Agilent MassHunter Walkup System

Setup Guide

This version of the Walkup software supports OpenLAB CDS ChemStation Edition software (C.01.05 or higher).

Agilent Technologies

What is the Agilent MassHunter Walkup System?

Agilent MassHunter Walkup System provides walk-up access to LC and LC/MS systems for lab users who lack experience with mass-spectrometry instrumentation and data systems. The software allows lab managers, analysts and operators in chromatography labs of pharmaceutical enterprises to do drug discovery and drug development under non-regulated conditions. It can also be used in chemical analysis labs in petrochemical, environmental, food, and other industries.

MS users such as medicinal and synthetic organic chemists can conveniently and easily submit samples. System administrators have a flexible way to manage the security and user access for the system. The system can be configured to email reports and data to users.

Where to Find More Information

You can access more information about Walkup System as follows.

Walkup online Help

Refer to the *Walkup online Help* for in-depth information about how to administer, configure, and use Walkup System.

- Press **F1** or the help button to get help on the pane or dialog box.
- Click **Help > Contents** in the main MassHunter Walkup window to get to the top level Help topic.

Walkup System Quick Start Guide

The *Walkup System Quick Start Guide* describes how to submit samples and manage the sample queue. It is available both in print and as a PDF file on the installation disc.

Agilent website

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

http://www.chem.agilent.com

Software Status Bulletin

A list of known problems and issues for 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.

Installation

Walkup software can be installed:

- in a small lab on standalone workstations
- in a large lab on networked workstations

In a large lab, the Walkup system consists of:

- Remote server that runs OpenLAB Shared Services
- Networked OpenLAB workstations
- Office computers that are used to manage Walkup and lab data remotely

NOTE OpenLAB CDS Distributed System is not supported.

Walkup supports only these instruments, software and hardware revisions:

- Agilent 1100 or 1200 Series Liquid Chromatograph
- Agilent 1290 Infinity LC System
- Agilent Infinity LC Injector HTS/HTC or equivalent
- Agilent 6100 A/B Series Single Quad LC/MS (fraction collection not supported in this release)
- MS firmware 3.02.42 or higher
- Windows 7 (64-bit)
- M8301AA OpenLAB CDS ChemStation Edition software (C.01.05 or higher)

Step 1. Install the OpenLAB Shared Services Server (large labs only)

1 Install the OpenLAB Shared Services software on a server system.

Follow instructions in the *Agilent OpenLAB Chromatography Data System (CDS) Networked Workstation Installation Guide (p/n M8203-90002)*.

2 Make sure that the system is completely verified.

Step 2. Install and configure OpenLAB workstation

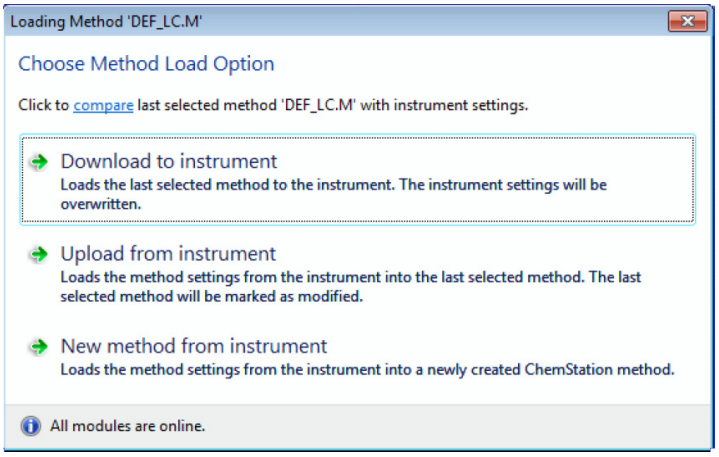
Do this step on all data acquisition workstations in your lab.

For large labs, refer to the *Agilent OpenLAB Chromatography Data System (CDS) Networked Workstation Installation Guide (p/n M8203-90002)*.

For small labs, refer to the *Agilent OpenLAB Chromatography Data System (CDS) Workstation Installation Guide (p/n M8301-90005)*.

1 Install all hardware as instructed in the appropriate installation guide.
2 Install the OpenLAB CDS ChemStation Edition software on each workstation, as described in the installation guide. Verify that the software functions properly.
   - In the System Configuration Check step, select **ChemStation Edition C.01.xx**.
   - Make sure that **IO Libraries** are installed.

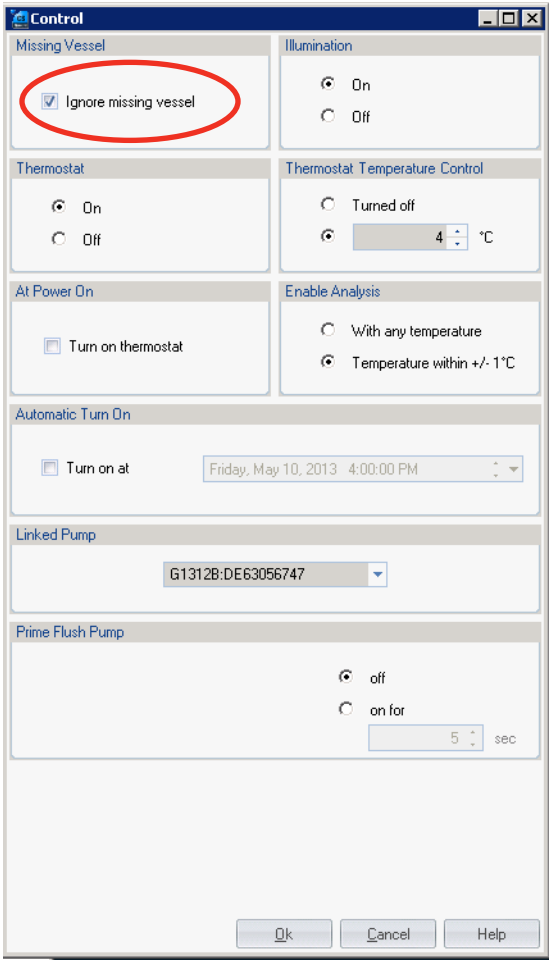
- Make sure all required patches and hot fixes are installed.
- When the ChemStation workstation is started for the first time, and when prompted, select the appropriate LC/MS model. For the Method Load Option, click **Download to instrument**.



