



MassHunter Workstation 11.0

## Administration Guide

# Notices

## Document Identification

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## Software Revision

This guide is valid for the 11.0 revision of MassHunter Data Acquisition for Agilent LC/TOF and LC/Q-TOF and compatible MassHunter Workstation programs, until superseded.

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# In This Book

This book provides instructions and reference material to configure and maintain your MassHunter Workstation.

MassHunter can be used in one of two configurations: Workstation or Networked Workstation.

The Networked Workstation requires an OpenLab Server/ECM XT server. For more details on server administration tasks, refer to the OpenLab Server/ECM XT server *Administration Guide*.

## **1 Licensing**

This chapter describes how to obtain and install a MassHunter Workstation license.

## **2 System Administration**

This chapter contains administration and troubleshooting tasks for your MassHunter Workstation.

## **3 Regulated Laboratory Features**

This reference chapter describes the technical control features and how they support compliance.

## Where to find more information



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## Licensing

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This chapter describes how to obtain and install a MassHunter Workstation license.

## Getting and Installing the License

You have two options to get a license:

- From SubscribeNet
- Offline (from an Agilent representative)

Before you begin, make sure you have:

- The authorization code label provided in the lavender envelope containing your Software Entitlement Certificate.

If you have not received a lavender envelope for your product, contact your vendor or internal support.

- The URL for SubscribeNet from the Software Entitlement Certificate.
- The host name of the computer where OpenLab Control Panel is running.
- The MAC address.

To retrieve your MAC address from a computer where MassHunter Workstation is already installed, refer to the MassHunter Help & Learning.

During this process you need to provide the MAC address of your license server. For MassHunter Workstation, this is the standalone computer. For Networked Workstation, this is the content management server.

### NOTE

If any changes are made to the computer name or domain reference after the license is installed, remove the license. A new license will need to be created in SubscribeNet, downloaded, and installed.

### NOTE

If the network adapter that provides the MAC address used during license creation is removed from the machine, your license will no longer be valid. A new license will need to be generated with a currently available MAC on the license server.

## To get a license from SubscribeNet

You will need an Internet connection to access SubscribeNet. If you do not have one, go to **“To get a license offline”** on page 11.

- 1 If you are new to SubscribeNet:
  - a Go to <https://agilent.subscribenet.com/control/agil/AgilRegisterToAccount> to register the product with SubscribeNet.
  - b On the registration page, enter the authorization code from the label and complete the profile information (required fields are marked with an asterisk \*).

The email address you enter will become your login ID.
  - c Click **Submit**. The system will generate and display an account name for you. SubscribeNet will send a welcome email with your login ID and password.
- 2 Go to <https://agilent.subscribenet.com/>.
- 3 Log in to SubscribeNet using your login ID and password.

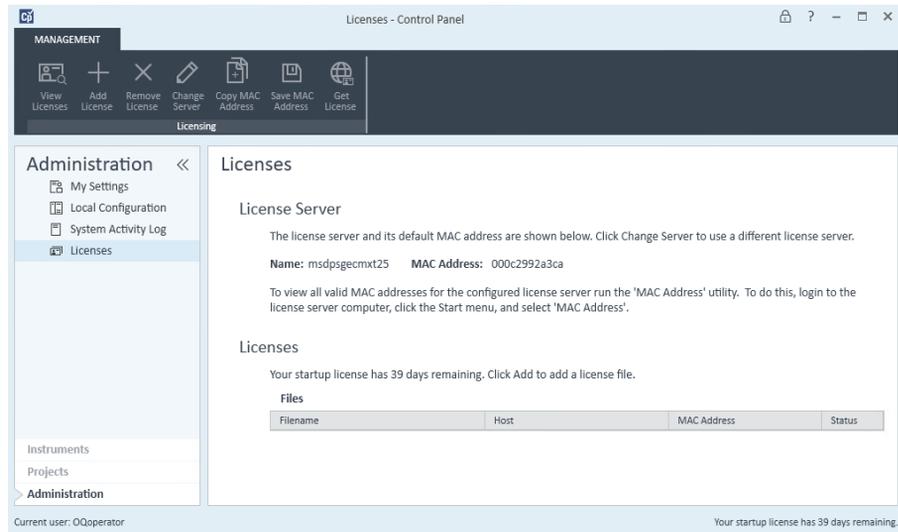
Once you log in, you can use the user manual link for help with any questions you have.
- 4 If you are an existing SubscribeNet user:
  - a If you have more than one account, select the SubscribeNet account associated with this authorization code.
  - b In the navigation pane, select **Register Authorization Code**.

