MassHunter Quantitative Analysis Compliance Software

Quick Start Guide

This guide contains information to install and use the MassHunter Quantitative Analysis Compliance Software.

What is MassHunter Quantitative Analysis Compliance Software?

21 CFR Part 11 is a result of the efforts of the US Food and Drug Administration (FDA) and members of the pharmaceutical industry to establish a uniform and enforceable standard by which the FDA will consider electronic records equivalent to paper records and electronic signatures equivalent to traditional handwritten signatures. For more information, see www.fda.gov/ora/compliance_ref/part11/frs/background/11cfr-fr.htm.

MassHunter Quantitative Analysis Compliance Software includes the following features which support 21 CFR Part 11 compliance:

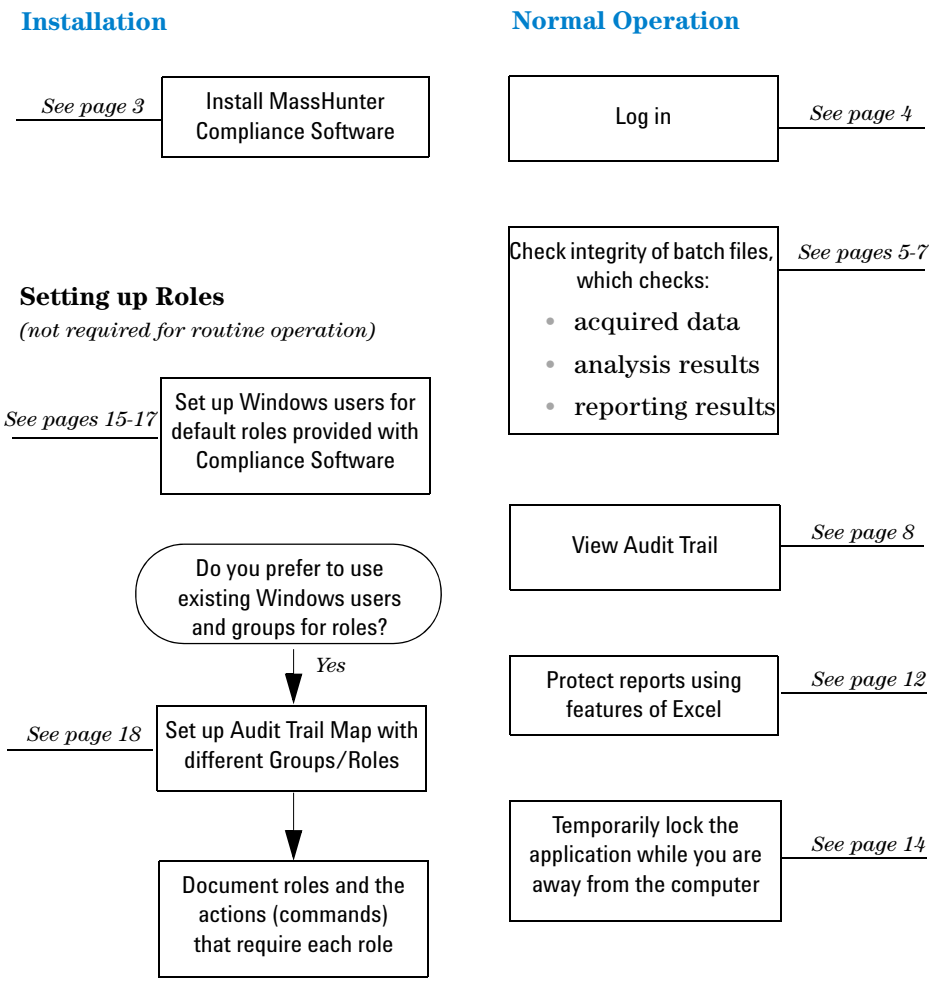
- Security (tamper detection) of data, batches, and results
- Quant Audit Trail
- Roles that restrict actions to certain users

See the online help for more information on these features.

Agilent Technologies

Getting Started Roadmap

The following diagram shows the steps for administrators and other users to get started with MassHunter Quantitative Analysis Compliance Software. This guide and the online help explain these steps.



Installation

Use the following procedure to install Compliance software. This installation procedure will install and enable Compliance software for Data Acquisition and Quantitative Analysis if those are present on the computer where you are installing Compliance.

