program. You need to enter the name and password of a user that has permission to stop the Walkup program.

Samples Management

Abort Run Stop data acquisition of the current running sample. You can only abort a run if you have the appropriate permission.

Reprocess Sample Reprocess the acquired data for the selected sample.

Instrument

Standby Put the instrument in standby. If the MassHunter Data Acquisition program or ChemStation console is hidden, then you can still put the instrument in standby.

Clear Tray

Sampler Reset the sample tray assignments to allow new samples to be added. Incomplete samples may prevent the sample tray from being cleared.

Fraction Collector Opens the **Clear Fraction Collector** dialog box. You can select which plates/trays to clear in the Fraction Collector. This tool is only available if you have a Fraction Collector.

Queue Status

The status of the queue. Possible values include "No Samples in Queue", "Paused for Error. <error message>", "Paused by Administration", and Queue Pausing. This box can also be blank if the Queue just has entered into the ready state, if Walkup has just started with pending samples in queue, or if the Queue is pausing with no further samples in queue.

Queue Runtime

The estimated time necessary to run all of the items in the queue. This value is only an estimate.



Figure 3 Tools tab in the Walkup ribbon

Remote tab in the Ribbon

Remote Instrument Workload Opens the **Instrument Workload** program. See “[To view Instrument Workload](#)” on page 34.

Submit Remote Samples Opens the **Remote Sample Login** program. See “[To submit samples remotely](#)” on page 31.

Remote Samples Dashboard Opens the **Remote Dashboard** program. You can review samples that have been submitted remotely. You can also delete samples that you have submitted.

Help tab in the Ribbon

Help View Help Start online Help.

About View the Walkup system and data system software versions.

Status Bar

The status bar is located below the ribbon and contains status indication of the **Walkup Queue**, **Walkup System**, **ChemStation** or **MassHunter Acquisition**, **Instrument**, and **Injector**.



Figure 4 Walkup Status Bar for ChemStation (top) and MassHunter (bottom)

The typical status states shown in **Table 1** use colors to help you quickly identify the Walkup system status.

- Green: Ready status
- Blue: Running status
- Yellow: Standby status
- Grey: Walkup System notification message
- Violet: Instrument and Injector notification message
- Orange and Red: Walkup Queue paused

Table 1 Typical indicators and colors in the Status Bar

Walkup Queue	Walkup System	ChemStation or MassHunter Acquisition	Instrument	Injector
Waiting	Ready	Ready	Idle	Ready Inj. Done
Running	In run 7.35 minute(s) left in run	Data acquisition	Injecting Running Post run	Injecting
Startup	Pre-standby	Not ready	Not ready	Not ready
Wakeup	Standby w/ lamp on System startup System wakeup Starting run Injecting Run is about to end Standby w/ lamp off		Pre-run	Preparing
	Paused by Administrator			
	Error paused			

Main Window

The main window is divided into two panes: **Plate Tray Diagram** and **Sample Queue Table** (see Figure 5 on page 17). A third **Fraction Collection** pane is visible if a Fraction Collector is configured.







Plate Tray Diagram The tray diagram on the left of the main window shows the position of the samples in the autosampler. Sample positions in the diagram are color-coded to indicate the status of each sample as described in **Table 2**.

- For vial trays, the graphic is updated to show vial status as they are run.
- For well-plates, the individual sample wells within the well plate are updated as they are run.

The tray diagram is reset by a **Clear Sampler Tray** operation; see **“To clear the sampler tray”** on page 29.

You can minimize the Plate Tray diagram by clicking the yellow icon in between the two panes.

Table 2 Typical status indicators and colors in the Plate Tray Diagram

Plate Tray Diagram Color	Status Description
 Green	Pending sample, in queue to run
 Blue	Current sample running
 Purple	Completed sample
 Red	Missing vial, sample aborted during run, or other error
 Grey	Position available for a new sample
 Grey with a Red X	Reserved by the Walkup System

Sample Queue Table The list of active samples in the queued run order is shown on the right of the main window.

The sample queue is divided into the following sections. Note that if priority or delayed sample submission is not enabled on your system, then those sections do not appear and the queue is not separated into sections.

Table 3 Typical sample order and color in the Sample Queue Table

Queue Row Positions	Color of Rows	Sample Priority
Upper	Green	High
Middle	Blue	Normal
Lower	Gray	Delayed

The information shown for each sample row in the queue may include: Index number in the queue, Status icon (current, pending, or manually moved), Sample Name, User Name (Submitter), Sample Position, Completion Time, Walkup Method, Injection Volume, Number of Injections, Description, Data File Name, Tray Type, Tray, Target(s), Department ID, Job ID, and Retain.

If you have proper user permissions, you can change the order of samples in the queue as described on **“To view or edit the list of active samples”** on page 40.

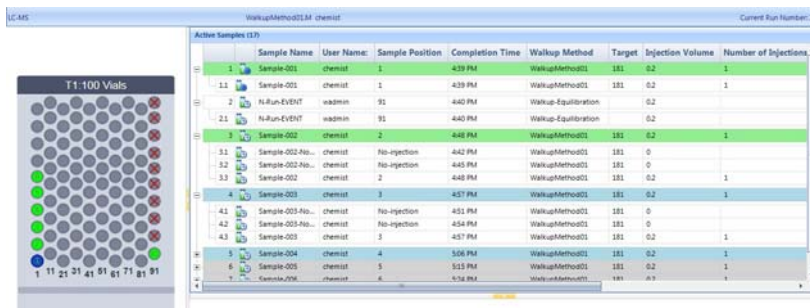


Figure 5 Plate Tray Diagram (left) and Sample Queue Table (right) in the main window

Fraction Collector Pane Images of each of the fraction collector plates.

Table 4 Color of positions in the Fraction Collector

Color of Position	Meaning
	Empty spot in the Fraction Collector tray
	The next spot to use in the Fraction Collector
	The first fraction for a sample
	Additional fractions for a sample

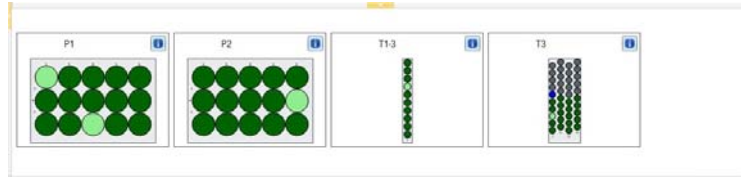




Figure 6 Fraction Collector Pane

Sample Bar

The Sample Bar contains three buttons - two buttons that change to either **hide**  or **show**  the main window and a **Submit Samples** button.