3 Create and configure all instruments in the OpenLAB Control Panel.

Note that Walkup supports only one instrument on each workstation.

For the AutoSampler or HiP-Sampler, make sure that the **Ignore missing vessel** check box is marked.



4 Create shortcuts for the ChemStation program:

   a In the OpenLAB Control Panel ribbon, click the **Create Shortcuts** icon.

   b Click **OK**.

NOTE When you install MassHunter Analytical Studio Reviewer or configure ChemStation, you can be asked one or more times whether to allow a program from an unknown publisher to make changes to the computer. Click **Yes**.

5 Install MassHunter Analytical Studio Reviewer software. Refer to the Analytical Studio Reviewer *Quick Start Guide* for installation instructions and requirements.

- MassHunter Analytical Studio Reviewer program (B.02.01).
- MassHunter ASR File Generator for ChemStation (with Patch 2), if you want to create custom reports for MS results.

If your operating system is Windows 7 and you are warned that you are installing on an unsupported Windows system, click **Yes** to continue the installation.

6 Configure ChemStation:

a Start the Online ChemStation Console. To do so, click the ChemStation icon for online analysis if a shortcut was created. As an alternative, in the OpenLAB Control Lab **Start Instrument** panel, click the **Launch** button for the instrument that you will use with Walkup.

b Create a method in ChemStation console.

c Save the method as **WalkupStandby.m**.

This method does not need to contain data analysis components. It is used as an idle method to lower the flow rates to reduce solvent consumption after the last sample is run.

d Test the ChemStation to make sure the system operates properly. Tune the LC/MS instrument before you continue.

Step 3. Install and start the Walkup program

Do this on each workstation after ChemStation is installed and verified.

1. Log in to an account that has administrator rights.
2. Close the ChemStation program.
3. Insert the Walkup System installation disc into the disc drive.
4. Under **Instrument Workstation** for either Small Lab or Large Lab, click **Install**.
5. Click **Run** when given the option to run or save the file.

   Do not save the installation program to your computer before you run it. The installation program will not run properly if you do.

6. If .NET Framework 4.0 is not already installed, the .NET Framework installation program runs. Follow the instructions to install .NET Framework.
7. If Walkup already exists on the computer, you are given the option to remove or repair Walkup. Select to remove Walkup if you want to do a fresh installation.
8. When the Agilent MassHunter Walkup System Setup dialog box appears, click **Next** to continue.
9. Read the license agreement. Click **Yes** to accept its terms and continue the setup program.
10. When the Choose Destination Location dialog box appears, click **Next** to accept the default folder, or click **Browse** to select a different location. The default installation folder is:
    C:\Program Files (x86)\Agilent\MassHunter\Walkup
11. Review the settings when presented and click **Next** to continue.
12. Click **Finish** when the Walkup installation is complete.
13. If no other MassHunter program was previously installed, you are prompted to select a **Customer Home** path.
14. Start the Walkup program. See "To start the Walkup program" on page 23.

Step 4. Configure the Walkup workstation

You can configure the Walkup workstation in one of three ways:

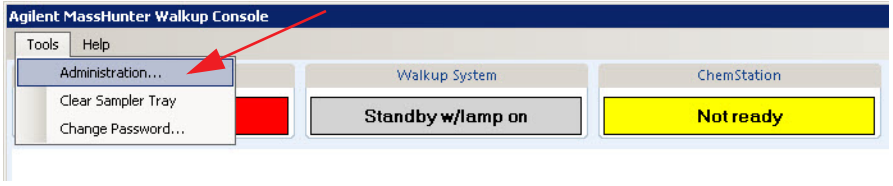
- Use the Walkup Administration tool to manually configure the system.
- Import configuration settings from another computer.
- Migrate configuration settings from Easy-Access installations.

After you configure the first workstation in your lab, you can export the configuration and import it to all of the other workstations in your lab.