NOTE

You must have the following minimum version numbers of MassHunter Workstation software components installed or Compliance installation is skipped for those components:

- Data Acquisition B.01.03
- Quantitative Analysis B.01.03

1 Put the Compliance setup CD in the drive.

2 Double-click on the **setup.vbs** file on the CD.

For Data Acquisition

3 These steps apply to the installation of Compliance for Data Acquisition only:

   a When the confirmation message appears, click **OK** to start the installation.

   b When complete, you will see the message: "Compliance installation for MassHunter Workstation Acquisition software is successful". If the Acquisition Compliance installation fails, you are given a chance to view the log file.

Successful install

If installation for all components present on the computer is successful, the following message appears: "Compliance Installation Finished".

Failed install

If installation for any component present on the computer is *un*successful, then following message appears: "Compliance Installation Failed".

NOTE

Once Acquisition Compliance is installed, it can only be uninstalled by uninstalling MassHunter Workstation software.

Normal Operation

This section describes using MassHunter Quantitative Analysis Compliance Software.

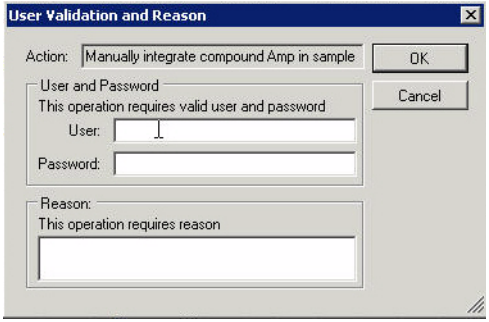
Log on to MassHunter Quantitative Analysis Compliance Software

1 Double-click the **Quantitative Analysis** program icon on your desktop or select **Programs > Agilent > MassHunter Workstation > Quantitative Analysis** from the Windows Start menu.

2 Depending on how the MassHunter Quantitative Analysis Compliance Software is configured, you may be prompted for your user name and password. If your account is in a domain, enter your user name and domain into the **User** field in the format **user@DNS_domain_name**. To configure the login option, see "Change global settings" on page 19.

User Validation and Reason

If your Compliance system has been customized with roles, some commands in the Quantitative Analysis software may not be available to you. Other actions may require you to reenter your logon information or supply a reason. Some examples of this might be manually integrating a peak or disabling a calibration point. In that case, the following dialog box will be displayed when you initiate the command:



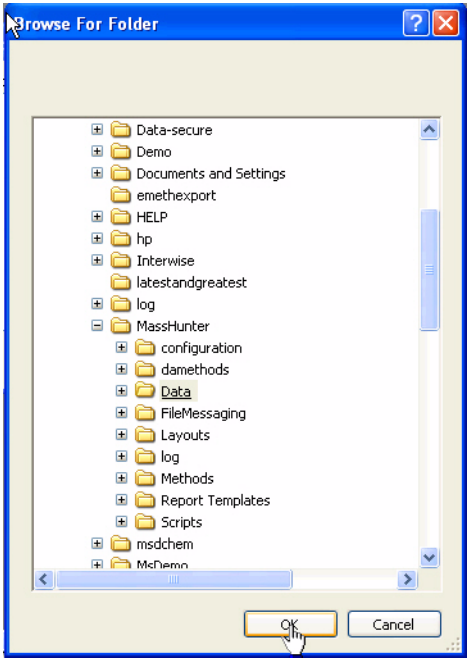
For more information on configuring these options, see:

- "Assign users to the appropriate user groups/roles" on page 16
- "Customize roles" on page 18

Check integrity of batch files

Use this procedure to check whether any files in a batch have been tampered with. This tool checks all files that are in a selected folder, such as batches (*.batch.xml files), acquired data (*.d files), report results (*.report.results.xml files). Checksum values (Hash codes) are checked for all file types. In addition, Audit Trail values are checked for batch and results files.

