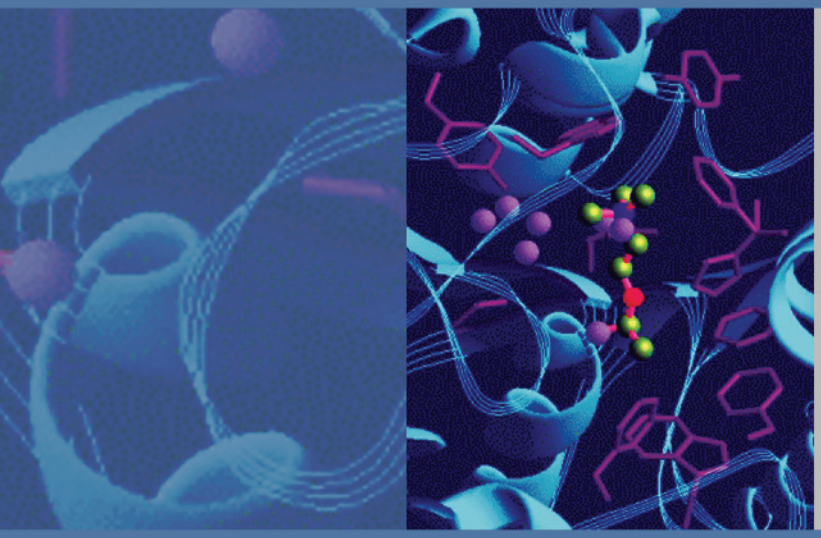

Xcalibur

Thermo LCquan

Version 2.7

Administrator Guide

XCALI-97238 Revision D September 2011

DOCUMENTATION SURVEY

Part of Thermo Fisher Scientific

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Software version: (Thermo Scientific) Foundation 2.0 SP1 and later, Xcalibur 2.2.0 SP1 and later, LCquan 2.7 and later, LC Devices 2.5 SP1 and later, Q Exactive 2.0 and later, Exactive 1.1 SP4 and later, TSQ Quantum 2.3 SP3 and later; (Microsoft) Windows 7 Professional SP1 32-bit and Office 2010

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Contents

Preface

The LCquan™ 2.7 application is part of the Xcalibur™ mass spectrometry data system. This administrator guide describes how to configure the Xcalibur and LCquan applications for security and compliance. The intended audience includes both laboratory administrators and local IT professionals who have administrative privileges for the system.

IMPORTANT Some of the instructions in this guide assume an understanding of the security settings for Microsoft™ Windows™ operating system. Thermo Fisher Scientific strongly recommends that you enlist your local IT professional to perform these tasks.

Note With Revision D, these instructions change the Microsoft™ Windows™ operating system from Windows XP or Vista™ to Windows 7.

Contents

❖ **To suggest changes to documentation or to Help**

Complete a brief survey about this document by clicking the button below. Thank you in advance for your help.

Related Documentation

The following LCquan manuals are available on the LCquan software CD as PDF files:

- *LCquan Administrator Guide* describes how to configure the LCquan application for security and compliance.
- *LCquan User Guide* describes how to use the LCquan application to perform quantitative analysis of compounds.
- *LCquan Tutorial* describes step-by-step procedures to perform quantitative analysis with sample data.

If you are using a Watson laboratory information management system (LIMS), refer to *Installing and Using the Peak View Gateway Between Watson and LCquan*.

If you are using the Thermo Scientific Web Access Suite™, refer to the *Web Access Administrator Guide* for instructions on adding the LCquan application to the programs served by Web Access.

❖ **To view the installed LCquan manuals**

Go to **Start > All Programs > Thermo Xcalibur > Manuals > LCquan**.

❖ **To open the LCquan Help**

1. From the LCquan window, choose **Help > LCquan Help**.
2. To locate a particular topic, use the Help Contents, Index, or Search panes.

Safety and Special Notices

Make sure you follow the precautionary statements presented in this guide. The safety and other special notices appear in boxes.

IMPORTANT Highlights information necessary to prevent damage to software, loss of data, or invalid test results; or might contain information that is critical for optimal performance of the system.

Note Highlights information of general interest.

Tip Highlights helpful information that can make a task easier.

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- Send an e-mail message to the Technical Publications Editor at techpubs-lcms@thermofisher.com.