To manually configure Walkup workstation

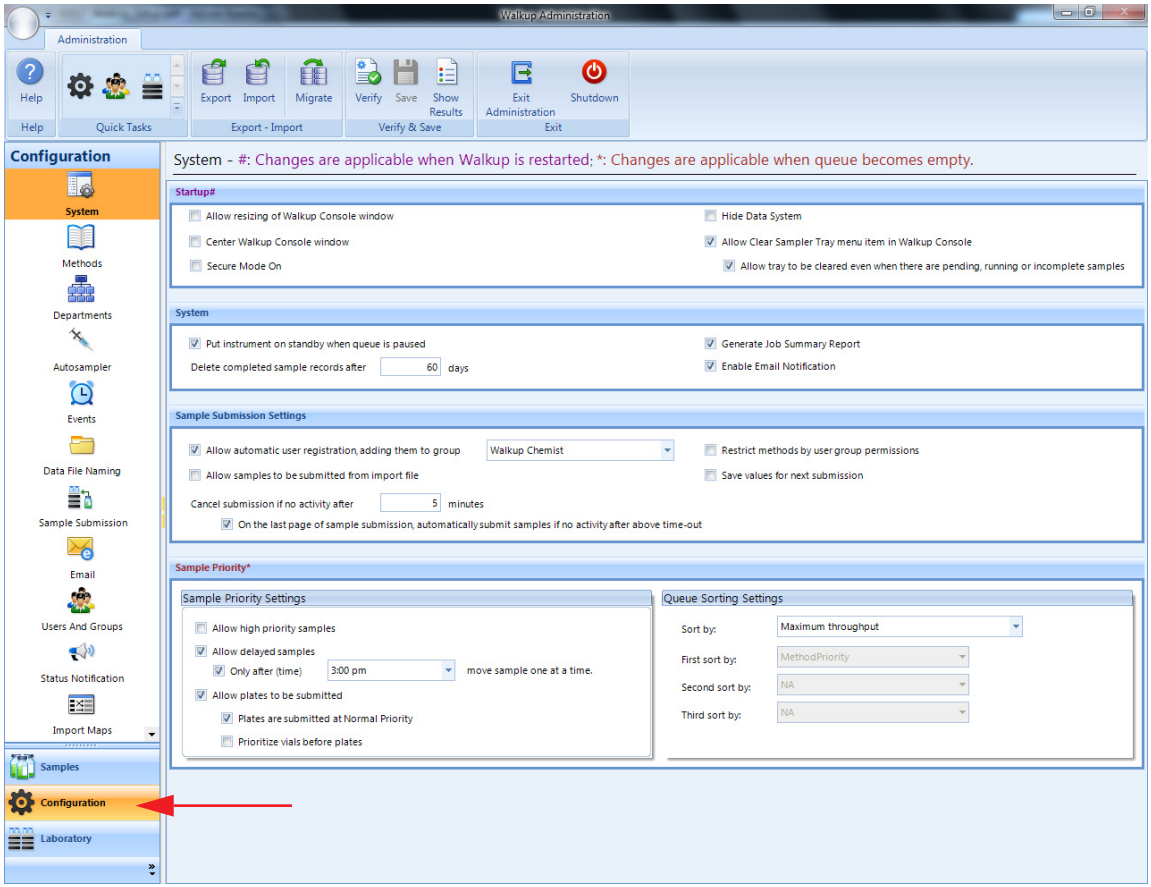
1 Open the Walkup Administration window:

a Click **Tools > Administration**.



b Enter the appropriate user name and password.

c When the Walkup Administration window appears, click the **Configuration** button in the lower left area of the screen (shown in the next figure).



2 From the left side of the screen, click **Events**, then under **Standby**, for **Idle Method**, select **WalkupStandby**.

3 Use the buttons on the left side of the screen to guide you through the remaining configuration tasks. For more information, refer to the online Help tasks under **Configure Walkup**.

4 When you are finished, verify and save the configuration. Refer to online Help if needed. In a networked system, the configuration is stored on the OpenLAB Shared Services server.

5 Click **Exit Administration** on the ribbon to close the Walkup Administration window and return to the MassHunter Walkup console.

6 To use the same configuration for another Walkup workstation, export the configuration. Refer to “To export a Walkup configuration” in the online Help.

To import configuration from another Walkup workstation

If you want to use the configuration from another Walkup workstation:

1 Export the configuration from the configured workstation. See “To export a Walkup configuration” in the online Help.

2 Import the configuration. See “To import a Walkup configuration” in the online Help.

To migrate settings from Easy-Access

If you installed Walkup on a system that was running Easy-Access, you can migrate the database and configuration settings from Easy-Access.

- To migrate Walkup configuration settings from Easy-Access, see “To migrate an Easy-Access configuration” in the online Help.

Step 5. Configure Analytical Studio Reviewer for Walkup

Analytical Studio Reviewer (ASR) lets you view, print, and export your data without having to purchase and run full analytical software on every desktop. To use Analytical Studio Reviewer, the ChemStation results file is converted to ASR format. With Walkup, ASR files can be emailed to users who can review the results on client computers where Analytical Studio Reviewer software is installed.

1. Start the ChemStation console.
2. Open a valid ChemStation method and data file.
3. Set up ASR File Export options in ChemStation:
   a. In **Data Analysis** view, click **ASR > ASR File Options**.
   b. Mark the **Generate ASR File** check box.
   c. Mark the **Automatically Print Single Sample Report** check box.
   d. Select **Print report after each run**.
   e. Click **OK**.