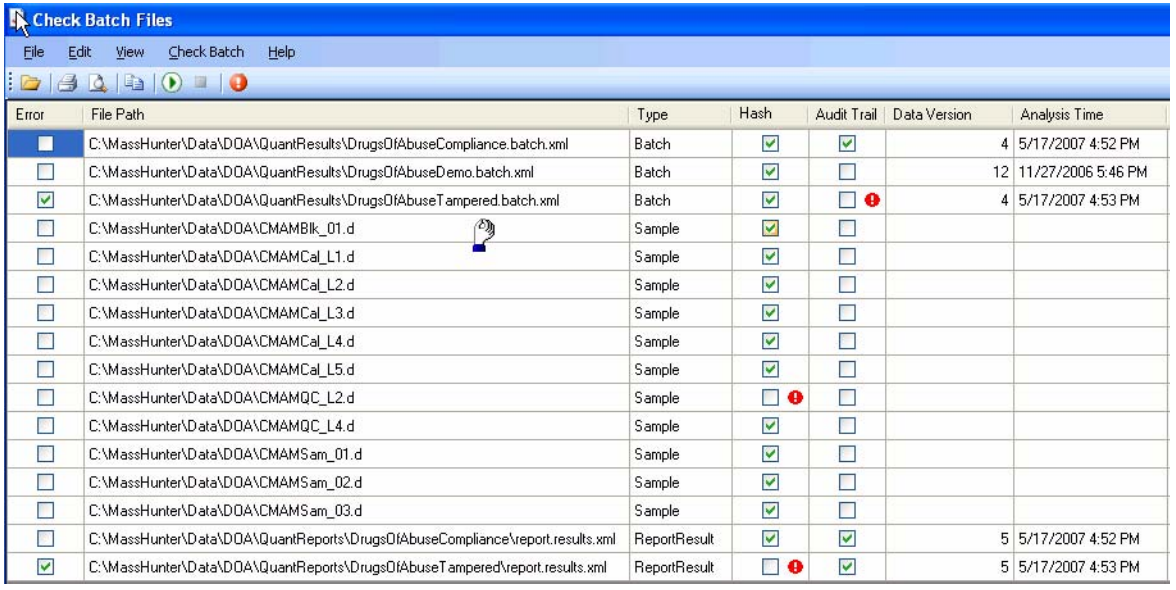
1. Select **Programs > Agilent > MassHunter Workstation > Quant Tools > Check Batch Files** from the Windows Start menu.
2. Select **Select Folders** from the File menu in the Check Batch Files window.
3. Click the **Add** button in the Check Batch Files Folder dialog box.
4. Select the folder of interest in the Browse For Folder dialog box. Often you will select the MassHunter Workstation Data folder or a subfolder as shown below.



5. Click **OK** on the Browse For Folder dialog box, then click **OK** on the Check Batch Files Folder dialog box.

6 Click the Run button in the toolbar or select **Start Check Batch** from the CheckBatch menu to start checking files in the selected folder.

7 Review the results displayed in a table in the Check Batch File window. Files that have a security problem are indicated with an exclamation mark (!) in a red circle in the first column of the table. If a problem was detected with either the **Hash Code** (Checksum) or the linked **Audit Trail** for that file, an exclamation mark (!) in a red circle also appears in those columns as shown in the example below.



Error	File Path	Type	Hash	Audit Trail	Data Version	Analysis Time
☐	C:\MassHunter\Data\DOA\QuantResults\DrugsOfAbuseCompliance.batch.xml	Batch	☑	☑	4	5/17/2007 4:52 PM
☐	C:\MassHunter\Data\DOA\QuantResults\DrugsOfAbuseDemo.batch.xml	Batch	☑	☐	12	11/27/2006 5:46 PM
☑	C:\MassHunter\Data\DOA\QuantResults\DrugsOfAbuseTampered.batch.xml	Batch	☑	☐ !	4	5/17/2007 4:53 PM
☐	C:\MassHunter\Data\DOA\CMAMBlk_01.d	Sample	☑	☐		
☐	C:\MassHunter\Data\DOA\CMAMCal_L1.d	Sample	☑	☐		
☐	C:\MassHunter\Data\DOA\CMAMCal_L2.d	Sample	☑	☐		
☐	C:\MassHunter\Data\DOA\CMAMCal_L3.d	Sample	☑	☐		
☐	C:\MassHunter\Data\DOA\CMAMCal_L4.d	Sample	☑	☐		
☐	C:\MassHunter\Data\DOA\CMAMCal_L5.d	Sample	☑	☐		
☐	C:\MassHunter\Data\DOA\CMAMQC_L2.d	Sample	☐ !	☐		
☐	C:\MassHunter\Data\DOA\CMAMQC_L4.d	Sample	☑	☐		
☐	C:\MassHunter\Data\DOA\CMAMSam_01.d	Sample	☑	☐		
☐	C:\MassHunter\Data\DOA\CMAMSam_02.d	Sample	☑	☐		
☐	C:\MassHunter\Data\DOA\CMAMSam_03.d	Sample	☑	☐		
☐	C:\MassHunter\Data\DOA\QuantReports\DrugsOfAbuseCompliance\report.results.xml	ReportResult	☑	☑	5	5/17/2007 4:52 PM
☑	C:\MassHunter\Data\DOA\QuantReports\DrugsOfAbuseTampered\report.results.xml	ReportResult	☐ !	☑	5	5/17/2007 4:53 PM

8 (optional) Select **Show Error Records Only** from the View menu to display only the rows (files) that have error conditions. Select the menu item again to return to the full display of data.