This will allow you to enter your new authorization code and make available the new license entitlements.
- 5 In the navigation bar on the left side of the page, select **Generate or View licenses**.
- 6 Follow the prompts to generate your new license.

## Licensing

### To get a license from SubscribeNet

You will be prompted for the HOST NAME of the computer. The host name you enter must match with the network name of the computer where OpenLab Control Panel is running. Do not include any DNS suffix (domain.com) references in the entered machine name.



- When the system generated the license, view its details, and then click **Download License File**. Save the license file to your computer and to a backup location (such as a portable storage device).

Use your login ID and password when you revisit the Agilent SubscribeNet site to regenerate a license file, add new authorization codes, or further configure the license for your system.

Refer to the *MassHunter Help & Learning* to learn how to add a license to your workstation.

## To get a license offline

If you are unable to generate a license, contact Agilent technical support. Agilent collects the necessary information from you to create a license account on your behalf. See **“Sales and Support Assistance”** on page 2 for contact information.

### 1 Collect profile information:

Your account name will be your company name and lab name separated by a comma. Employee information provided here will be used to define the first administrator of your account for future access to the system as required.

- Company Name
- Lab/Department Name
- First Name
- Last Name
- E-mail address
- Job
- Title
- Phone number
- Address, City, State/Province, Postal Code, Country

### 2 Collect Authorization Code(s).

The authorization code is an alpha-numeric code provided on a label which is enclosed in a lavender envelope. If you received more than one code, provide all codes to ensure that all ordered licenses are granted to your account.

### 3 Contact your Agilent representative and provide the collected information for Agilent to generate a license through SubscribeNet.

Once the license file is generated, it will either be sent to your shipping address, or your local Field Service Engineer will deliver it in person.

Refer to the *MassHunter Help & Learning* to learn how to add a license to your workstation.

## About MassHunter Workstation Licensing

### **Software subscriptions and Software Maintenance Agreement (SMA)**

Bundled into MassHunter Workstation is a one-year software subscription which provides access via SubscribeNet to new software updates, product upgrades, familiarization and media.

Renew subscriptions annually so as to maintain licenses and have full access to the newest updates, upgrades, media and familiarization. To manage software entitlements and download software, log in to SubscribeNet by going to <http://agilent.subscribenet.com/>.

Software subscriptions do not include installation services. Installation or upgrade services must be purchased by contacting your sales representative in your region.

### **License Types**

In Workstation configuration, a MassHunter license is good for all users, but only one user can run MassHunter Workstation at a time.

In Networked Workstation configuration, MassHunter uses floating user licenses. Licenses are not permanently assigned to any one user. Instead they are automatically assigned to users as they log on. The licenses are automatically returned when the user logs off. The license management program controls license issuance and retrieval.

A startup license allows you to run a MassHunter program for 60 days after the installation. In order to run the MassHunter after the 60-day period, you must install your license file.

## License File

A license file contains your software license.

In Workstation configuration, this file is installed on the workstation. The license file is bound to this computer, and cannot be moved to another workstation without regenerating the license in SubscribeNet.

In Networked Workstation configuration, this file is installed on the OpenLab Server/ECM XT server.

Information in the license file defines the number of users that can concurrently run the MassHunter program.

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This chapter contains administration and troubleshooting tasks for your MassHunter Workstation.

## Administration

MassHunter Workstation administration is done through the OpenLab Control Panel. The Control Panel ribbon changes depending on the objects that are selected in the navigation pane, the MassHunter programs that are installed, and the instrument that is configured.

For more information on the buttons of the Control Panel, refer to the *MassHunter Help & Learning*.

The tasks in this section are not covered in the *Help & Learning* or are done outside of Control Panel.

### To open OpenLab Control Panel

- 1 From the desktop, double-click the **Control Panel** icon.