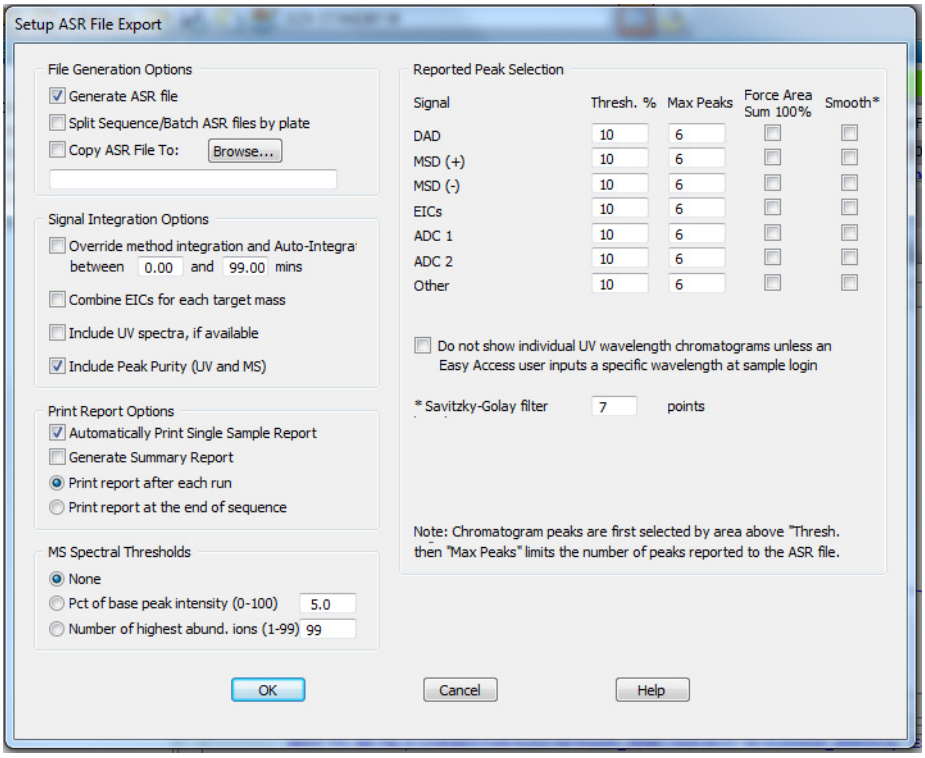


Figure 1 Setup ASR File Export dialog box

4 Set up Sample Purity Options:

- **a** In **Method & Run Control** view, click **Method > Sample Purity Options**.
- **b** Select the appropriate adducts.
- **c** Mark the **Enable purity calculations** check box.
- **d** Select **Use target mass from Easy-Access**.
- **e** Select signals for **Qualitative Calculations**.
- **f** Click **OK**.

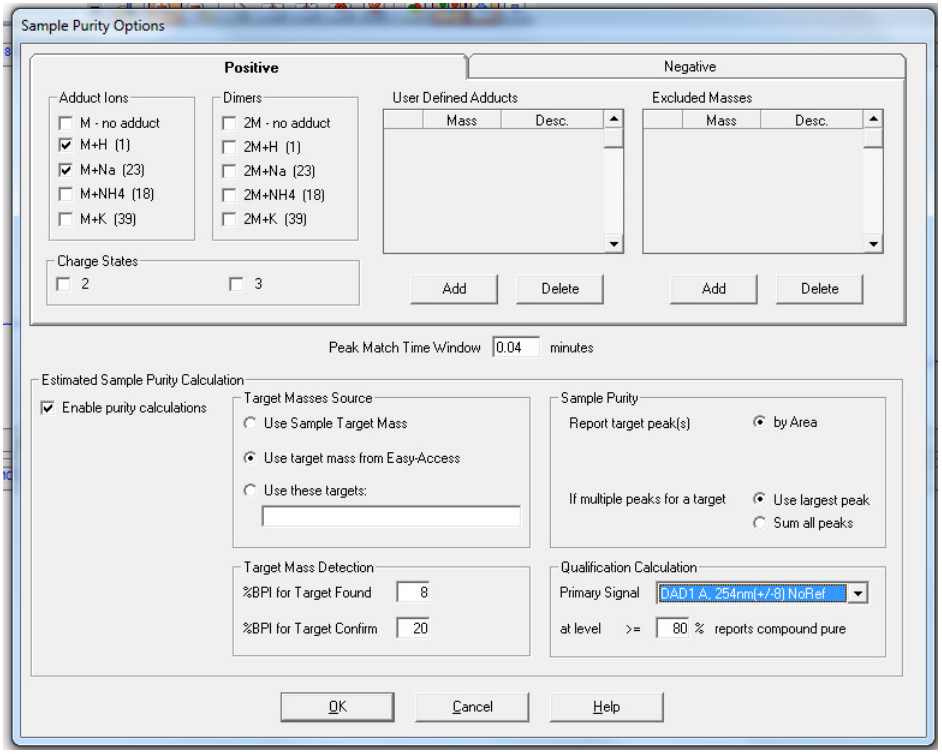


Figure 2 Sample Purity Options dialog box

5 Save the method with a new name, such as `Walkup_ASR1`.

6 Repeat step 2 through step 5 for each method that you want to use with Walkup and Analytical Studio Reviewer.

7 Set up Analytical Studio Reviewer options for Walkup:

   a Start MassHunter Analytical Studio Reviewer.

   b Click **Report > Setting > Single Sample Report**.

   c Mark the check box for **Adobe Acrobat**.

   d In the **General** tab, select **Save to specified directory**.

   e Click **Save**.