9 (optional) To copy the *entire table* to another application:

- **a** Select **Select All** from the Edit menu.
- **b** Select **Copy** from the Edit menu.
- **c** The data can then be pasted into a word processing or spreadsheet application.
- **d** To “deselect” the entire table, select other cells, rows, or columns with the mouse.

10 (optional) To copy *selected data* to another application:

- **a** Drag the mouse to select the cells, rows, or columns of interest.
- **b** Select **Copy** from the Edit menu.
- **c** The data can then be pasted into a word processing or spreadsheet application.

11 (optional) To save the results in a file:

- **a** Select **Export** from the File menu.
- **b** Select a location for the export file.
- **c** Enter a name for the export file.
- **d** Select the format for the export file: .CSV, Tab-delimited (.TXT), or .XML.
- **e** Click the **Save** button.

12 When you have finished checking files, select **Exit** from the File menu to close the Check Batch Files window.

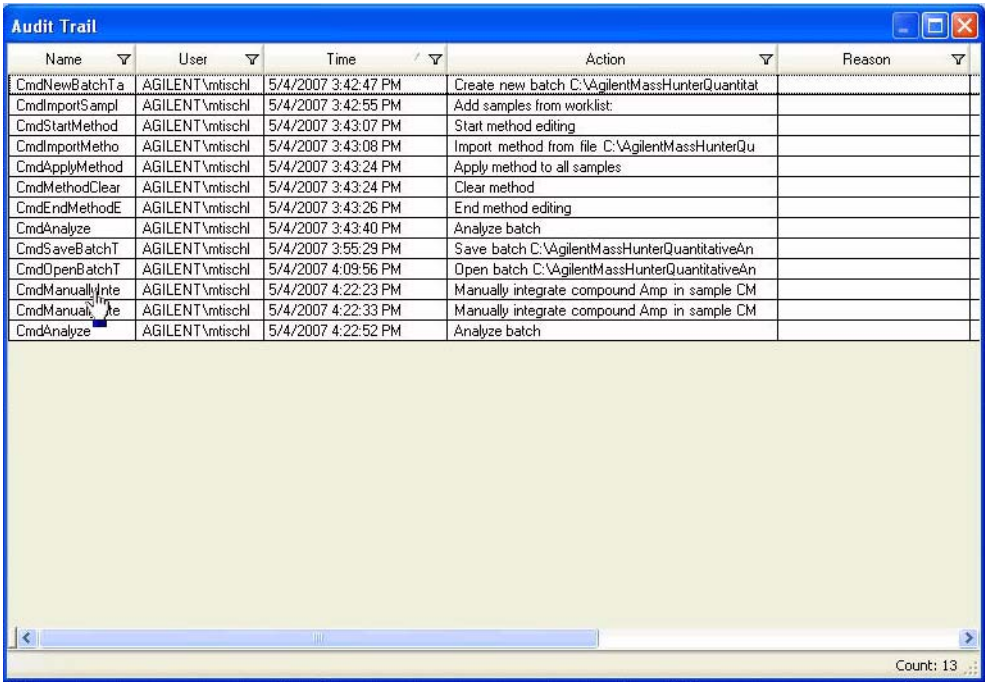
View Audit Trail

Use this procedure to check audit trail entries for a batch. Audit trail information is available for all batches that were created with the **Enable Audit Trail** checkbox selected on the New Batch dialog box.

1 If not already open, open the batch of interest by selecting **Open Batch** from the File menu.

2 If the batch has not yet been analyzed, select **Analyze Batch** from the Analyze menu.

3 Select **Audit Trail** from the Tools menu in the Quant application window to open the Audit Trail dialog box. An example is shown below:

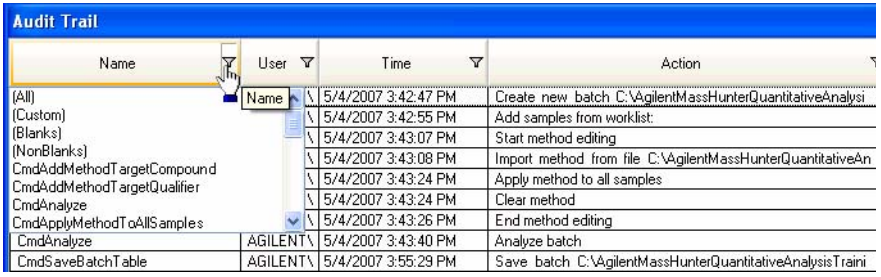


4 You can change or add entries in the **Comment** column for actions that were performed in the current session. Actions from the current session are indicated by a marked checkbox in the **InSession** column for their row.