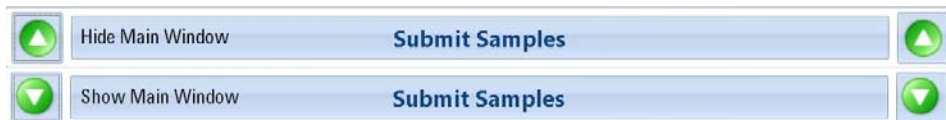


Figure 7 Sample Bar buttons shown with the main window displayed (top) and the main window hidden (bottom)

Submit Samples button Click **Submit Samples** to begin a new sample submission.

Submit Samples and Create New Users

Your user name and password are required to submit a new sample into the MassHunter Walkup System sample queue. If enabled by your system administrator, you can register a new user and password when you submit a new sample. For more information, see **“To view Walkup online Help”** on page 11.

To submit samples



The Submit Samples wizard has three (3) pages that guide you through the steps to enter a new sample into the Sample Queue table.

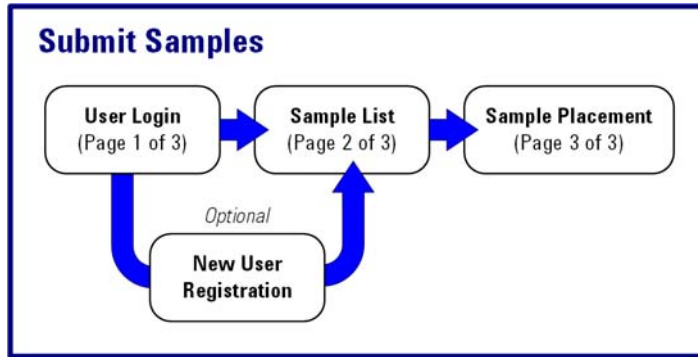


Figure 8 Submit Samples wizard

If the Allow Custom Sample Import check box in the Workflow Configuration pane is marked, then you do not see this dialog box. Instead, you see the user interface from the **Sample Import Program** that was entered.

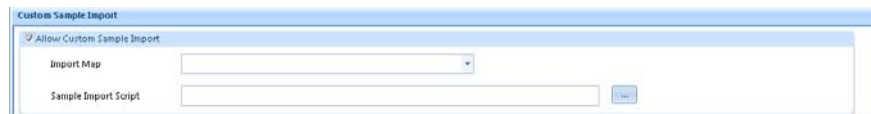


Figure 9 Custom Sample Import in the Workflow Configuration section

Submit Samples and Create New Users

To submit samples

User Login (Page 1 of 3)

- 1 Click **Submit Samples** **Submit Samples** in the Sample Bar at the bottom of the Walkup Console.
- 2 Enter information on the **User Login** page.
 - a (Optional) Mark **Register New User** if you are a new user. Registering a new user is only available if user registration is enabled on your system (see **Figure 18** on page 27).
 - b Type your **User Name**.
 - c Type your **Password**, if required and if you are not a new user.
 - d Select the **Workflow** to apply to your sample.
 - e Type the **Number of Samples** you are adding to the run queue.

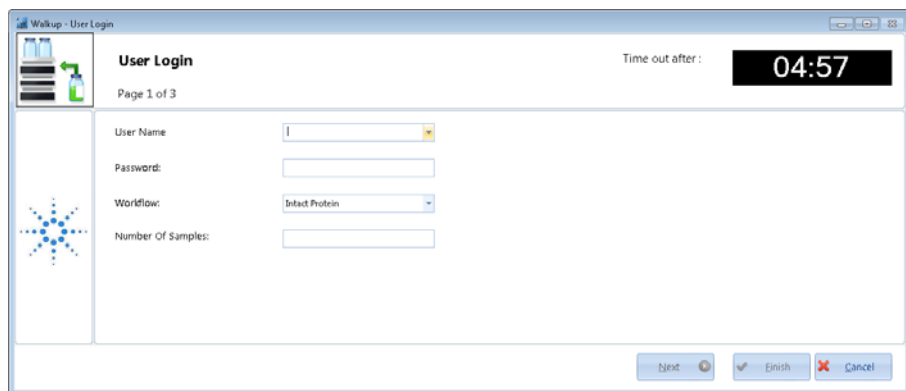



Figure 10 User Login (Page 1 of 3)

- f (Optional) Import samples from a file as an alternate to entering a value for the number of samples as shown in **Figure 11**, if sample import is configured for your user group:
 - Click **Import Samples**.
 - Select the **Import Map**
 - Select a name for the **Import Data File**. The Import Data file must be in Unicode format. The Browse button  is available if your user account is configured to select the path for Import Data Files.

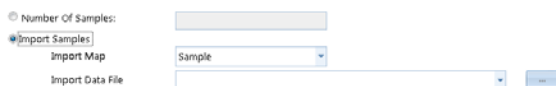


Figure 11 Import Samples options in the User Login (Page 1 of 3)

- g Enter and select additional information that may be required, such as Department ID, Job ID, or Vial Type.

3 Click **Next**.

Register New User (Page 1 of 3)

- 4 (Optional) Enter information on the **Register New User** page if **Register New User** was marked on the **User Login** page. See **“To register a new user”** on page 27 and then return to **step 5** below.

Sample List (Page 2 of 3)

- 5 Enter information on the **Sample List** page.
 - a Mark **Automatically copy down columns** to replicate the information for the current sample to the sample rows below. If your **Sample Name** ends in a number, the number is automatically incremented for the subsequent rows.

Sample Name may have constraints if your system administrator has set up a Sample Name Template.

- b Type and select your sample information in the sample list table. Fill out a row of the table for each sample. Enter information such as **Description**, **Formula**, **MethodName**, **Sample Priority**, **Sample Name**, **Position**, and **Target**. The column headings are customized by the system administrator; your **Sample List** page may appear different from the example in **Figure 12**. Additionally, many of the parameters available to the system administrator are customizable; the **MethodName** parameter is mandatory.