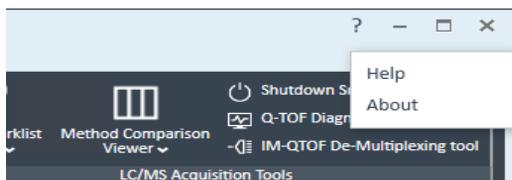
The Control Panel is the administrative and management center of MassHunter, offering:

- In Networked Workstation configuration:
  - Full instrument status information of your entire laboratory
  - Central configuration and administration of users, instruments, and security settings
- Full system documentation and built-in reports

### To open the Help & Learning

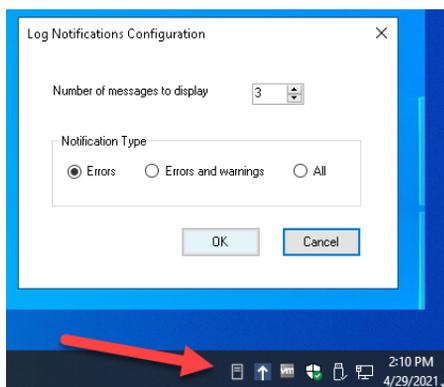
The Help & Learning contains instructions to manage your MassHunter workstation.

- To get context-sensitive help, press **F1**.
- To open the main Help & Learning, click **?** in the upper right corner of OpenLab Control Panel, and then click **Help**.



### To configure log notifications

- 1 Click the notification button in the system tray. This button is available only if MassHunter Data Acquisition is installed.
- 2 Select the number of notification to receive.
- 3 Select **Errors**.
- 4 Click **OK**.

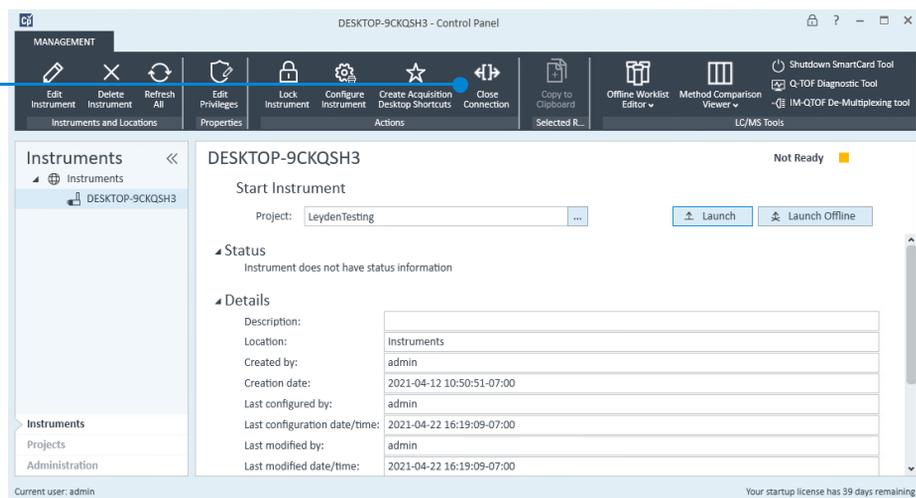


## To stop MassHunter Engines

MassHunter engines are started when an instrument is launched. MassHunter engines are stopped in one of two ways.

- In OpenLab Control Panel, on the ribbon, click **Close Connection**, or
- Log off the computer.

Close Connection  
button



## To configure the network interface card

The computer that is shipped with your instrument is equipped with two network cards (LAN-cards). The first LAN-card is for connection to the “house network” (via 10/100/1000 Base-T network card). The IP address for this card can either be “static” or dynamically assigned (e.g. obtained by a DHCP server). By default, TCP/IP is configured as the network protocol for this card, which is built-in to the PC.

The second LAN card (in slot #1) is dedicated for instrument communication with the mass spectrometer and the InfinityLab Series LC system. *This network card should NOT be connected to the site LAN.*

To verify that the Instrument LAN network card settings are correct, follow these steps.

- 1 Click **Start > Settings > Control Panel**.
- 2 Double-click **Network Connections**.
- 3 Right-click the icon for the network card for the house LAN, click **Properties**, and then configure the network card as needed.

Because this network card is independent from the card used for instrument control, it may be configured using a static IP address or using a DHCP server.

- 4 Right-click the icon for the network card for the mass spectrometer, click **Properties**, and then check that these parameters are set:
  - IP Address (Default): 192.168.254.1
  - Subnet Mask 255.255.255.0
  - Gateway - leave blank

### NOTE

Because network configurations vary widely from site to site, get assistance from an IT representative when you connect to the site network. Configuration by an Agilent Field Service Engineer is on a best-effort basis only.