Filter by Name

5 Audit information can be filtered to make it easier to review as shown in the following example.

a Click on the **Filter** icon in the **Name** column heading to open a list of commands:



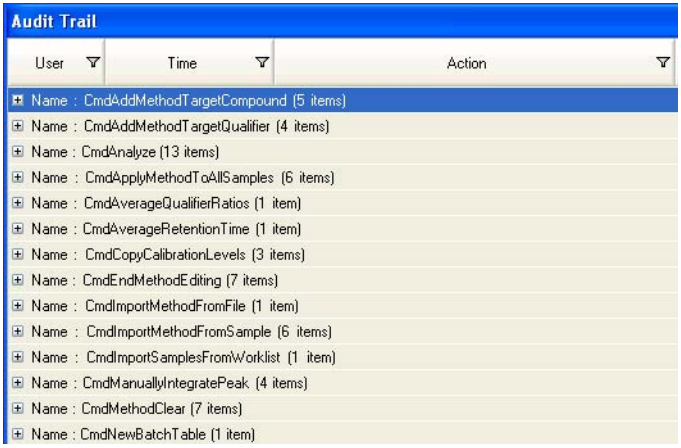
b If you select **CmdManuallyIntegratePeak**, then only the manual integration actions will appear in the Audit Trail table:

c To return to the full display, click on the **Filter** icon in the **Name** column heading and select **All** from the list of commands.

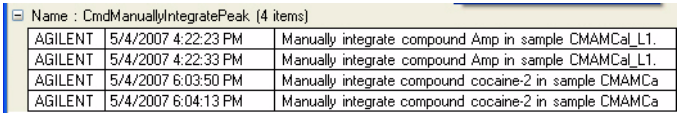
Group by Command

6 Audit information can be grouped by command as shown in the following example.

a Right-click in the **Name** column, and select **Group by Name** from the shortcut menu, which results in a list of commands:



b To view the actions for a particular command, click on the **+** icon next to the command name of interest, as shown for manual integration below:



c Click on the **-** icon to close the list.

d To return to the regular display, right-click in the **Name** column, and *deselect* **Group by Name** from the shortcut menu.

Sort Table

7 To sort the actions in the audit trail table, click on the column heading that you want to use for sorting.

Export Table

8 Right-click in the table and select **Export** from the shortcut menu.

a On the Export dialog box, select the folder and enter a **File name** for the export file.

b Select the **Type** for the export file (Excel .xls, CSV .csv, Tab Delimited .txt, or XML .xml).

c Click the **Save** button.

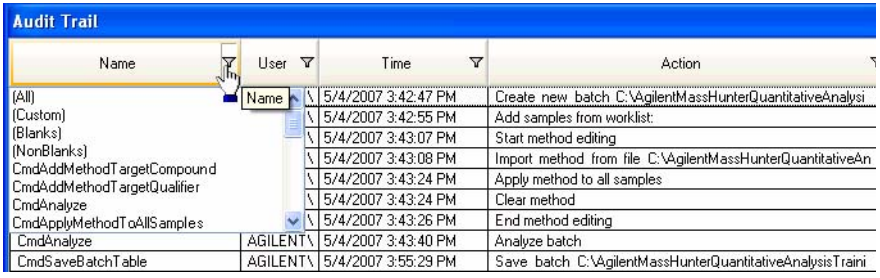
Print or Preview Table

9 Right-click in the table and select **Print** or **Print Preview** from the shortcut menu.

Custom Filtering

10 You can select other criteria for filtering audit trail information as follows:

a Click on the **Filter** icon in the column heading of interest to open a list of commands, as shown for the Command Name column below:



b Select **Custom** to open the Filter Criteria dialog box.

c Open the list of **Operators** and select one, such as Equals, Does not equal, Less than, and Greater than.

d Open the list of Operands and select one. The items in the list depend on which column you select in step a).

e (optional) To add more criteria to the filter, click the **Add a condition** button. Select either **And conditions** or **Or conditions** for the filter.

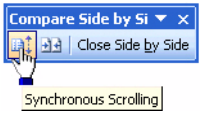
f Click **OK** to filter the Audit Trail table using the specified criteria.

g To return to the full display, click on the **Filter** icon in the column heading and select **All** from the list of commands.

Protect reports

Reports generated by MassHunter Workstation Quantitative Analysis software as Excel worksheets (.xls files) are not intended to be edited. The following features help ensure that these report files are not tampered with after they are generated.