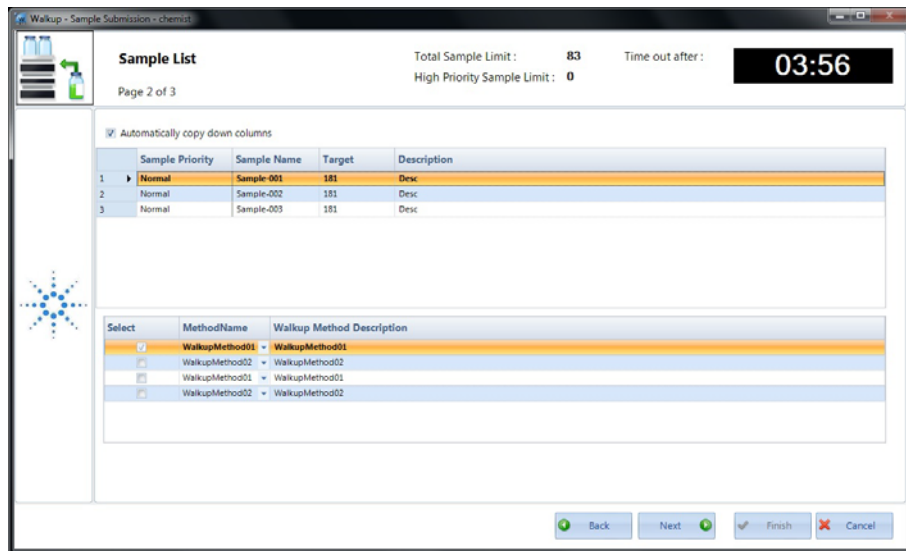


Figure 12 Sample List (Page 2 of 3)

Submit Samples and Create New Users

To submit samples

- c Set the queue priority for running the sample as **High**, **Normal**, or **Delayed**, if priority samples are allowed. There may be limits to how many priority samples are allowed per user per day.

Delayed samples are added as a third (bottom) section of the sample queue and are run when no **Priority** or **Normal** level samples are present in the queue. Delayed samples entered using the *after a specified period of time* feature are run after the specified time, even if the sample queue does not contain **High** and **Normal** samples.

- d Enter the **Position** of the sample on the plate. This is not displayed if Vials are configured.
- e (*Optional*) Enter information such as a molecular **Formula**, **Target Mass**, **Target Column**, or **Custom Column** if they are configured for this Workflow. Other columns include **DA Workflow**, **Condition**, **Mass Confirmation**, **Sequences**, **Modification Profiles**, and **Enzymes**.

An entry for **Formula** or **Target Mass** can be used for SIM ions or Sample Purity/Compound Confirmation calculations. Enter the target mass value with up to two decimal places, or enter a molecular formula, or enter both the expected molecular weight and formula separated by a colon (:). Molecular formulas are validated, and the corresponding molecular weight is displayed along with the formula in the Target column.

- f Assign a method for each sample from the list of available methods after the samples have been entered. If multiple method settings are enabled, you can submit a single sample with multiple methods without adding additional rows in Sample List.

- 6 Click **Next**.

Sample Placement (Page 3 of 3)

7 Review the information on the **Sample Placement** page.

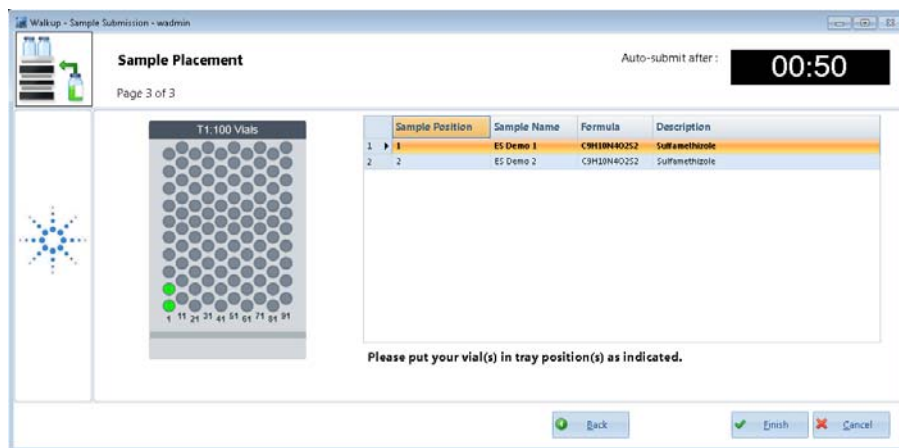




Figure 13 Sample Placement (Page 3 of 3)

- Review the sample information table.
- Click **Back** if you need to make any corrections in previous sample submission pages.
- Place your samples in the autosampler according to the diagram.

Sample status is color-coded as follows:

- Positions ready to accept your samples are **Green** .
- Positions available to submit additional samples using **Submit Samples** are **Grey** .

You may have to wait to place the vials if the autosampler is injecting. When the injection is done, the tray door is unlocked.

- (Optional)* Set options to retain vials, receive email reports, and print reports, if these are configured for your user group.

8 Click **Finish**.

NOTE

Sample submission may be customized in either of the following ways:

- Sample submission is canceled if not completed in a preset amount of time.
- Sample submission is automatically completed and your sample(s) are submitted if the timeout occurs on the last page of sample submission.

Submit Samples and Create New Users

To reprocess sample

- 9 Review the Walkup Console. Your samples appear in the Sample Queue table in the main window. Sample priority is indicated by row colors as described in **Table 3** on page 17.
- 10 Retrieve your analysis report. Reports are created and emailed to you when the sample analysis is completed, if this option is configured and selected by your system administrator.

To reprocess sample



The Reprocess Sample wizard has three (3) pages that guide you through the steps to reprocess one or more samples.

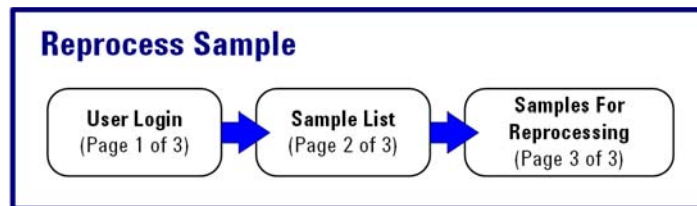



Figure 14 Reprocess Sample wizard

- 1 Click **Reprocess Sample**  in the Walkup ribbon.
- 2 Enter information on the **User Login** page.
 - a Select your **User Name**.
 - b Type your **Password**.
 - c Select **Samples Submitted By**. Typically the selection is **Myself** but the system administrator can configure the system to allow you to select other users.
 - d Select **When** the samples were originally processed.
 - e Select the **workflow** with which the samples were submitted.