Introduction

You can use the LCquan application to develop methods, create or import sequences, acquire, process, and review data, and create reports, all within a secure environment. This chapter provides an overview of security and compliance considerations and how to use the Xcalibur and LCquan applications to address them.

Contents

System Security

To prevent unauthorized access to data, most organizations implement strict security procedures for their computer networks. In this context, *unauthorized access* means:

- Access by an individual (external or internal to the organization) who has not been granted the authority to use, manipulate, or interact with the system
- Access by using the identity of another individual—for example, by using a colleague's user name and password

The Xcalibur data system directly implements some of these controls and relies on the security functions in the Microsoft Windows 7 Professional operating system for other controls, for example:

- The Finnigan™ Security Server controls secure file operations.
- The laboratory administrator restricts user software access through Thermo Foundation Authorization Manager (an administrative utility), which relies on Windows user groups. The Authorization Manager does not configure user access to the workstation. It can, however, define application roles for the users.

- The laboratory administrator controls software feature access through the Thermo Foundation Authorization Manager application.
- Windows security functions handle user authentication.
- Windows security functions maintain electronic record security and, in particular, the NTFS permission rights.

Configuring Software Applications

To fully implement these security features of the Xcalibur data system, the laboratory administrator must work with the IT professional to achieve the proper data system configuration. Configuring applications for security and compliance requires two steps:

- Protecting Records
- Setting Up User Access Controls

Protecting Records

To establish secure file operations, as the laboratory administrator, you must restrict access permissions for specific folders and files. Set permissions so that only you can delete or alter records. The use of protected folders and files ensures that unauthorized users cannot obscure previous records by using a utility such as Windows Explorer.

Setting Up User Access Controls

To control user access, you must define secure user groups and grant access permissions for each group. You can restrict defined groups of users from performing various functions within the application. This restriction can range from complete prohibition, through several levels of password-required access, to no restrictions. You set user access controls by using Thermo Foundation Authorization Manager.

After the security settings are defined for at least one group, users who are not in a secure group are denied access to the application.

IMPORTANT If no secure groups are defined, users have access to all features of the application.

Security Features Within the Xcalibur Application

After the appropriate file protections and user access controls are in place, the Xcalibur application employs several built-in features to ensure the security of the data.

The Xcalibur application performs Cyclic Redundancy Checks (CRCs) to protect against malicious changes to data files. A CRC can detect file corruption and attempted changes to data files outside the application. The CRC calculates checksums for sets of data, using mathematical formulas, and embeds the value within the file. Each time you open the file, the CRC recalculates the checksums and compares them with the stored values. When you modify or process data within the application, the CRC recalculates and stores new checksums.

In addition, the Xcalibur application includes a file tracking system that maintains a database of the files created in or used by the application. When you open an existing project, the Xcalibur application displays a warning if files within that project have been moved or modified (as determined from the CRC value).

A comprehensive audit trail ensures that you can generate all electronic records from the raw data. The audit trail comprises three parts: the history log, the event log, and the file tracking log. The history log contains information about every parameter change a user has made within an LCquan workbook. The event log contains information about all the events that have occurred within the application, such as the creation of a workbook or the execution of a command that is under authorization control. The file tracking log tracks changes made to files contained within an LCquan workbook.

Prerequisites to Configuring the System

As the laboratory administrator, you must plan how the laboratory will function before performing the procedures in this guide. At a minimum, address the following:

- How Users Perform Sample Acquisition
- LCquan Folder Structure
- Secure User Groups

How Users Perform Sample Acquisition

The Scenarios for LCquan sample acquisition diagrams illustrate how users can perform sample acquisitions and where the LCquan system can store the acquired sample data:

- Scenario A—Acquired sample data stored on a standalone workstation (local users)
- Scenario B—Acquired sample data stored on a workstation that is on a network (domain users)
- Scenario C—Acquired sample data stored on a network server (domain users)

A scenario B or C configuration can be integrated with a laboratory information management system, such as the Watson LIMS. If you are using a Watson LIMS, refer to *Installing and Using the Peak View Gateway Between Watson and LCquan*.

For scenario C, the LCquan system supports the Thermo Scientific Web Access Server environment for LCquan workstations that are for data review only. Web Access can provide application virtualization to manage LCquan configuration and maintenance. An instance of the LCquan application running on a Web Access server cannot be used for acquisition. The IT professional is responsible for installing LCquan software on the Web Access server.