1. The templates used to generate the reports can be customized to use password protection. This causes an error message to be displayed when a user tries to edit any cell in the worksheet. This option can be set in the Options section of the template.
2. The reports can be reviewed with the Excel Viewer, which does not allow files to be edited. Another benefit of using the Excel Viewer, in addition to security, is that it loads more quickly than the full Excel product.
3. You can visually compare Excel reports to detect changes as follows:
   a. Open both reports in Excel and select the **Calibration** tab in each report.
   b. Mark the **Compare Side by Side** option on the Excel Window menu and visually compare the two reports, such as calibration curves, final concentrations, etc.
   c. Click the **Synchronized Scrolling** icon shown below to facilitate reviewing and comparing the two documents.



4. You can use a third-party tool to compare two Excel documents, such as the one available from Formula Software, Inc. This tool allows you to compare all sheets that have the same names in two workbooks and is most useful for Quant reports that have been generated with the same template. You can specify that deleted, added, and changed data be reported on separate worksheets, and that the compared sheets be replicated into a new report workbook for easy review.

5 You can generate PDF files of your reports as follows:

   a Install Adobe Acrobat and specify a folder to store the generated PDF files.

   b Analyze your batch with MassHunter Workstation Quantitative Analysis software.

   c Select **Report > Generate** to open the Report dialog box. Select the reports to be generated, assign unique output file names, and specify Adobe PDF as the printer for each report. Click **OK** to begin processing the reports.

   d Open the **Queue Viewer** from the Report menu to monitor the progress of report generation.

   e The PDF report files (.pdf) that are generated can have signatures, approval workflows, comments, and password-protection features enabled.

Lock your computer screen when unattended

When you are going to be away from your computer for awhile, use the following procedure to lock your computer so that it can't be accessed by others.

1 Press **Ctrl+Alt+Delete**.

2 Click **Lock Computer**.

To unlock your computer on your return, press **Ctrl+Alt+Delete**, type in your password and click **OK**.

Using Roles to Restrict Actions

What are roles?

Roles are groups that users can be assigned to that establish the actions (or commands) that users can perform in MassHunter Quantitative Analysis Compliance Software. The software defaults to four roles: **QuantBatchAnalyzer**, **QuantBatchReviewer**, **QuantMethodDeveloper**, and **QuantReportGenerator**, which are automatically installed with the Compliance software. If desired, roles can be set up using your own Windows group names as described in "Set up roles using existing Windows groups", and roles can be customized as described in "Customize roles" later in this section.

Set up Windows user groups for Quantitation Compliance roles

Use the following procedure to create user groups for the above four roles on the computer where you are running MassHunter Quantitative Analysis Compliance Software.

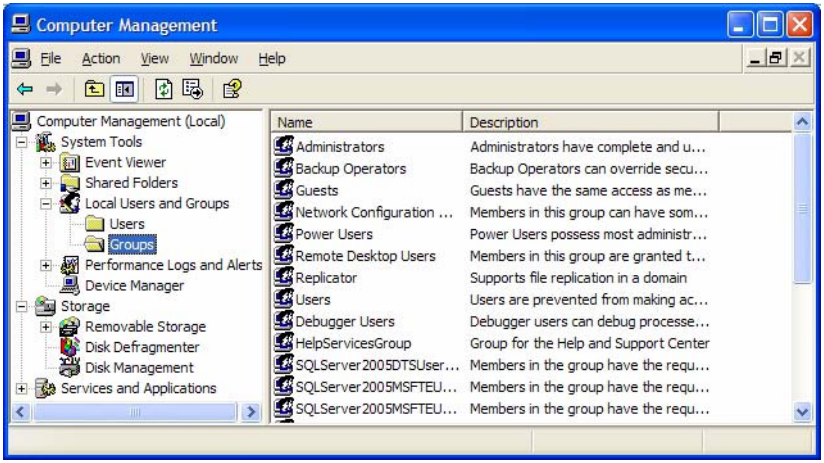
NOTE Skip this section if you prefer to set up roles using your own Windows groups instead.