User Login
(Page 1 of 3)

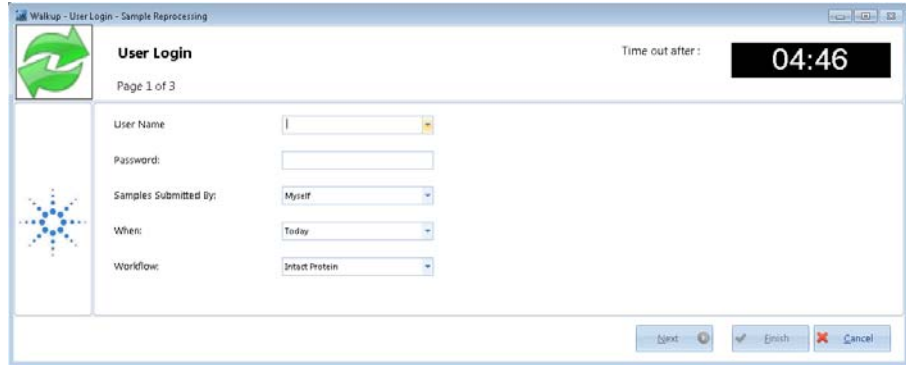


Figure 15 User Login (Page 1 of 3)

3 Click **Next**.

Sample List
(Page 2 of 3)

4 Mark the samples you want to reprocess on the **Sample List** page.

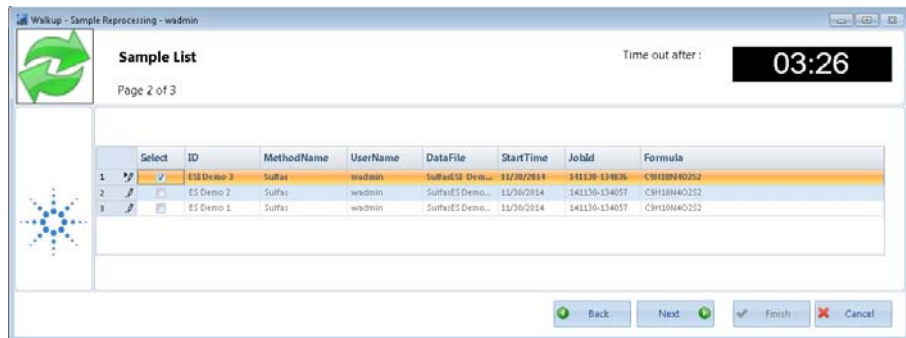


Figure 16 Sample List (Page 2 of 3)

5 Click **Next**.

Sample Placement
(Page 3 of 3)

6 Review samples scheduled for reprocessing in the **Sample Placement** page.

7 Click **Back** if you need to make any corrections in previous sample reprocess sample pages.

Submit Samples and Create New Users

To view email reports

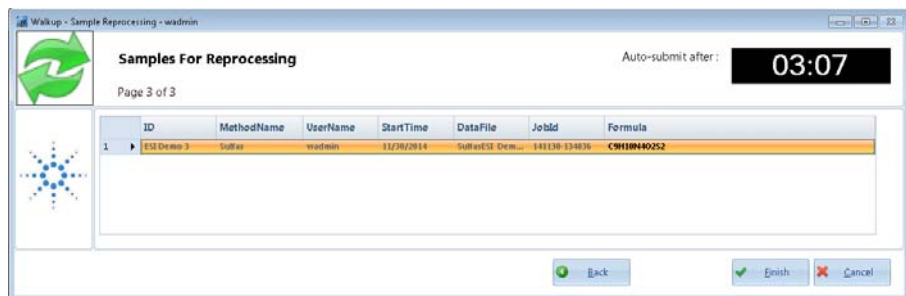


Figure 17 Samples For Reprocessing (Page 3 of 3)

8 Click **Finish**.

To view email reports

Use this procedure to view Walkup results that you receive by email in **.zne** format.

NOTE

This procedure assumes that the Unpack Utility is on the computer where you are opening the **.zne** attachment. See your system administrator if the Unpack Utility is not already installed on your computer.

- 1 Double-click the **.zne** file that is attached to an email or a **.zne** file that you have saved to disk. The Unpack Utility starts automatically and opens the **.zne** file.
- 2 Mark **View Report** in the Unpack Utility window.
- 3 Click **Unpack**.

The ChemStation report files are extracted and displayed in your Internet browser window.

Tip

You can also use WinZip or PKZip decompression program to open a **.zne** file that has been saved to disk.

To register a new user



New user registration during sample submission is a feature that can be enabled by the system administrator. If enabled on your system, the new user is added to the group specified in the Walkup System Configuration pane.

- 1 Click **Submit Samples** [Submit Samples](#) in the Sample Bar at the bottom of the Walkup Console.
- 2 Enter information in the **User Login** page.
 - a Mark **Register New User** (see [Figure 18](#)).
 - b Type your **User Name**.
 - c Enter and select additional information requested in the User Login page.

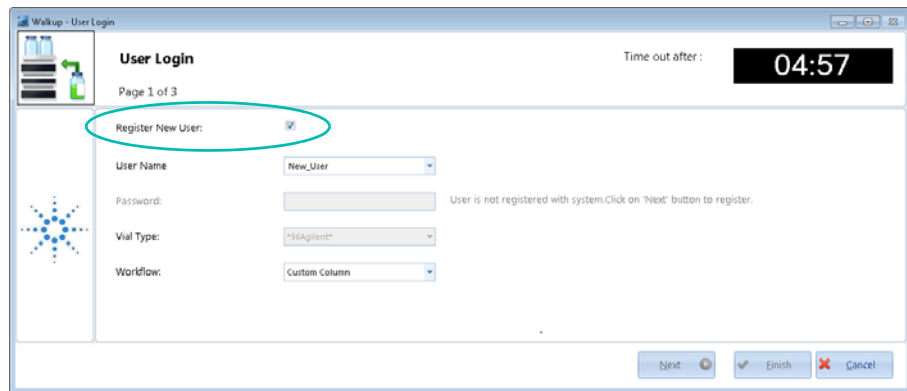


Figure 18 Register New User option in the User Login (Page 1 of 3)

- 3 Click **Next**.
- 4 Enter information in the **New User Registration** page.
 - a Type your **Full Name**.
 - b Type your **Password**.
 - c Type the same password in **Confirm Password**.
 - d Enter additional information, depending on how your system and group is configured. For example, you may need to type the **Email Address** where you want Walkup results to be sent and click **Send Test Email** to confirm that you receive email from the Walkup System.
 - e View the **Full Data Path** where the data files are stored for the new user.