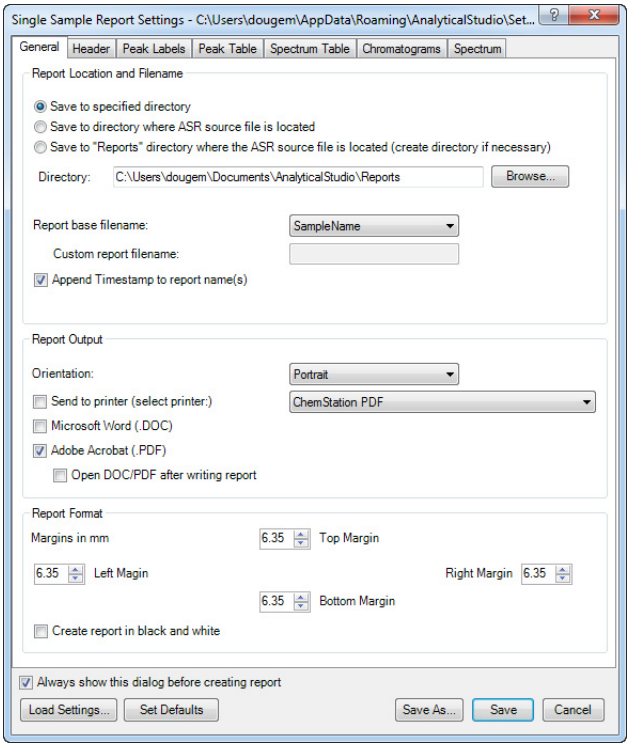


Figure 3 Single Sample Report Settings dialog box in Analytical Studio Reviewer.

8 Set up Walkup options for Analytical Studio Reviewer:

- **a** Start the Walkup Console.
- **b** Click **Tools > Administration**. Log in as an administrator.
- **c** In **Configuration** view, click **Methods**.
- **d** Click **<Add New Method>**. Give the new Walkup method a name and description.
- **e** Mark the check box for **Make available for sample submission**.
- **f** For **Data System Method**, select a method that you just created, such as `C:\Chem32\1\METHODS\WALKUP_ASR1.M`.
- **g** Repeat step 8 for every method that you created for use with Analytical Studio Reviewer and Walkup.

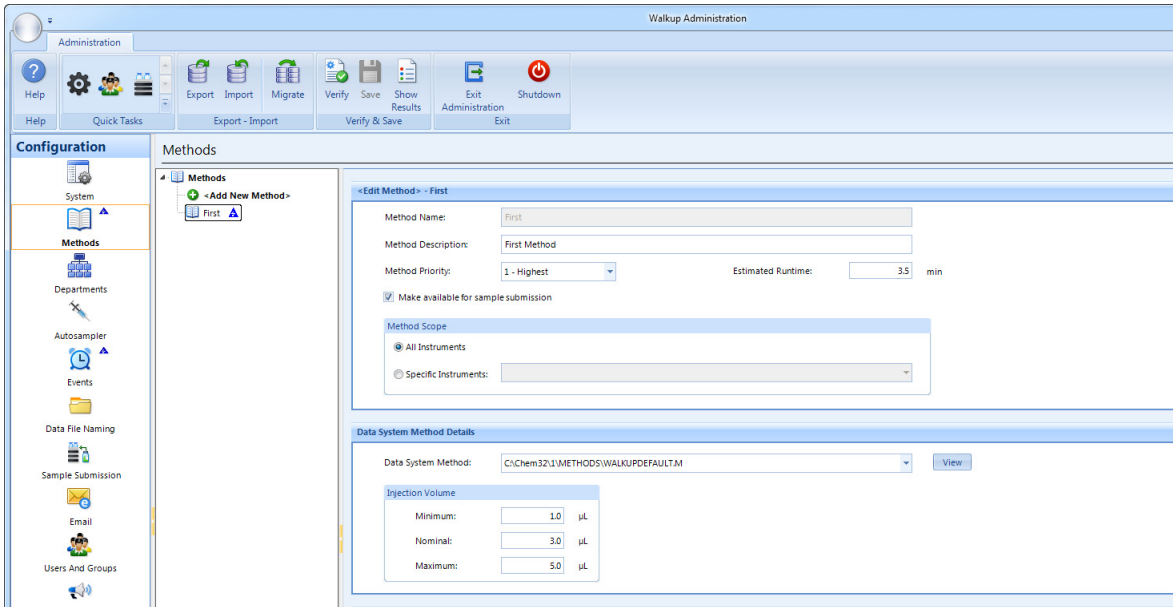


Figure 4 Methods pane in Walkup

h In **the** Navigation Pane, click **Email**.

i In the **Content** group, mark the check boxes for **ASR Report** and **Custom**.

j Type `PDF` as the custom file type.

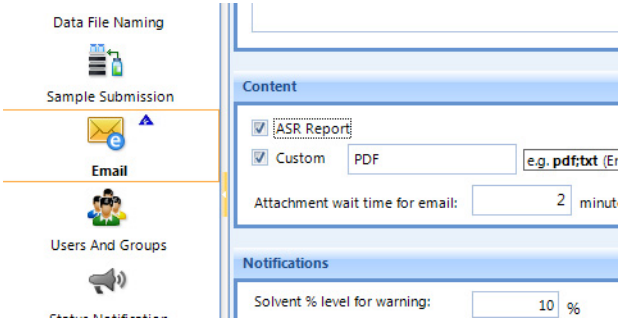


Figure 5 Email options in Walkup.

k In **the** Navigation Pane, click **Users And Groups**.

l For each group that is to receive ASR reports, select the group name, and then make sure that the **Email report** check box is marked.