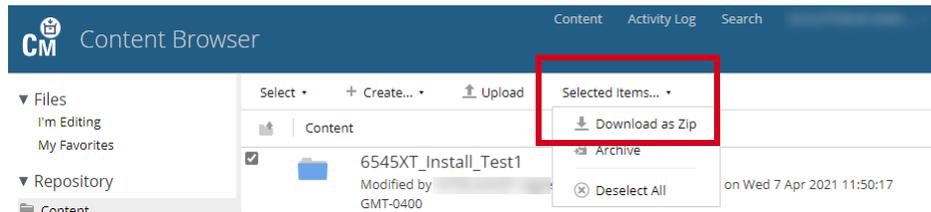
## To retrieve data from the content management server

You can retrieve data from the content management server onto your local computer and run it in Qualitative Analysis, but the data will be considered to be uncontrolled.

- 1 From the Networked Workstation, open a browser and connect to the Content Browser on the OpenLab Server/ECM XT server.

Use the URL of the server to connect to the server. The Content Browser page is displayed.

- 2 Find and select the data files that you want to retrieve.
- 3 Click **Selected Items > Download as Zip**.



- 4 Unzip the file to the appropriate local folder, such as **D:\MassHunter\Data** or one of its subfolders.
- 5 Open the data file in Qualitative Analysis and use as you would any uncontrolled MassHunter data.

## To import Quantitative Analysis report templates

Quantitative Analysis report templates must be imported to the MassHunter project before you can generate Quant reports.

### Workstation configuration

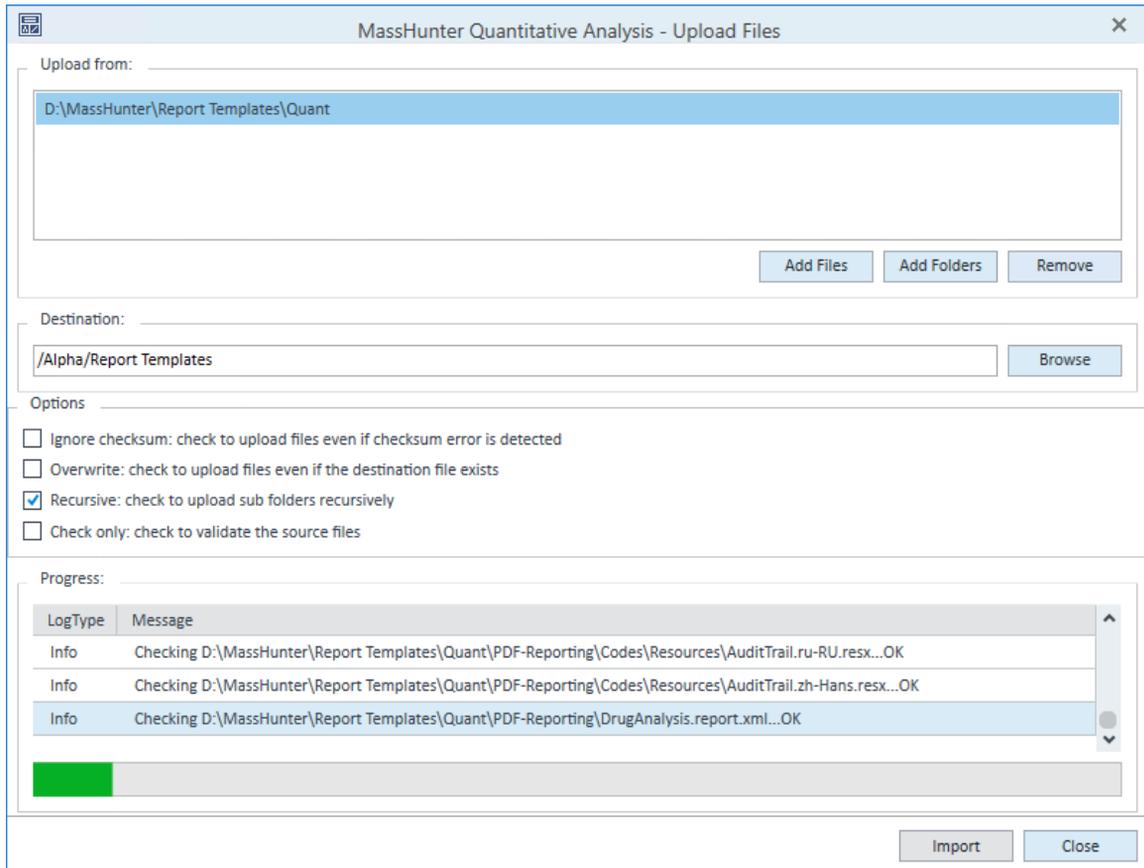
- 1 Open File Explorer.
- 2 Copy the contents of the folder **D:\MassHunter\Report Templates\Quant** into the folder **D:\Projects\projectname\Report Templates**. Make sure to copy all subfolders.

