

MassHunter Quantitative Analysis Compliance Software

Quick Start Guide

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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 http://www.fda.gov/ICECI/EnforcementActions/default.htm.

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

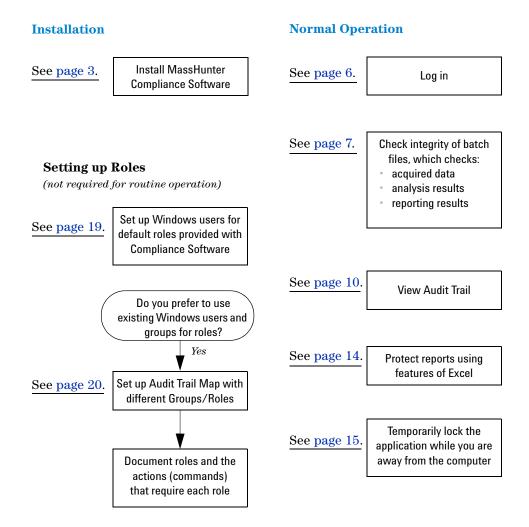
- Security (tamper detection) of data, batches, and results
- Quant Audit Trail
- · Roles that restrict actions to certain users

See the online help for more information on these features.



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 the Quantitative Analysis Compliance software. This installation procedure will install and enable Compliance software for Quantitative Analysis if it is present on the computer where you are installing Compliance.

To install the compliance program from version 4.00 - 6.00:

Quantitative Analysis version B.04.00 or later must be installed before the Compliance program is installed.

- 1 Double-click on the **setup_quantcompliance.exe** file on the MassHunter Workstation Quantitative Analysis Software DVD.
- **2** Select the language to use for the installation and click **OK**.

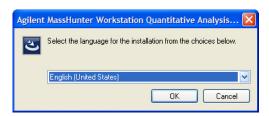


Figure 1 Selecting a language

- **3** Click **Next** in the Welcome dialog box.
- 4 Click the I accept the terms in the license agreement button and then click Next. You can click the Print button to print the license agreement.
- **5** Click **Install** in the Ready to Install the Program dialog box.

Installation

What is MassHunter Quantitative Analysis Compliance Software?

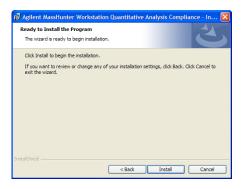


Figure 2 Ready to Install the Program page in the Installation program

Successful install

If installation for all components present on the computer is successful, you are shown this message: "The InstallShield Wizard has successfully installed Agilent MassHunter Workstation Quantitative Analysis Compliance."

Failed install

If installation for any component present on the computer is un successful, you are shown this message: "Compliance Installation Failed".

NOTE

You can remove the Compliance for Quantitative Analysis program by using Add/Remove programs.

To install compliance for version B.07.00:

When you install version B.07.00 of the MassHunter Quantative Analysis software, the compliance software is automatically installed if you choose the **Complete** installation procedure. You can determine if the program was installed by checking your **Windows Control Panel Program** list.

If the compliance program was not installed follow this procedure.

- 1 Verify that no other program is running on your system. Installation of the Quantitative Analysis Compliance program will fail if Windows Update is running, even in the background.
- **2** From the MassHunter Quantitative Analysis Disk 1/2 installation DVD, right-click **Setup_Quant**, and then select **Run** as administrator.
- **3** In the **Welcome to the InstallShield Wizard** window, click **Next** to continue with the installation.

- 4 In the **Program Maintenance** page, choose **Modify** and click **Next**.
- 5 In the Custom Setup page, Compliance list, choose This feature, and all subfeatures, will be installed on local hard drive.

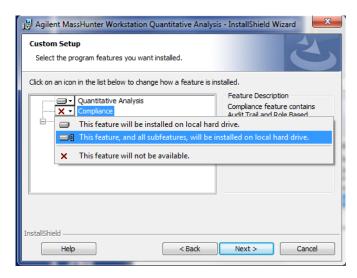


Figure 3 This feature is installed on local hard drive

- 6 In the Ready to Modify the Program page, click Install to begin. The Installing Agilent MassHunter Workstation Quantitative Analysis window is displayed.
- 7 When the InstallShield Wizard Completed page is displayed, click Finish.

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 21.

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 enter your user name and password or supply a reason. For example, you may need to give a reason when you manually integrate a peak or disable a calibration point. The User Validation and Reason dialog box is displayed when you do the action.