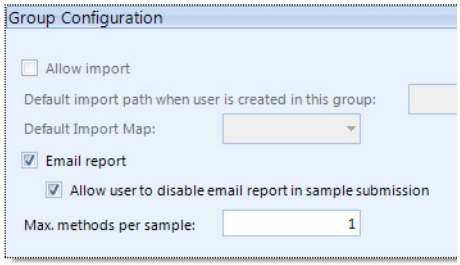
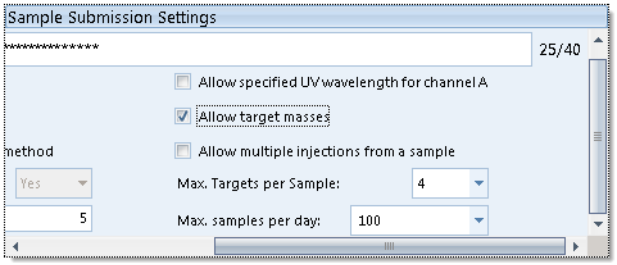


Figure 6 Group Configuration options in Users And Groups view

m For each group in which you want to let users enter target masses, select the group name, and then make sure that the **Allow target masses** check box is marked.



n In the toolbar, click **Verify** and then click **Save**.

The Save button is not enabled until configuration errors are resolved.

o Click **Exit Administration**.

9 Run a few samples in the Walkup program. In the Sample List screen, make sure you specify a **Target Mass** or **Molecular Formula**.

10 Verify that the samples are successfully completed.

11 Open the completed sample data file in MassHunter Analytical Studio Reviewer.

12 Verify that the Target column appears with data for target sample.

Step 6. Install other tools and programs on office computers

You can install these tools and programs on other computers to help you remotely manage data and Walkup workstations in your laboratory network.

These programs are installed on computers other than Walkup workstations and OpenLAB Shared Services servers.

Remote Administration software (networked labs only)

The Remote Administration software lets you manage your lab from anywhere on the network.

1 Make sure that OpenLAB is installed in Network Client mode and verified. Refer to the *Agilent OpenLAB Chromatography Data System (CDS) Networked Workstation Installation Guide (p/n M8203-90002)*.

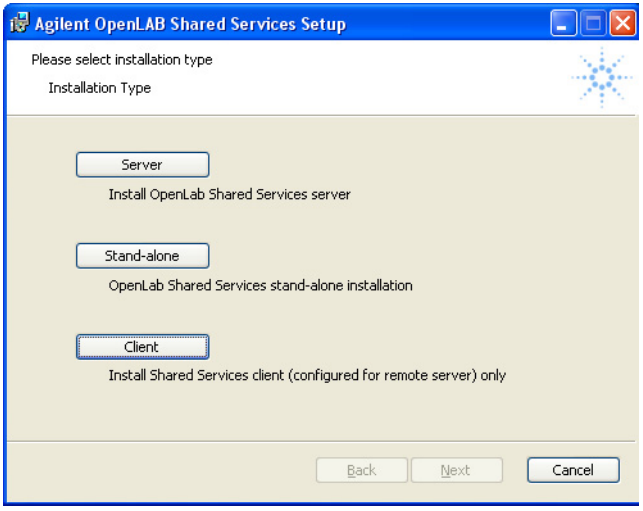
   a Insert Disk1 of the OpenLAB installation software media into the disc drive.

   b In File Explorer, locate the **OLSS** folder.

   c Double-click **OpenLabSharedServices.msi**.

   d Agree to the licensing agreement.

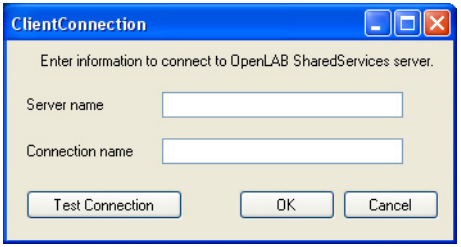
   The Installation Type screen is displayed.



e Click **Client**.

f In the ClientConnection dialog box, for both the **Connection name** and the **Server name**, type the name of the OpenLab Shared Service computer.

g Click **OK**.



h When the installation completes, the OpenLAB Control Panel icon is placed on the desktop.

2 Install the Walkup Remote Administration:

a Insert the Walkup installation disc into your disc drive.

b Under **Any Other Computer**, click **Install**.

c Click **Run** in the File Download message box.

Do not save the installation program to your computer before you run it. The installation program will not run properly if you do.

d Follow the prompts to install the Remote Administration program.

Unpack Utility

Install the Walkup Unpack Utility on all computers that will receive HTML reports in .zne format from Walkup workstations.

You can configure Walkup software to send sample results to users by email. The results are compressed into a .zne file.

1. Insert the Walkup installation disc into the disc drive.
2. Under **Additional Software**, click **Install**.
3. Follow the prompts to install the Unpack Utility.

Analytical Studio Reviewer

Analytical Studio Reviewer lets you view ASR reports remotely. Additional license may be required.

- Refer to the Analytical Studio Reviewer *Quick Start Guide* to install Analytical Studio Reviewer.