### Networked Workstation configuration

- 1 In **File Manager**, open **C:\Program Files\Agilent\MassHunter\Workstation\Quant\bin\QuantFileUploader.UI.exe**.
- 2 When prompted, log into the server as a user who has the privilege to upload Quant report templates, and has permission to modify the content of the project.
- 3 Select the destination project for the report templates.



- 4 For **Upload from**, select the report templates folder. This folder exists on the Networked Workstation only if MassHunter Quantitative Analysis is installed.



- 5 For **Destination**, create a new folder in the Project folder for the report templates, such as **Report Templates**.
- 6 Select **Recursive: check to upload sub folders recursively**.
- 7 Click **Import** to begin the import.

## To import acquisition data, methods, and worklists into a project

Do these steps to import acquisition data, methods, and worklists into MassHunter in either Workstation or Networked Workstation configuration. For MassHunter programs other than Data Acquisition, to import objects that are specific to that program, use the import tool that is included with that MassHunter program.

- 1 Under **Projects**, select a project.
- 2 On the ribbon, click **Import Files > Launch Application**.
- 3 Specify the **File type**, **Source Folder**, and **Destination project location**.
- 4 Click **Import**.

## To remove the MassHunter Workstation software

- 1 If you have any data, methods, libraries, or other files or directories that you want to save, move or copy them to a folder outside of those to be deleted.
- 2 Close all MassHunter Workstation programs, including the Data Acquisition, Qualitative Analysis, BioConfirm, Quantitative Analysis, and Report Builder programs.
- 3 Click **Start > Control Panel > Programs and Features**.
- 4 Remove programs in which the name starts with **Agilent MassHunter Workstation**
- 5 Close *all* applications.
- 6 Reboot the computer. You are now ready to install new software.

## Troubleshooting

### If the system hangs when you start MassHunter Data Acquisition

When MassHunter Data Acquisition starts, it waits up to five minutes for all the physical instruments to respond.

- ✓ Wait for the timeout period to end to see entries in the logbook. Check for an entry that indicates that an instrument is turned off. The device could be turned off for a number of reasons:
  - Incorrect bootp setup.
  - Incorrect LAN connection.
  - Instrument not powered up or defective.
  - Some other program is using the instrument. An example is the LC Firmware Update Tool. This can also happen if the instrument is on a network with multiple PCs.
- ✓ Check that all LC modules have the same or correct version of firmware.
- ✓ Open a command window. At the DOS prompt, type `ping 192.168.254.12` to test the communication with the mass spectrometer.

To test the communication with the LC, type `ping 192.168.254.11`.

If you see lines that begin with **Reply from *ip\_address***, then the computer is communicating with the instrument.

## If you are unable to log into the system when the lock screen is activated

In Authentication mode, application(s) cannot be unlocked when OLSS server, domain controller, or the ECM XT server is not reachable.

- ✓ Check that the computer is communicating with the domain server.
- ✓ Reboot the computer to reset all communications.

### NOTE

If any runs are in progress, the data for the currently running sample will be lost.

## If the log file says that no communication with the instrument exists

- ✓ This problem could be similar to those in **“If the system hangs when you start MassHunter Data Acquisition”** on page 24. Use the same steps to try to troubleshoot the problem.
- ✓ Select the communication error entry in the logbook and press **F1** on the keyboard. Search on the error message, follow the list of possible causes for this condition, and correct as needed. If this fails, repeat the instrument configuration steps for the instrument.

## If the MassHunter Workstation reports “Method Pane Initialization Failure”

- ✓ One or more instrument modules cannot be accessed.
  - 1 Shut down the MassHunter Workstation user interface and stop the MassHunter engines. (See **“To stop MassHunter Engines”** on page 18.)
  - 2 Turn the HPLC modules off, and then on.
  - 3 Press the reset button on the instrument.
  - 4 Wait for at least two minutes or until you hear the solvent selection valve change position twice.
  - 5 Restart the MassHunter Data Acquisition program.