Submit Samples and Create New Users

To change your password

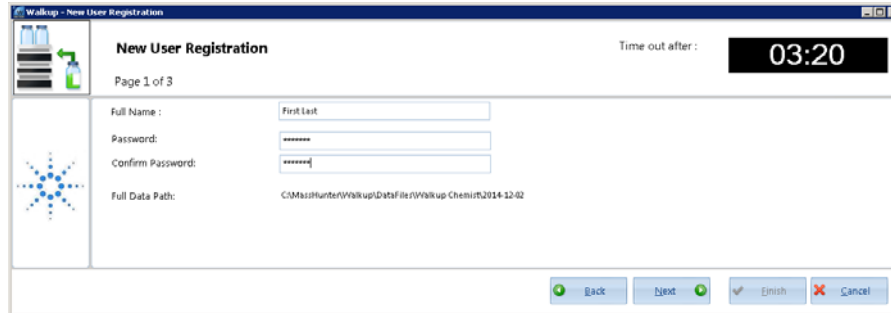



Figure 19 New User Registration page

- 5 Click **Next**.
- 6 Continue with your sample submission as described in “**To submit samples**”, **step 5** on **page 21**.

To change your password



You can change the password for your Walkup user account in a few steps.

- 1 Click **Change Password**  in the Walkup ribbon.
- 2 Enter the information in the **Change Password** dialog box appears:
 - a Type your **User Name**
 - b Type your current password in **Old Password**.
 - c Type your **New Password**.
 - d Type the same password in **Confirm New Password**.
- 3 Click **OK**.

To shut down the Walkup program




You can shutdown the Walkup program if you have the correct permission.

- Click **Shutdown Walkup**  in the Walkup ribbon. You need to enter a user name and password.

To clear the sampler tray



When the sampler tray becomes full of sample vials, or when you simply want to reset the sample tray, completed samples must be removed. Incomplete samples may prevent the sampler tray from being cleared.

- Click **Sampler**  in the Walkup ribbon to clear the sampler tray.
- Click **Fraction Collector** to clear the Fraction Collection tray, if a Fraction Collector is configured.




NOTE

If you have more than one tray to clear, this button opens the Clear Tray dialog box. You can mark which trays to clear.

NOTE

This option may not be configured on your system. In this case see the alternate method below.

Alternate method to clear the trays

- 1 Click **Administration**  in the Walkup ribbon.
- 2 Type your **User Name** and **Password** in the **Login to Walkup Administration** dialog box.
- 3 Click **OK**.
- 4 Click **Samples/Events**  from the list of actions along the left side of the Administration main window (see **Figure 20**). See **“To open the Samples and Events pane”** on page 38.
- 5 Click **Sampler**  or **Fraction Collector** in the **Clear Tray** group of the ribbon.

If you have more than one tray to clear, this button opens the Clear Tray dialog box. You can mark which trays to clear.

Submit Samples and Create New Users To clear the sampler tray

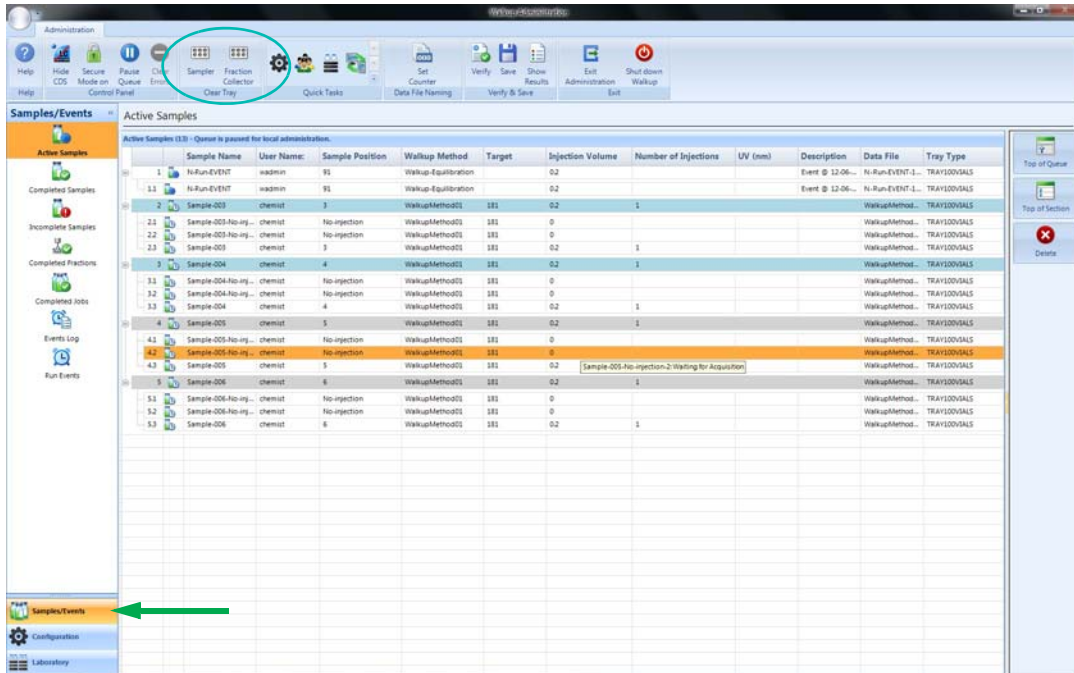



Figure 20 Clear Sampler Tray in the Samples/Events ribbon

6 Click **Exit Administration**  in the *Exit* group of the ribbon.

Submit Samples Remotely

In a Walkup Networked System only, you can submit your samples remotely. Your user name and password are required to submit a new sample. You use three different programs to submit a sample remotely.

- Submit Remote Samples program - submit the sample
- Instruments Workload program - review the workload on each instrument
- Walkup program - assign your samples to an instrument

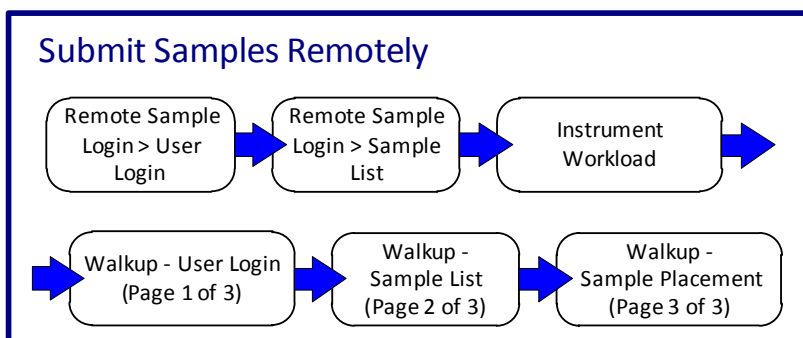


Figure 21 Workflow for Submit Samples Remotely

To submit samples remotely



User Login page

The Remote Sample Login wizard has two (2) pages that guide you through the steps to enter a new sample into the Remote Dashboard.