For scenario C, the LCquan system supports remote acquisition. During remote acquisition, you can have the application time-stamp raw files and create a time-stamped folder:

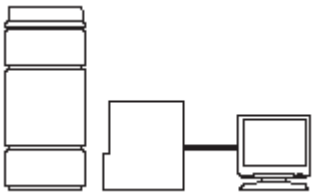
- Remotely stored raw files are time-stamped with the submission time.
- All raw files in a sequence share the same time stamp.
- Pausing during acquisition does not change the time stamp.
- The time stamp for the raw files folder and the time stamp for the raw files are not necessarily the same.

Or, you can prevent the LCquan application from time-stamping the raw files during a remote acquisition by setting the permission from the Expand Tree list: LCquan > Acquisition Section > Prevent Raw File Time-Stamping When Doing Remote Acquisition to Allowed in the Thermo Foundation Authorization Manager.

IMPORTANT The LCquan application can overwrite a raw file of the same name if you turn off time-stamping.

Figure 1. Scenarios for LCquan sample acquisition

A. Acquisition to a standalone LCquan system

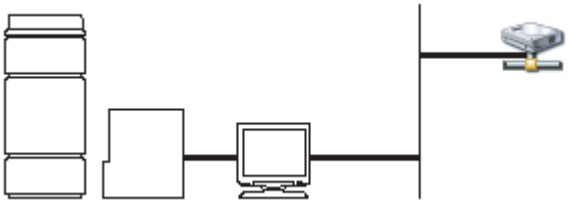


LCMS system

Workstation **(LCquan data storage)**

Local acquisition
Local user
Standalone workstation

B. Acquisition to a standalone LCquan system on a network



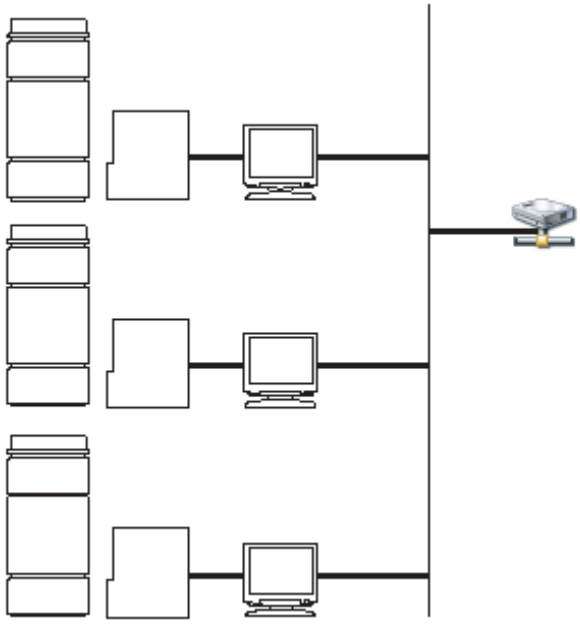
Server

LCMS system

Workstation **(LCquan data storage)**

Local acquisition
Domain users
Networked workstation but data stored locally
(LIMS option)

C. Acquisition to a network server



Server **(LCquan data storage)**

LCMS system

Workstations

Network acquisition
Domain users
Networked workstations
(LIMS option, Web Access option)

LCquan Folder Structure

The LCquan folder structure includes the following:

- Security folder—Contains the configuration files. Thermo Foundation Authorization Manager retrieves the controlled feature information from the configuration files in the Security folder. The file path for the security folder is as follows:

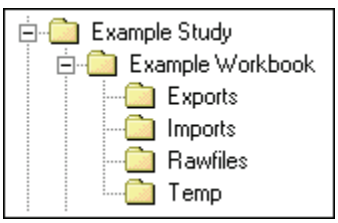
  C:\ProgramData\Thermo Scientific\INI

- Root folder or folders—Contain the LCquan projects.
  - For storing the acquired data locally, you can use the default folder, \Xcalibur\QuanRoot, or you can create your own LCquan root folder. Go to Scenarios for LCquan sample acquisition, scenario A.
  - For storing the acquired data on a network server, you must designate a folder on the network server as the LCquan root folder.

For each new project, the LCquan application creates the following hierarchical folder structure within the designated root folder (see Figure 2).