Figure 4 User Validation and Reason dialog box

For more information on configuring these options, see "Assign users to the appropriate user groups/roles" on page 18 or "Customize roles" on page 20.

Check integrity of batch files

Do this step 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.bin files), acquired data files (*.d files), and 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 Click Select Folders from the File menu in the Check Batch Files program.
- **3** Click the **Add** button in the Check Batch Files dialog box.
- **4** Select the folder of interest in the Browse For Folder dialog box. Often, you will select the *MassHunter/Data* folder or a folder in that folder.

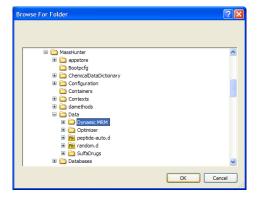


Figure 5 Browse For Folder dialog box

- **5** Click **OK** on the Browse For Folder dialog box, then click the **OK** button in the Check Batch Files dialog box.
- **6** Click the **Run** button on the toolbar or click **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 a marked check box in the **Error** 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 appears in those columns as shown in Figure 6.

In this example, the checksum file is missing from several data files. If a data file is acquired when the Data Acquisition Compliance software is disabled, the checksum file is not created.

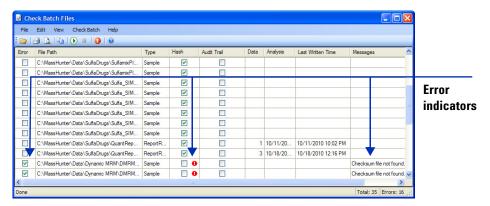


Figure 6 Errors after running the Check Batch Files tool

- **8** (optional) Click **Show Error Records Only** from the View menu to display only the rows (files) that have error conditions. Click the command again to return to the full display of data.
- **9** (optional) Copy the entire table to another application.
 - a Click Edit > Select All.
 - **b** Click **Edit > Copy**.

The data can then be pasted into a word processing or spreadsheet application.

To cancel the selection for the entire table, select other cells, rows, or columns with the mouse.

- **10** (optional) Copy selected data to another application.
 - **a** Drag the mouse to select the cells, rows, or columns of interest.
 - **b** Click **Edit > Copy**.
 - **c** The data can then be pasted into a word processing or spreadsheet application.

- **11** (*optional*) Save the results in a file.
 - a Click File > Export.
 - **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, click **File > Exit** to close the Check Batch Files window.

View Audit Trail

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

- 1 If not already open, open the batch of interest by clicking File > Open Batch.
- 2 If the batch has not yet been analyzed, click **Analyze > Analyze Batch**.
- **3** Click **Tools > Audit Trail** in the Quant application window. The Audit Trail dialog box opens. See Figure 7.

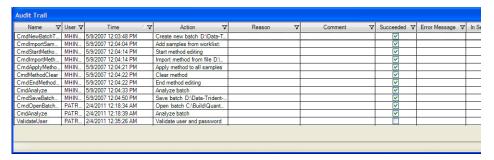


Figure 7 Audit Trail dialog box

4 (optional) Click a cell in the Comment column for an action that was performed in the current session. You can change or add entries in the Comment column for actions that were performed in the current session. These actions are indicated by a marked check box in the InSession column for their row.



Figure 8 Adding a comment to an action performed in this session

Filter by Name

- **5** Audit information can be filtered to make it easier to review as shown in the following example.
 - a Click the Filter icon in the Name column heading to open a list of commands.

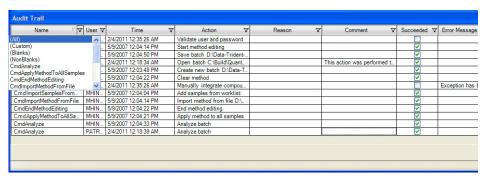


Figure 9 Filter options in the Audit Trail program

b If you select **CmdAnalyze**, then only the analyze actions will appear in the Audit Trail table.

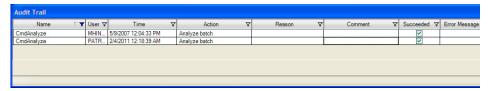


Figure 10 Filtered results in the Audit Trail program

c To return to the full display, click 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 the **Name** column, and click **Group by Name** from the shortcut menu. The results are listed grouped by the name of the command.

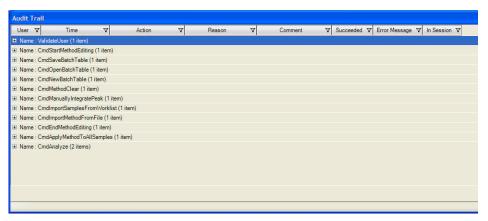


Figure 11 After using the Group by Name command

b To view the actions for a particular command, click the + icon next to the name of the command. See Figure 12.