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This reference chapter describes the technical control features and how they support compliance.

## 21 CFR Part 11 Compliance

MassHunter 11.0 provides technical controls to fulfill the FDA rules and guidelines for compliant electronic records and computerized systems.

The basic aspects of secure data handling are described here.

- **Data security:** physical protection of data by limiting access to the system and preventing unauthorized access.
- **Data integrity:** protecting raw data and metadata and preventing these from unauthorized modification, and linking raw data and results to reproduce the original results at any time, for example, in an audit situation, and document each new result copy.
- **Audit traceability:** documenting who did what to the results and when, and tracing the user adding new reanalyzed versions to the original raw data.

## Data Security

The data security functionality includes the following (see **“Control Panel Overview”** on page 70 for details):

- System Activity Log
- Selection of authentication provider
- Management of users, groups, roles, and privileges
- Security Policy

Data Security is available for Workstation (when Authentication Mode is turned on) and Networked Workstation.

### CAUTION

#### Data integrity risk

**Customers subject to regulations from US FDA or similar organizations are cautioned that FTP services are enabled by default. This may be considered as a data integrity risk.**

- **Impacted customers are advised to disable or block FTP services when not needed. Please refer to the section on FTP administration in the OpenLab Server Administration Guide.**

## Data Integrity

The Content Management component of OpenLab Server/ECM XT stores data in a manner that ensures compliance with 21 CFR Part 11. It provides secure data storage with access control and an audit trail. Data files are versioned to ensure data integrity and traceability. In addition, OpenLab Server/ECM XT provide electronic signatures, which allows users to sign off on data.

OpenLab Server/ECM XT is available for use with Networked Workstations only.

## Audit traceability

Different types of audit trails are provided, depending on the MassHunter programs that are installed. The specific behavior of an audit trail depends on the project settings in the OpenLab Control Panel. Refer to the *MassHunter Help & Learning* for more details.

Audit traceability is available for Workstation (when Authentication Mode is turned on) and Networked Workstation.

## Networked Workstations

MassHunter Workstation can be configured as either a standalone Workstation or a Networked Workstation. Networked Workstations require an OpenLab Server or ECM XT product on a separate server.

### OpenLab Server/ECM XT Products

OpenLab Server/ECM XT software products provide secure file storage for scientific data. These products are installed on a separate network server.

- **OpenLab Server** supports the storage of data acquired, analyzed, and processed by Agilent data systems, such as MassHunter and OpenLab CDS.
- **OpenLab ECM XT** extends the storage scope to support data generated by third party data systems, office files and any other type of file.

OpenLab Server/ECM XT software is comprised of two core components, Content Management and Shared Services.

- **Content Management** software component includes functions to store and manage files. Content Management's interface for accessing the stored files is called Content Browser.
- **Shared Services** software component includes functions to manage users, roles, and privileges. The interface for managing users, roles, and privileges is called OpenLab Control Panel.

## Compatibility

With the exception of data collected from these instruments:

- Agilent 6560 IM-QTOF LC/MS
- Agilent 1290 Infinity II 2D-LC System

Content Management is compatible with these MassHunter programs:

- MassHunter Data Acquisition for LC/TOF and LC/Q-TOF
- MassHunter BioConfirm
- MassHunter Quantitative Analysis

MassHunter data stored in the Content Management component can be used in other MassHunter programs, including MassHunter Qualitative Analysis. To do so, MassHunter data must be retrieved from the Content Management component onto your local computer. Note that the data will be considered to be uncontrolled. See **“To retrieve data from the content management server”** on page 20.

## Retrieve versus Checkout (Content Management)

When users log into the Content Browser directly from a web browser, they may, depending on their privilege, be able to retrieve or checkout a file.

- Retrieved files are not locked in the Content Management component.  
The file in the Content Management component is still available to anyone else.
- Checked out files are locked in Content Management.  
Only the individual who checked out the file can check the file back in to content manager, or undo the Checkout. However, with appropriate permissions, users can retrieve a copy of a checked out file.

Any file that is checked out of the Content Management component remains unavailable to MassHunter until it is checked back in or the checkout is canceled.

Batches that are opened in Quantitative Analysis or an Analysis in Unknowns Analysis are automatically checked out by default.

## Networked Workstation versus Workstation

This topic lists the differences between a Networked Workstation and a standard MassHunter Workstation.