Startup

To start the Walkup program

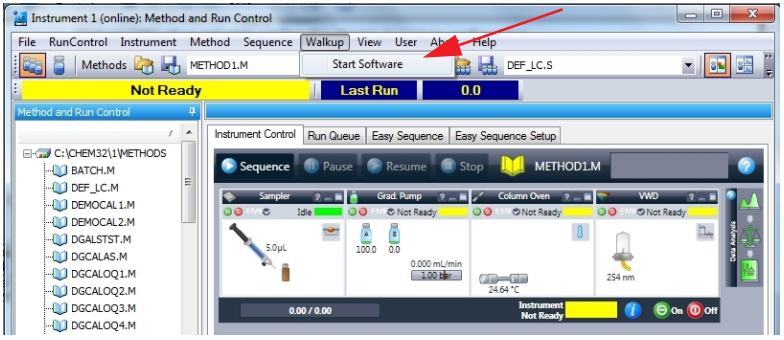
Do the following procedure from a Windows account with administrator rights.

1 Start the Online ChemStation Console.

Click the ChemStation icon for online analysis if a shortcut was created. As an alternative, in the OpenLAB Control Lab **Start Instrument** panel, click the **Launch** button for the instrument that you will use with Walkup.

2 Start the Walkup program:

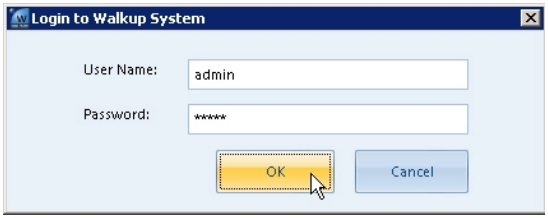
a In ChemStation console, click **Walkup > Start Software**.



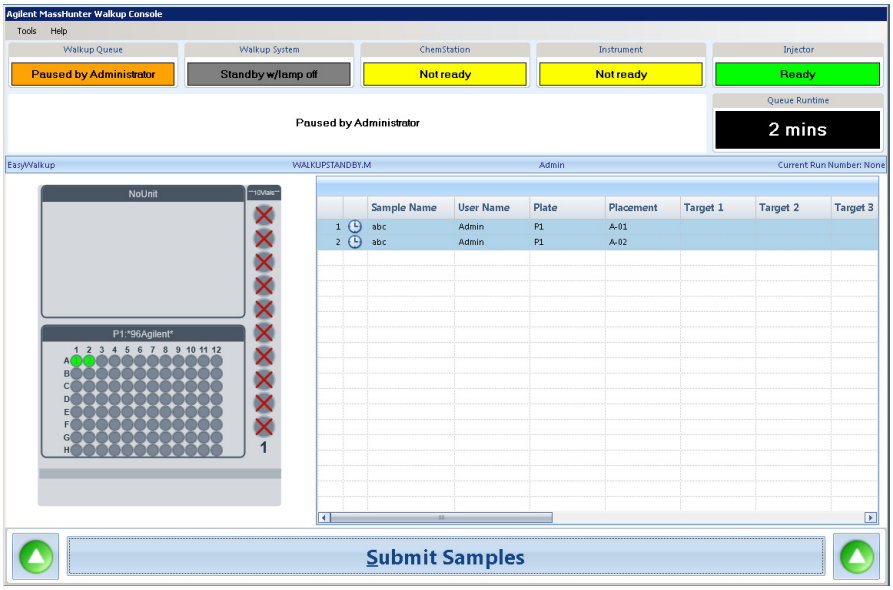
3 If the **Login to Walkup System** dialog box appears:

a Enter the user name and password for a valid administrator on the OpenLAB workstation.

b Click **OK**.



The MassHunter Walkup Console appears.



Walkup users will click the **Submit Samples** button at the bottom of the MassHunter Walkup Console to begin the sample submission process. The options that are displayed on the sample submission screens can be configured. Refer to online Help for more information.

To shut down the Walkup program

1 Open the Walkup configuration pane.
   - See "To open the Configuration pane" on page 28.

2 Click the **Shutdown** icon on the ribbon at the top of the window:

If you shut down the Walkup program while samples are running:

- The current sample run does not complete.
- The Sample Queue stops.
- Pending samples resume when Walkup starts again.
- An email is sent to notify that the sample run failed.

Samples

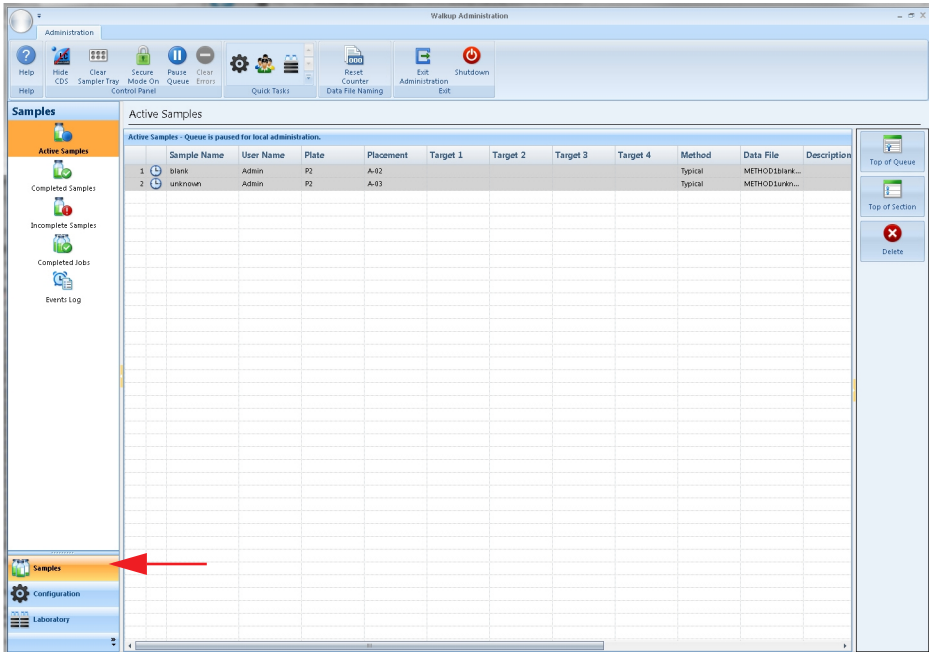
The Samples view lets you see and manage information for the following types of samples:

- **Active Samples** (shown in the example screen below)
- **Completed Samples**
- **Incomplete Samples**

You can also view a list of **Completed Jobs** and the **Events Log** and manage the Sample Queue.

To open the Samples view

1. Click **Tools > Administration** on the MassHunter Walkup window.
2. After you enter your **User Name** and **Password** on the **Login to Walkup Administration** dialog box, the Walkup Administration window appears.
3. Click the **Samples** button in the lower left corner of the window.



To learn how to manage samples

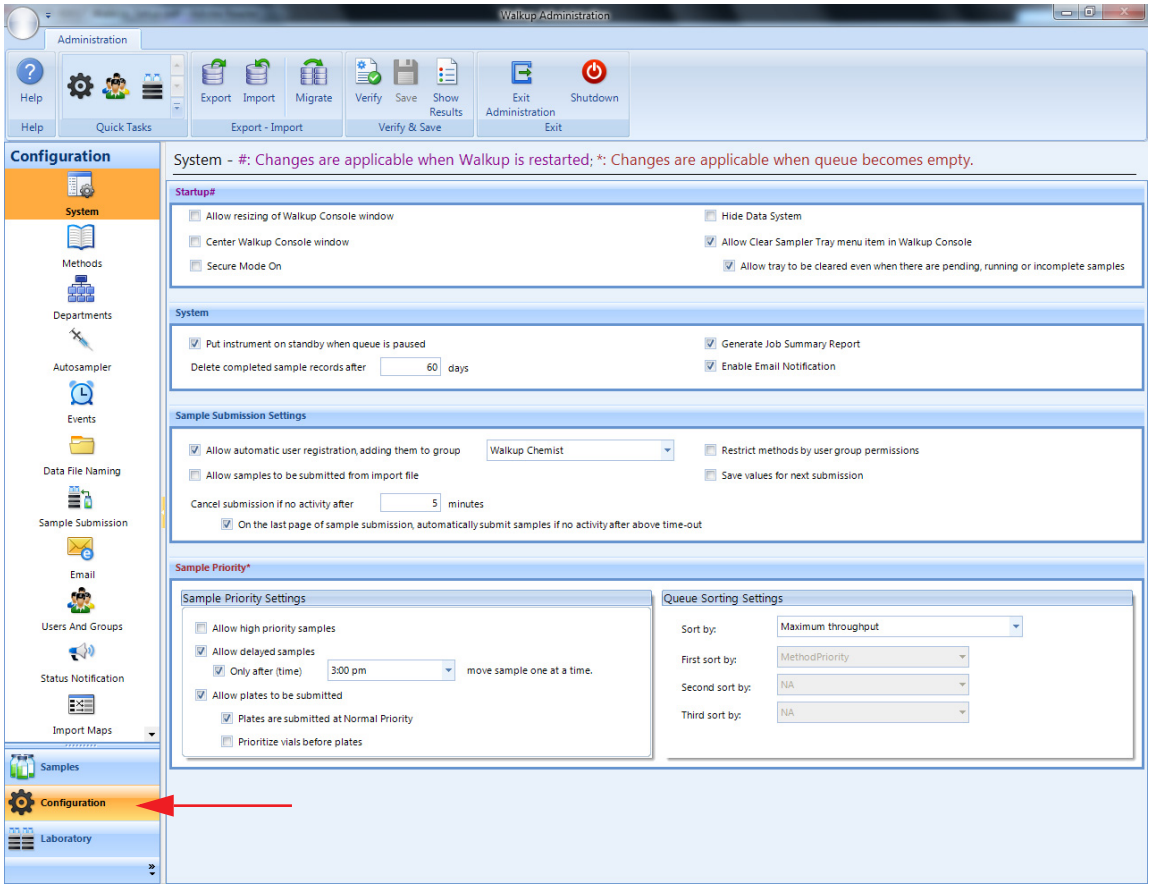
- In the Walkup online Help, refer to the tasks under **Manage Samples**.

System Administration and Configuration

The Configuration pane of the Walkup Administration window lets you set many parameters to customize the appearance and operation of the Walkup System.

To open the Configuration pane

1. Click **Tools > Administration** on the MassHunter Walkup window.
2. Enter your **User Name** and **Password** on the **Login to Walkup Administration** dialog box.
3. When the Walkup Administration window appears, click **Configuration** in the lower left corner of the window to display the Configuration pane.



4 Use the icons in the navigation pane on the left side of the window to view different configuration parameters described in online Help.

5 When you have finished setting all the configuration parameters, verify and save the configuration. Refer to online Help if needed.

To learn how to configure the system

- In the online Help, refer to the tasks under **Configure Walkup**.

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In this Book

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

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