- 1 Click **Submit Remote Samples** in the Agilent MassHunter Walkup Remote Tools program group. The Remote Sample Login dialog box opens.
- 2 Enter information on the **User Login** page.
 - a Type your **User Name**.
 - b Type your **Password**, if required.
 - c Select the **Data System** to use for this sample. You select either **OpenLab ChemStation System** or **MassHunter Acquisition System**.

Submit Samples Remotely

To submit samples remotely

- d Enter the **Remote Samples Name**.
- e Enter the **Description**.
- f Select the **Workflow** to apply to your sample.
- g Click either **Number of Samples** or **Import Samples**.
- h If you click the **Number of Samples** option, then type the **Number of Samples** you are adding to the run queue. If you click the **Import Samples** option, then select the **Import Map** and the **Import Data File**.

The screenshot shows a web application window titled "Remote Sample Login" with a sub-section "User Login". The form includes the following fields and options:

- User Name: [text input]
- Password: [password input]
- Data System: [radio buttons for OpenLab ChemStation System and MassHunter Acquisition System]
- Remote Samples Name: [text input with value S-001]
- Description: [text input with value S-001]
- Job ID: [text input with value S-001]
- Department ID: [dropdown menu with value Bio-Chemistry]
- Workflow: [dropdown menu with value CS-All Workflow]
- Number of Samples: [radio button selected, text input with value 5]
- Import Samples: [radio button unselected]
- Import Map: [dropdown menu]
- Import Data File: [text input]

At the bottom right, there are four buttons: Back, Next, Upload, and Cancel.

Figure 22 Remote Sample Login > User Login

- i Enter and select additional information that may be required, such as Department ID, Job ID, or Vial Type.

3 Click **Next**.

Sample List page

- 4 Enter information on the **Remote Sample Login > Sample List** page.
 - a Mark **Automatically copy down columns** to replicate the information for the current sample to the sample rows below. If your **Sample Name** ends in a number, the number is automatically incremented for the subsequent rows.

Sample Name may have constraints if your system administrator has set up a Sample Name Template.

- b Type and select your sample information in the sample list table. Fill out a row of the table for each sample. Enter information such as **Barcode**, **DA Workflow**, **Masses**, and **Walkup Method**. The column headings are customized by the system administrator; your **Sample List** page may appear different from the example in **Figure 23**. Additionally, many of the parameters available to the system administrator are customizable; the **Walkup Method** parameter is mandatory.

Sample Priority	Barcode	Accepted DAR Range	Condition	CC	DA Workflow	Enzymes	Expected Dar	Masses	Mod_Pro	Qual_W	Seq	DAR 0 Mass	Theoretical Drug	Walkup Method
1 High	S001	01-10	Reduced	Custom	Intact Protein	Non-specific	10	150	.mAb .P.	CompoundClass	Bovine carbonic ..	200	300	First
2 Normal	S002	01-10	Reduced	Custom	Intact Protein	Non-specific	10	150	.mAb .P.	CompoundClass	Bovine carbonic ..	200	300	Second
3 Normal	S003	01-10	Reduced	Custom	Intact Protein	Non-specific	10	150	.mAb .P.	CompoundClass	Bovine carbonic ..	200	300	First
4 Normal	S004	01-10	Reduced	Custom	Intact Protein	Non-specific	10	150	.mAb .P.	CompoundClass	Bovine carbonic ..	200	300	Second
5 Delayed	S005	01-10	Reduced	Custom	Intact Protein	Non-specific	10	150	.mAb .P.	CompoundClass	Bovine carbonic ..	200	300	First

Figure 23 Remote Sample Login > Sample List

- c (Optional) Enter information such as a molecular **Formula**, **Target Mass**, **Target Column**, or **Custom Column** if they are configured for this Workflow. Other columns include **DA Workflow**, **Condition**, **Mass Confirmation**, **Sequences**, **Mod_Pro**, **Expected DAR**, and **Enzymes**.

An entry for **Formula** or **Target Mass** can be used for SIM ions or Sample Purity/Compound Confirmation calculations. Enter the target mass value with up to two decimal places, or enter a molecular formula, or enter both the expected molecular weight and formula separated by a colon (:).

Molecular formulas are validated, and the corresponding molecular weight is displayed along with the formula in the Target column.

- d Assign a method for each sample from the list of available methods after the samples have been entered. If multiple method settings are enabled, you can submit a single sample with multiple methods without adding additional rows in Sample List.
- 5 Click **Upload**.

To view Instrument Workload



The Instrument Workload program lets you see the Queue Length and Queue RunTime for each data instrument in the system. These values help you to determine which instrument to use to submit the remote samples.

- 1 Click **Instrument Workload** in the Agilent MassHunter Walkup Remote Tools program group. The Instrument Workload program opens.
- 2 View the Queue Status, Queue Length, and Queue RunTime for each instrument that has the data system that you selected when you remotely submitted your sample.
- 3 Determine the instrument to use when you submit your sample.

Name	Description	Controller	Data system	Status	Queue Status	Queue Length	Queue RunTime	Last Update Time
LC		V-MMWIN0764-01	ChemStation	Available	Running	3	9 mins	11/23/2017 3:40:51 PM
MhInst-01		V-MMWIN0764-02	LCMS MassHunter	Available	Standby	0	0	11/23/2017 3:54:09 PM
Instrument 1		V-MMWIN1054-04	LCMS MassHunter	Available	Ready	6	12 mins	11/23/2017 3:40:19 PM

Figure 24 Instrument Workload program

To assign remote samples to an instrument



After you remotely log the samples, you need to assign them to an instrument and place the samples.

User Login
page

- 1 Click **Submit Samples** in the Agilent MassHunter Walkup Remote Tools program group. The **Walkup - User Login** dialog box opens.
- 2 Enter information on the **User Login** page.
 - a Type your **Login**.
 - b Type your **Password**, if required.
 - c Click the **Remote Samples** option.
 - d Select which remote samples to submit.