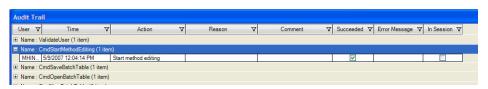


Figure 12 After clicking + icon in the Audit Trail program

- **c** Click the icon to close the list.
- **d** To return to the regular display, right-click the **Name** column, and click **Group by Name** again from the shortcut menu.

Sort Table

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

Export Table

- **8** Right-click the table and click **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 .xlsx, CSV .csv, Tab Delimited .txt, or XML .xml).
 - c Click the Save button.

Print or Preview Table

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

Custom Filtering

10 You can select other criteria for filtering audit trail information.

a Click the **Filter** icon in the column heading of interest to open a list of commands, as shown for the **Name** column in Figure 13.

Name ∇ ∇	User ♥	Time	V	Action 🔽	Reason	7 Comment ▽	Succeeded V	Error Messag
All)	^ -	2/4/2011 12:35:26 AM	T	Validate user and password				
Custom)		5/9/2007 12:04:14 PM	П	Start method editing			~	
Blanks)		5/9/2007 12:04:50 PM		Save batch D:\Data-Trident			✓	
NonBlanks)		2/4/2011 12:18:34 AM	П	Open batch C:\Build\Quant		This action was performed t	✓	
mdAnalyze mdApplyMethodToAllSample		5/9/2007 12:03:48 PM	П	Create new batch D:\Data-T			V	
CmdEndMethodEditing CmdImportMethodFromFile		5/9/2007 12:04:22 PM	\neg	Clear method			<u> </u>	
		2/4/2011 12:35:26 AM	П	Manually integrate compou				Exception has
CmdImportSamplesFrom	MHIN_	5/9/2007 12:04:04 PM	\neg	Add samples from worklist:			V	
CmdImportMethodFromFile	MHIN_	5/9/2007 12:04:14 PM	T	Import method from file D:\			▽	
CmdEndMethodEditing	MHIN_	5/9/2007 12:04:22 PM		End method editing			V	
CmdApplyMethodToAllSa	MHIN_	5/9/2007 12:04:21 PM	╗	Apply method to all samples			<u>~</u>	
CmdAnalyze	MHIN_	5/9/2007 12:04:33 PM	П	Analyze batch			V	
CmdAnalyze	PATR	2/4/2011 12:18:39 AM	\neg	Analyze batch			✓	
	•							

Figure 13 Commands available after clicking the Filter icon in the Name column

- **b** Select **Custom** to open the Custom Filter dialog box.
- c Open the list of **Operators** in the Name field and select one, such as **Equals**, **Does not equal**, **Less than**, and **Greater than**.
- **d** Select the operand to use from the **Operands** list. 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. Click either **And conditions** or **Or conditions** for the filter. If you click **And conditions**, then all conditions must be true to include the row.
- 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 (.xlsx 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. The Excel Viewer loads more quickly than the full Excel product.
- 3 You can visually compare Excel reports to detect changes.
 - a Open both reports in Excel and select the Calibration tab in each report.
 - **b** Click the **View Side by Side** button on the View menu.
 - c Click **Synchronous Scrolling** on the View menu if it isn't selected.
- 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.
 - **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 Save the batch. Click either File > Save or File > Save As.
 - **d** Click **Report > Generate** to open the Report dialog box.
 - **e** If **Adobe PDF** is not the default printer, then click **Advanced**. Click **Next** until the Reports page in the Report wizard is displayed. Select a

- template and a printer. Click the **Next** button until the final page of the wizard. Then, click the **Finish** button.
- f If Adobe PDF is the default printer, then select a Template file and click the OK button.
- **g** Open the **Queue Viewer** program from the Report menu to monitor the progress of report generation.
- **h** 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, do this step to lock your computer so that it can't be accessed by others.

- 1 Press Ctrl and Alt and Delete.
- 2 Click the Lock Computer button.

To unlock your computer on your return, press **Ctrl** and **Alt** and **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 five roles:

QuantAdministrators, QuantBatchAnalyzer, QuantBatchReviewer, QuantMethodDeveloper, and QuantReportGenerator. These roles must be manually created using the exact names shown here. 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

Do this step to create user groups for the above five 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 Computer Management.
 - **a** Click **System Security >Administrative Tools** from the Control Panel.
 - **b** Click Computer Management.
- 2 In the Computer Management window, click System Tools > Local Users and Groups > Groups from the navigation pane on the left side of the window.