1 Open C**omputer Management**.

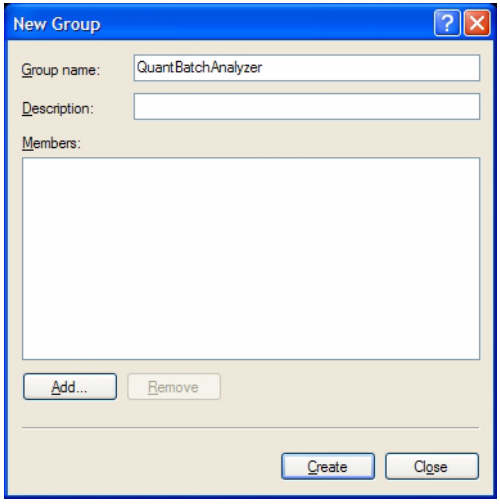
   a Select **Administrative Tools** from the Control Panel.

   b Select **Computer Management**.

2 In the Computer Management window, select **System Tools > Local Users and Groups > Groups** from the navigation pane on the left side of the window.



3 Select **New Group** from the **Action** menu to open the New Group dialog box.



4 Type in a name for the new group (i.e. **QuantBatchAnalyzer**, **QuantBatchReviewer**, **QuantMethodDeveloper**, or **QuantReportGenerator**).

5 (*optional*) Type in a description of the group.

6 (*optional*) Click the **Add** button to add users to the group at this time. This can also be done later as described in "Assign users to the appropriate user groups/roles" on the following page.

7 Click the **Create** button.

8 Repeat Steps 3-7 for the other three groups.

Assign users to the appropriate user groups/roles

Use this procedure to add users to the appropriate user groups, keeping in mind the privileges and restrictions of each role in MassHunter Quantitative Analysis Compliance Software described on the previous page.

1 Open C**omputer Management** as follows:

   a Select **Administrative Tools** from the Control Panel.

   b Select **Computer Management**.

2 In the Computer Management window, select **System Tools > Local Users and Groups > Groups** from the navigation pane on the left side of the window.

3 Right-click on the group of interest (i.e. **QuantBatchAnalyzer**, **QuantBatchReviewer**, **QuantMethodDeveloper**, or **QuantReportGenerator**) and select **Properties** from the shortcut menu.

4 Click the **Add** button on the Group Properties dialog.

5 On the Select Users dialog box, type in the user names in the text box that you want to add to the group, then click the **Check Names** button. The complete computer name and user name will be filled in for each user.

6 Click **OK** to complete the process.

Alternate method

If you are adding a single user to a group, it may be easier to access User Accounts as follows:

1 Select **User Accounts** from the Control Panel.

2 Select the user you want to add to the group on the **Users** tab in the User Accounts window, then click the **Properties** button to assign that member to one of the Quantitation Compliance groups.

3 If the user you want to add to the group *does not already exist on the local machine*, click the **Add** button to add them to the local machine and to the desired Quantitation Compliance group.

Set up roles using existing Windows groups

Instead of using the roles provided with MassHunter Quantitative Analysis Compliance Software, you can use existing Windows groups or create new ones as follows.

1 Set up Windows user groups, using your own names.

2 "Assign users to the appropriate user groups/roles", as described above.

3 Open the Audit Trail Map (ATM) Configuration window by clicking the program icon on the desktop or by selecting **Programs > Agilent > MassHunter Workstation > Quant Tools > ATM Configuration** from the Windows Start button.

4 Log in using the appropriate account name and password.

NOTE

You must be a member of a group called **QuantAdministrators** in order to open the ATM Configuration window. If this group does not already exist, you must create it and add a user account to it before you proceed.

5 Delete the existing roles (i.e. **QuantBatchAnalyzer**, **QuantBatchReviewer**, **QuantMethodDeveloper**, or **QuantReportGenerator**) as follows:

   a Right-click on the role in the Required User Role pane and select **Remove User Role** from the shortcut menu. Click **Yes** to confirm the deletion.

   b Repeat Step 5a) for all the roles you want to remove.

6 Create new roles using the Windows user groups you created in Step 1 as follows:

   a Right-click on a role in the Required User Role pane and select **Add User Role** from the shortcut menu.

   b Repeat Step 6a) for all the roles you want to add.

7 Customize roles as described below.

Customize roles

Use this procedure to assign the roles are required for various actions or commands in the MassHunter Quantitative Analysis Software. Assigning a role to an action or command means that a user must be a member of that role in order to run that action or command.

1 If the Audit Trail Map (ATM) Configuration window is not already displayed, open it by clicking the program icon on the desktop or by selecting **Programs > Agilent > MassHunter Workstation > Quant Tools > ATM Configuration** from the Windows Start menu. Log in using the appropriate account name and password.

NOTE You must be a member of a group called **QuantAdministrators** in order to open the ATM Configuration window. If this group does not already exist, you must create it and add a user account to it before you proceed.

2 Select a command from one of the four command groups (**Batch Analysis**, **Batch Review**, **Method Development**, or **Report**) on the left side of the ATM Configuration window.