Submit Samples Remotely

To assign remote samples to an instrument

Walkup - User Login

User Login Time out after : **04:18**

Page 1 of 3

Register New User:

Login:

Password:

Remote Samples
 Number Of Samples:
 Import Samples

Import Map:

Import Data File:

Department ID:

Job ID:

Workflow: Click Next to bring up a dialog for entering inputs for this workflow

Figure 25 User Login (Page 1 of 3)

3 Click **Next**.

Sample List
page

4 Review the information on the **Sample List** page.

5 Click **Next**.

Sample
Placement
(Page 3 of 3)

6 Review the information on the **Sample Placement** page. Place your samples in the positions indicated.

Submit Samples Remotely

To assign remote samples to an instrument

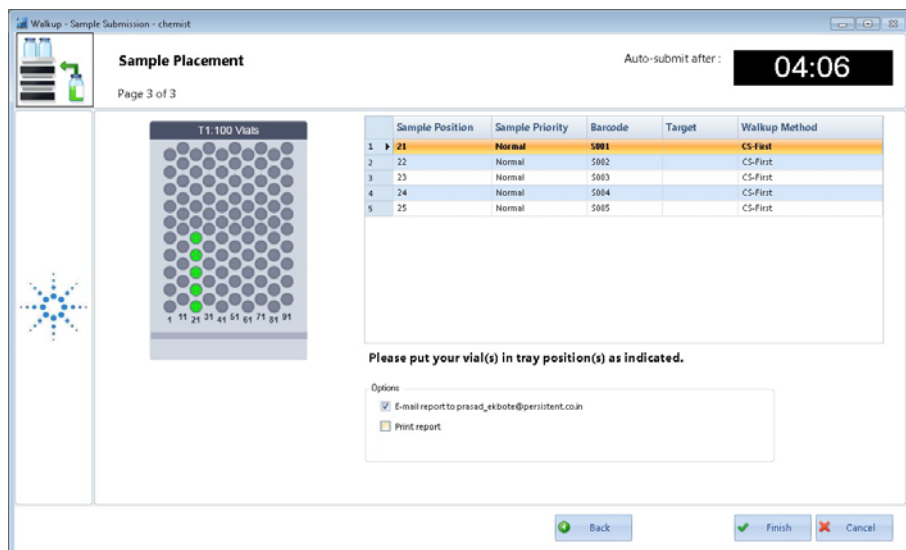




Figure 26 Sample Placement (Page 3 of 3)

- a Review the sample information table.
- b Click **Back** if you need to make any corrections in previous sample submission pages.
- c Place your samples in the autosampler according to the diagram.

Sample status is color-coded as follows:

- Positions ready to accept your samples are **Green** .
- Positions available to submit additional samples using **Submit Samples** are **Grey** .

You may have to wait to place the vials if the autosampler is injecting. When the injection is done, the tray door is unlocked.

- d (Optional) Set options to retain vials, receive email reports, and print reports, if these are configured for your user group.

7 Click **Finish**.

NOTE

Sample submission may be customized in either of the following ways:

- Sample submission is canceled if not completed in a preset amount of time.
- Sample submission is automatically completed and your sample(s) are submitted if the timeout occurs on the last page of sample submission.

Submit Samples Remotely

To assign remote samples to an instrument


- 8 Review the Walkup Console. Your samples appear in the Sample Queue table in the main window.
- 9 Retrieve your analysis report. Reports are created and emailed to you when the sample analysis is completed, if this option is configured and selected by your system administrator.

Manage Samples and Events

Samples and events management is accessed in the Administration window. You must log into the Administration window in order to access the tasks described in this section. A comprehensive guide to the features available in Administration is available in the online Help.

To log into Administration



- 1 Click **Administration**  in the Walkup ribbon.
- 2 Type your **User Name** and **Password** in the **Login to Walkup Administration** dialog box (see **Figure 27**).
- 3 Click **OK**.

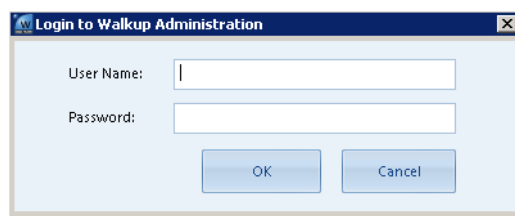



Figure 27 Login to Walkup Administration dialog box

To open the Samples and Events pane







- 1 Log into the **Administration** window as described in “**To log into Administration**” above.
- 2 Click **Samples/Events**  from the list of actions along the left side of the main window (see **Figure 20** on page 30).

To manage the sample queue and clear errors

- 1 Log into the **Administration** window and open the **Samples/Events** pane (see “**To log into Administration**” and “**To open the Samples and Events pane**”).
- 2 Review the new tools that are available in the ribbon (see **Figure 28**).



Figure 28 Administration ribbon

- 3 Click **Pause Queue**  in the *Control Panel* group of the ribbon to temporarily pause the sample queue. *This button may not be available for your user group.*
- 4 Click **Resume Queue**  in the *Control Panel* group of the ribbon to restart the sample queue.
- 5 Click **Clear Errors**  in the *Control Panel* group of the ribbon to clear the most recent error condition and restart the sample queue. The next sample in the queue is run immediately.
- 6 Click **Set Counter**  in the *Date File Naming* group of the ribbon when you want to reset the counter used in data file naming. You can enter the reset counter value in the **Set Data File Counter** dialog box (see **Figure 29**).

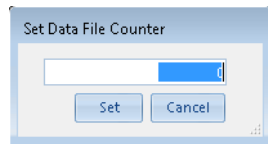








Figure 29 Set Data File Counter dialog box

- 7 Reorder samples in the sample queue as necessary to meet current needs by following the steps in the section “**To view or edit the list of active samples**” below.
- 8 Reset the sampler tray by following the steps in section “**To clear the sampler tray**” on page 29.


To view or edit the list of active samples

- 1 Log into the **Administration** window and open the **Samples/Events** pane (see “**To log into Administration**” and “**To open the Samples and Events pane**”).
- 2 Click **Active Samples**  from the list along the left side of the **Samples/Events** pane.
- 3 View the list of active samples displayed on the right side of the **Samples/Events** pane. The queue is divided into the following sections:
 - Upper: High priority samples in  green
 - Middle: Normal priority samples in  blue
 - Lower: Delayed samples in  gray

Event samples have no color coding in the Active Samples table.
- 4 Move a sample in the list to a new queue position:
 - a Click the sample row containing the sample you want to move.
 - b Click **Top of Queue**  on the right side of the pane to move the selected sample to the top of the entire Sample Queue.
 - c Click **Top of Section**  on the right side of the pane to move the selected sample to the top position within its *section* of the Sample Queue (Upper, Middle, or Lower).