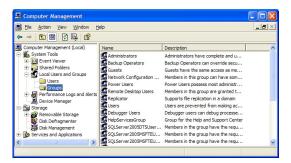


Figure 14 The Computer Management program

- **3** (optional) If the following groups are not available, create them.
 - a Click New Group from the Action menu to open the New Group dialog box.



Figure 15 Adding the group QuantBatchAnalyzer

- b Type in a name for the new group (i.e. QuantAdministrators,
 QuantBatchAnalyzer, QuantBatchReviewer, QuantMethodDeveloper,
 or QuantReportGenerator).
- **c** (optional) Type in a description of the group.
- **d** (*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 page 18.
- e Click the **Create** button.
- f Repeat step b to step e for the other four groups. Then, click Close.

Assign users to the appropriate user groups/roles

Do this step 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 in "What are roles?" on page 16.

If you are using the Study Manager program and submitting a Bioanalysis study, make sure that the person using the Study Manager program has the correct permissions for the Quantitative Analysis program. See the Study Manager Quick Start Guide for a list of the permissions that a person submitting a Bioanalysis study needs.

- 1 Open the Computer Management program.
 - 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 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 using the following steps.

- 1 Click **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. The QuantAdministrators can do every command, so you do not need to assign roles to that group.

- 1 Set up Windows user groups, using your own names.
- 2 "Assign users to the appropriate user groups/roles" on page 18.
- 3 Open the Audit Trail Map (ATM) Configuration window. Click **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).
 - **a** Click the **Batch Analysis Command Group** to open the Required User Role Window.
 - **b** Right-click the role in the Required User Role pane and click **Remove** User Role from the shortcut menu. Click **Yes** to confirm the deletion.
 - **c** Repeat step a for all the roles you want to remove.
- **6** Create new roles using the Windows user groups you created in step 1.
 - Right-click a role in the Required User Role pane and select Add User
 Role from the shortcut menu.
 - **b** Repeat step a for all the roles you want to add.
- 7 Customize roles as described in "Customize roles" on page 20.

Customize roles

Do this step to assign the roles that 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, click 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 under Required User Role.

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** check box under User Validation and Reason to optionally require that a user enter a reason when they run the selected command.
- **5** (*optional*) Mark the **Requires User Validation** check box under User Validation and Reason to optionally require that a user enter their user name and password when they try to run the selected command.
- **6** Repeat step 2 to step 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, click **Save** from the File menu.

Change global settings

Do this step to set certain global settings for MassHunter Quantitative Analysis Software.

1 If the Audit Trail Map (ATM) Configuration window is not already displayed, click 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.

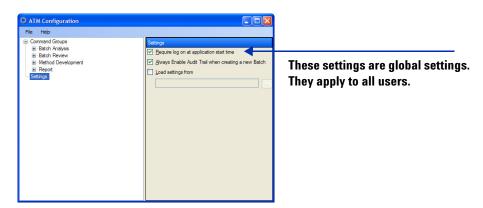


Figure 16 The Settings pane on the right side

3 Mark the **Require Logon at application start time** check box if you want to require users to log in with a Windows user account in order to start the

Using Roles to Restrict Actions

Change global settings

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 check box if you want to create audit trails for all batches. When marked, the Enable Audit Trail check box 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** check box is cleared, then users can choose to turn audit trails on or off when creating a new batch file as shown in Figure 17.

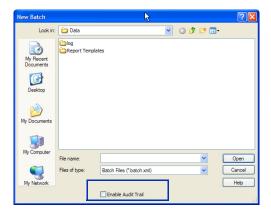


Figure 17 The Enable Audit Trail check box in the New Batch dialog box

- **5** Mark the **Load settings from** check box if you want to load an ATM Configuration from a specified path name. Then, click the Browse button to select the XML file to use. Loading settings from a file 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** Click **Save** from the File menu.

Where to find more information

You can access more information about the MassHunter Quantitative Analysis Compliance Software on the internet and in the online Help.

You can find more information on the MassHunter Data Acquisition Compliance Software in the online Help for the Compliance Software for Data Acquisition and in the MassHunter Data Acquisition Compliance Software Quick Start Guide.

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.

Where to find more information

MassHunter Workstation Software Online Help

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www.agilent.com

In This Book

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

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