3 Mark a **Required User Role** for the command in the upper right part of the window.

NOTE If no **Required User Role** is selected for an action or command, then that action or command can be run by *all users*.

4 (optional) Mark the **Requires Command Reason** option in the lower right part of the window to optionally require that a user enter a reason when they run the selected command.

5 (optional) Mark the **Requires User Validation** option in the lower right part of the window to optionally require that a user enter their user name and password when they try to run the selected command.

6 Repeat Steps 2 - 5 for all actions or commands that you want to assign to roles.

7 (optional) Add new command groups by right-clicking on **Command Groups** and selecting **Add Command Group** from the shortcut menu. Type in the name of the new group and click **OK**.

8 (optional) You can drag commands to move them from one group to another. A command can only be in one group. Be sure to mark the appropriate Required User Role for commands that you move.

9 When you have finished customizing ATM, select **Save** from the File menu.

Change global settings

Use this procedure to set certain global settings for MassHunter Quantitative Analysis Software.

1 If the Audit Trail Map (ATM) Configuration window is not already displayed, open it by clicking the program icon on the desktop or by selecting **Programs > Agilent > MassHunter Workstation > Quant Tools > ATM Configuration** from the Windows Start button. Log in using the appropriate account name and password.

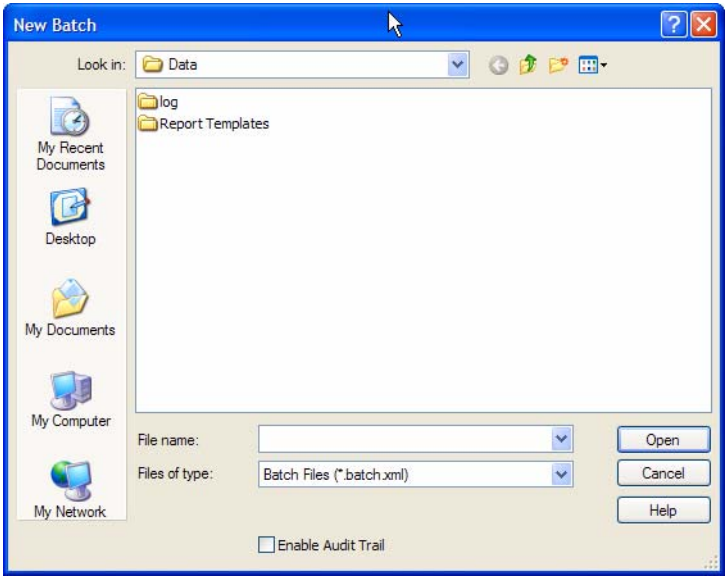
NOTE You must be a member of a group called **QuantAdministrators** in order to open the ATM Configuration window. If this group does not already exist, you must create it and add a user account to it before you proceed.

2 Click **Settings** on the left side of the ATM Configuration window. The global settings window appears in the right pane.

3 Mark the **Require Logon at application start time** option if you want to require users to log in with a Windows user account in order to start the MassHunter Quantitative Analysis Software. This user account is used for Audit Trail, User Validation, and Role-based command security. If not marked, then the user session account is used. This option is useful if you are running Quantitative Analysis on the same computer that is used to acquire data from the instrument. In that case, a different user can perform Quantitative Analysis while data is being acquired, and both users will be identified.

4 Mark the **Always Enable Audit Trail when creating a new Batch** option if you want to create audit trails for all batches. When marked, the **Enable Audit Trail** checkbox at the bottom of the New Batch dialog box will be unavailable at all times.

If the **Always Enable Audit Trail when creating a new Batch** option is *not* marked, then users can choose to turn audit trails on or off when creating a new batch file as shown below.



5 Mark the **Load settings from** option if you want to load an ATM Configuration from a specified path name. This is useful for larger labs that may want to maintain a central ATM configuration file for use on all systems and not have to configure settings on individual computers.

6 Select **Save** from the File menu.

Where to Find More Information

You can access more information about MassHunter Quantitative Analysis Compliance Software as follows.

Agilent Web Site

To view support information for MassHunter Quantitative Analysis Compliance Software and other Agilent products, see: **http://www.agilent.com/chem** and access the Mass Spectrometry products page.

MassHunter Workstation Software Online Help

You can access MassHunter Workstation online help from the **Help** menu in the software or by pressing F1 in the MassHunter Workstation dialog boxes.

www.agilent.com

In This Book

This guide contains information to install and use the MassHunter Quantitative Analysis Compliance Software.

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