Keep the following in mind when reordering samples in the queue:

- Once a sample is moved to **Top of Queue**, the moved sample is *not* considered in sample prioritization.
- Once a sample is moved to **Top of Section**, the moved sample is *not* considered in the sample prioritization for that section.
- A unique sample icon indicates samples that have been manually moved in the queue.
- The following types of samples cannot be moved: Running sample, Pre-fetched sample (in case of overlapped samples execution), Event sample, Plate sample, and Equilibration samples, which are samples for which equilibration is already triggered.

- 5 Remove a sample from the list:
 - a Click the sample row containing the sample you want to remove.
 - b Click **Delete**  on the right side of the pane. The following types of samples cannot be deleted: Running sample, Pre-fetched sample (for overlapped samples), and Equilibration sample (samples for which equilibration is already triggered).



When you close the Walkup Administration window, the changes you made are reflected in the Sample Queue table of the Walkup Console.

To view or export the list of completed samples

- 1 Click **Completed Samples**  from the list along the left side of the **Samples/Events** pane. A list of completed samples is shown on the right side of the pane.
- 2 Click **Export**  on the right side of the pane to export the list of completed samples as an Excel spreadsheet (.xls or .xlsx format).
- 3 Decide if you want to remove the completed sample queue data from the *Completed Samples* list after export. If you do, then when prompted, click **Yes** to delete the sample list data for the completed samples from the Walkup system. To save the completed sample queue data, click **No**.

Lists of completed samples are automatically deleted from the *Completed Samples* list after a period of time set by your system administrator. *The sample data files are not removed, only the record of the samples within Walkup are removed.*




To view or export the list of completed fractions

- 1 Click **Completed Fractions**  from the list along the left side of the **Samples/ Events** pane. A list of completed fractions is shown on the right side of the pane.
- 2 Click **Export**  on the right side of the pane to export the list of completed fractions as an Excel spreadsheet (.xls or .xlsx format).
- 3 Decide if you want to remove the completed fraction data from the *Completed Fractions* list after export. If you do, then when prompted, click **Yes** to delete the fractions list for the completed fractions from the Walkup system. To save the completed fractions data, click **No**.



Lists of completed fractions are automatically deleted from the *Completed Samples* list after a period of time set by your system administrator.

To view or edit the list of incomplete samples

Incomplete samples are samples that were not run because of a problem with the sample or the system or samples that you aborted.



- 1 Click **Incomplete Samples**  from the list along the left side of the **Samples/ Events** pane. A list of incomplete samples is shown on the right side of the pane. Note that incomplete samples may prevent the sampler tray from being cleared.
- 2 Click **Delete**  on the right side of the pane to remove a sample from the list. Deleted samples are moved to Completed samples list, marked with an "X" for that row.
- 3 Click **Resubmit**  on the right side of the pane to resubmit samples for analysis. Make sure the samples have sufficient sample volume and that they are actually in the specified position in the sampler.

To view or export a list of completed jobs

- 1 Click **Completed Jobs**  from the list along the left side of the **Samples/ Events** pane.
- 2 View the list of completed jobs.
- 3 Click **Export**  on the right side of the pane to export the list of completed jobs as an Excel spreadsheet (.xls or .xlsx format).
- 4 Decide if you want to remove the completed job queue data from the *Completed Job* list after export. If you do, then when prompted, click **Yes** to delete the job list data for the completed jobs from the Walkup system. To save the data, click **No**.

Lists of completed jobs are automatically deleted from the *Completed Jobs* list after a period of time set by your system administrator. *The sample data files are not removed*, only the record of the jobs within Walkup are removed.



To view or export the Events Log

- 1 Click **Events Log**  from the list along the left side of the **Samples/ Events** pane.
- 2 View the list of events for this instrument in the Events Log table.
- 3 Click **Export**  on the right side of the pane to export the list of completed jobs as an Excel spreadsheet (.xls or .xlsx format).
- 4 Decide if you want to remove the completed events queue data from the *Events Log* list after export. If you do, then when prompted, click **Yes** to delete the event list data for the completed events from the Walkup system. To save the data, click **No**.

Lists of completed events are automatically deleted from the *Completed Events* list after a period of time set by your system administrator. *The sample data files are not removed*, only the record of the events within Walkup are removed.

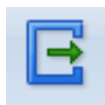
To run scheduled events immediately

When an instrument error occurs, some scheduled events do not run. The Run Events pane provides access for you to immediately run selected events.

- 1 Click **Run Events**  from the list along the left side of the **Samples/ Events** pane. A list of scheduled events that were previously configured are displayed in the table.
- 2 Select event rows you want to run. The order that the events are run is shown in the Run Order column.
- 3 Click **Run**  on the right side of the pane to run the selected events.

Events that run samples are added to the queue and run after you close the Walkup Administration window.

To close the Walkup Administration window




Use the following procedure to close the Walkup Administration window and return to the Walkup Console.

- Click **Exit Administration**  in the *Exit* group of the ribbon.

The Walkup Console is displayed.

NOTE

Do not click **Shutdown**  to close the Walkup Administration window. **Shutdown** closes the Walkup console, does not complete the current sample, and sends an email notice indicating that the sample run failed.

Tips and Tricks

Avoiding fraction collection contamination

- ✓ After a sample run failure (due to instrument error or if the user aborts the run), replace the container. Then in the Walkup program, in the **Clear Tray** ribbon tool tab, select **Fraction Collector**.

When fractions are successfully collected, fraction details are recorded in the data file. If the sample run ends unexpectedly, fraction details are not saved, and Walkup displays incomplete fraction data. Walkup also incorrectly calculates the next fraction location, which can cause contamination during fraction collection for the next sample.

When you clear the fraction collection tray, you refresh the system settings.

- ✓ Put a limit on how full a fraction collection tray can be so that fractions do not run over from one tray to the next.

Changing fraction configuration

- ✓ Do not change fraction configuration from the ChemStation Console during a run. Changes that you make in ChemStation after a run begins are ignored by Walkup.

If you need to make a change, wait until the run is complete, and close the Walkup program first.

Changing or adding a new Multisampler drawer

- ✓ When you change or add a new drawer to the Multisampler, do a test run outside of Walkup first. If the drawer configuration is not verified outside of Walkup, Walkup can report incorrect number of drawers.

In This Guide

The Quick Start Guide tells how to submit and manage samples and events in the MassHunter Walkup System.