### Login

On a Networked Workstation, the login dialog box lets you select the Content Management server to which to connect.

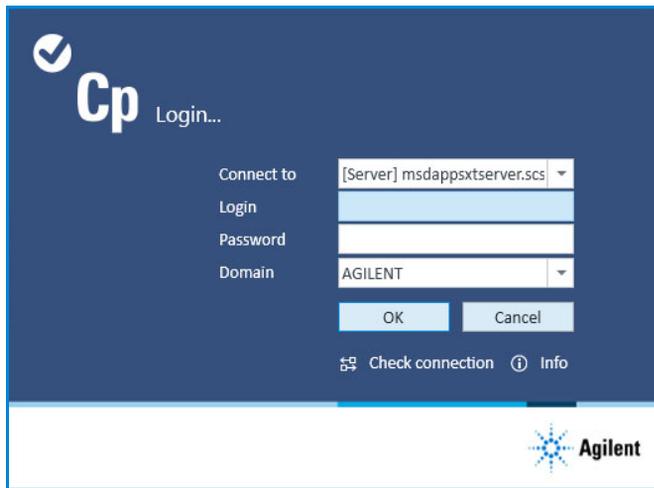


Figure 1. Networked Workstation Login

### User Access

On a Networked Workstation, user access to MassHunter commands and functions are controlled on the server. Users (and Groups) are assigned to Roles on the server. Privileges can be assigned to Roles on either the MassHunter Workstation or the Content Management server. See [“Users/Groups/Roles/Privileges”](#) on page 35 for more details.

### Paths

On a Networked Workstation, files that are stored on the Content Management server are indicated by a four-level path in the format **\\Location\Cabinet\Drawer\Folder**, and not by the standard Windows folder path. Files can be stored only at the *Folder* level.

#### Worklists and methods

For both the Workstation and Networked Workstation:

- Worklists and methods cannot be edited during data acquisition. Worklists must be paused, edited, and then saved to continue running.
- To run a single sample run, the Acquisition method must first be saved.
- To run a Worklist, the Worklist must first be saved.

#### MassHunter Qualitative Analysis support

MassHunter Qualitative Analysis is not supported in Content Management, so in a Networked MassHunter system, the Qual tab is not visible in the Data Acquisition program. You can still retrieve data from Content Management onto your local computer and run it in Qualitative Analysis, but the data will be considered to be uncontrolled. See [“To retrieve data from the content management server”](#) on page 20.

#### MassHunter Quantitative Analysis and BioConfirm support

MassHunter Quantitative Analysis and BioConfirm are supported in the Content Management component. In a Networked Workstation system, Quantitative Analysis methods, report templates, and report methods are stored in the Content Management component.

#### Method Development Tools

Source Optimizer and MRM Optimizer can be used to develop methods locally. In a Networked Workstation system, these methods can be imported into Content Management. Refer to the *MassHunter Help & Learning* for more information on importing methods.

#### Log books

In a Networked Workstation system, log books are archived on the content management server. You can only change or view log book settings if you have the appropriate permission.

## Authentication Mode

### Users/Groups/Roles/Privileges

In Authentication mode, access to MassHunter data and commands is controlled by how Users, Groups, Roles, and Privileges are set up. Access can also be set up for an individual instrument to overwrite access that is set up on the content management server.

Authentication mode is available for both Workstation and Networked Workstations.

On Networked Workstations, Users and Roles are assigned to Groups on the Content Management server. On Workstations, they are managed locally.

**Table 1 Authentication terms**

Term	Description
User	Each person who needs to run MassHunter software or access MassHunter objects (data, methods, worklists, sequences, and tune files) needs an individual User account. Users can be managed by your organization's Windows domain function, or added to the content management server in the BUILT-IN domain.
Groups	Similar Users can be organized into Groups. You can use Groups to control and change access and audit requirements to an entire group of Users at once. The use of Groups is optional. You can assign Roles directly to Users.
Privileges	Privileges determine the tasks that Users are allowed to do in the MassHunter or content management server programs.
Roles	Roles are used to link Privileges to Users. You can assign Roles to Users or Groups. Each Role determines what the Users in that Role can do (Privileges).

Refer to the *MassHunter Help & Learning* for a description of default MassHunter roles and privileges.

## In This Book

This book provides instructions and reference material to configure and maintain your MassHunter Workstation.

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