- Study folder—Top-level folder within the root folder. Each study folder contains one or more workbook folders. The study folder can contain any number of workbook folders, but each workbook must have a unique name.
- Workbook folder—Contains all the information that the LCquan application uses for an individual quantitative analysis project. The workbook folder contains the LCquan file (.lqn), the instrument method file (.meth), and an audit database (.mdb). The workbook folder also contains the following:
  - Exports folder—Stores copies of all files that the application exports, such as report files.
  - Imports folder—Stores a copy of legacy files that you import into the workbook, such as instrument method files, processing method files, or sequence files.
  - Rawfiles folder—Contains acquired data files (.raw files) and any imported raw data files.
  - Temp folder—Contains temporary files used by the LCquan application.

Figure 2. LCquan folder structure



Secure User Groups

The LCquan application requires both the security features of the Windows 7 operating system and the Thermo Foundation Authorization Manager to define the LCquan secure user groups and permissions. Typically, the IT professional is responsible for establishing Windows user accounts and user groups. The laboratory administrator is responsible for setting up the permission levels in the Authorization Manager and, if necessary, private groups.

- Windows user groups
  - The IT professional creates and manages domain user accounts and user groups. Go to Scenarios for LCquan sample acquisition, scenarios B and C.
  - You or the IT professional can create standalone workstation user accounts and user groups. Go to Scenarios for LCquan sample acquisition, scenario A.

  IMPORTANT Each Windows user account must be associated with a user ID, a password, and a full description. These items are required for the system to store the auditing information in the designated database.

- Authorization Manager private groups—A group can be either a preexisting Windows user group or a private group that you configure within the Foundation Authorization Manager.
  - Networked workstation—A user must be a member of a domain user group before you can add the user to a private group. If an intended user is not a user on the domain, the IT professional must create a user account for the user. Go to Scenarios for LCquan sample acquisition, scenarios B and C.
  - Standalone workstation—A user must have a logon account for the workstation before you can add the user to a private group. You or the IT professional must create a user account for each intended user. Go to Scenarios for LCquan sample acquisition, scenario A.

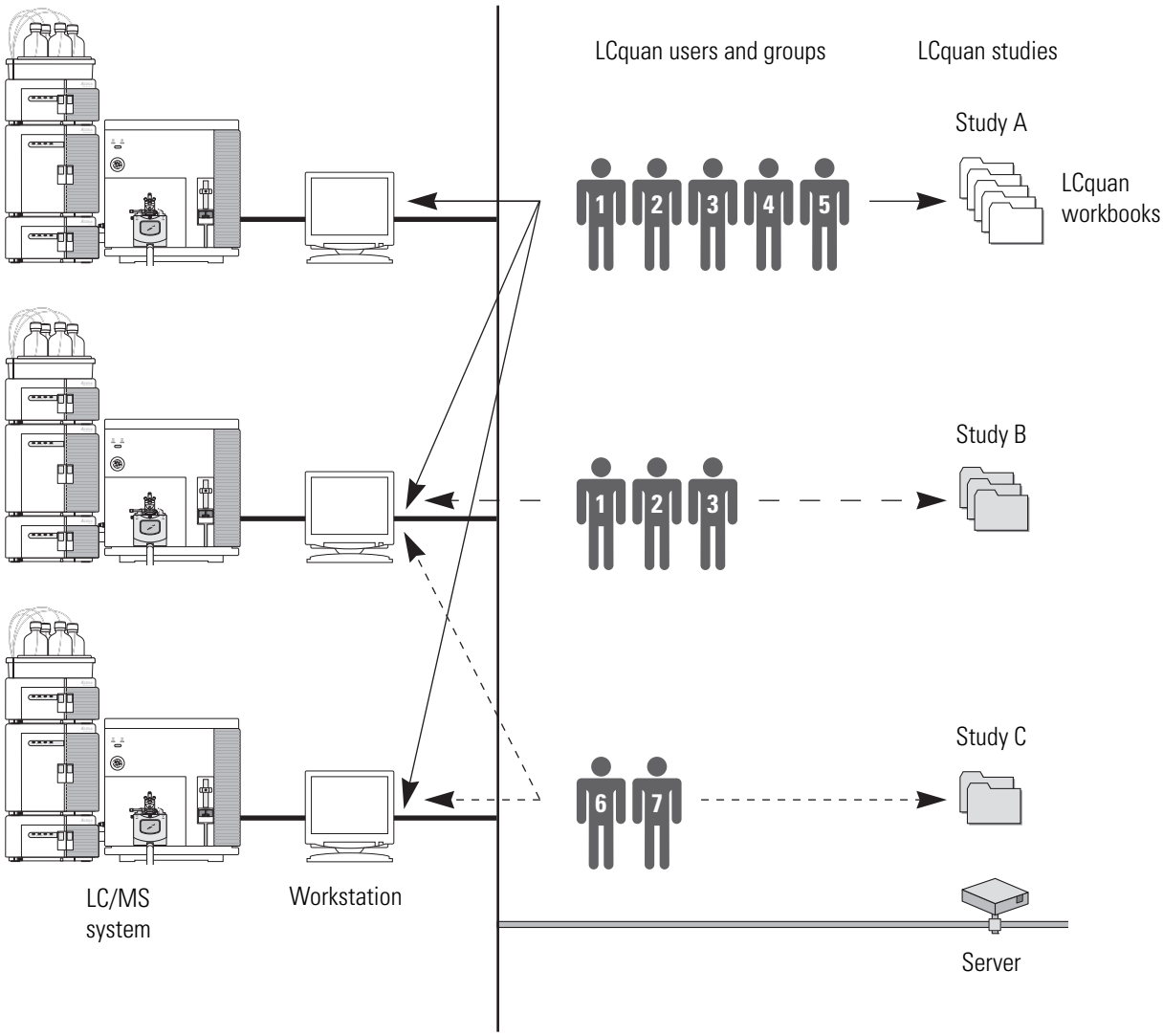
As the laboratory administrator, you must make the following decisions before asking your IT professional to configure Windows user groups for domain users or before configuring private groups in the Foundation Authorization Manager:

- Types of user roles, for example, administrator, supervisor, scientist, technician, auditor, or quality assurance
- Individuals assigned to each user role and their projects
- Permissions for a given user role, such as the authority to create methods and acquire data, signature authority, or read-only access to workbooks

For example, a laboratory might have standard operating procedures that prohibit technicians from performing certain operations with the software. But the same laboratory might not have any restrictions on software operations that the scientists can perform. In this case, you must create at least two user groups—one for scientists and one for technicians.

A user can belong to more than one user group. In the following example, users 1, 2, and 3 belong to more than one user group.

Figure 3. LCquan system users and user groups example



Configuration Tasks of the Laboratory Manager and IT Professional

As the laboratory administrator, you must work with your IT professional to configure the security features. Table 1 lists the tasks the laboratory administrator and IT professional perform.

IMPORTANT The local IT administrator must configure the security features and settings for Windows.

Table 1. Configuration tasks checklist (Sheet 1 of 2)

Task	Refer to topic	Role	Completed?
1. Install software for Xcalibur and LCquan on the designated workstations.	*Thermo LCquan 2.7 Installation Guide* in the LCquan 2.7 Upgrade Kit	IT professional or laboratory administrator	
2. Run the database configuration application.	Chapter 2, "Using the Database Configuration Manager."	IT professional (Oracle™ database) or laboratory administrator	
3. Ensure that the Finnigan Security Server is properly configured and running.	"Verifying the Properties of the Finnigan Security Server" on page 17.	IT professional or laboratory administrator	
4. Determine which folder to use as the LCquan secure root folder and identify the secure user groups.	"LCquan Folder Structure" on page 6 and "Secure User Groups" on page 7.	Laboratory administrator	
5. Configure security settings for Windows: a. Set up users and groups. b. Specify the password lockout parameters for failed logon attempts. Refer to your company's guidelines. c. Restrict access to the secure root folder. Ensure users have permissions to write to the secure root folder.	"Configuring Security Settings for Folders and Files" on page 22.	IT professional (Laboratory administrator can also restrict access to the secure root folder.)	
6. Configure sequential user logon and automatic logoff.	"Specifying the Way Users Log On and Off" on page 38.	IT professional or laboratory administrator	

Table 1. Configuration tasks checklist (Sheet 2 of 2)

Task	Refer to topic	Role	Completed?
7. Configure Authorization Manager settings for the LCquan application:	"Using the Authorization Manager" on page 44.	Laboratory administrator	
a. Define LCquan user groups.	"Setting Up Secure User Groups" on page 45.		
b. Set permission levels for software features for each LCquan user group.	"Setting Permissions" on page 48, and Appendix A, "Permission Level Settings in the LCquan Application."		
c. If users are permitted to change the secure root folder, define the list of secure folders.	"Defining the List of Secure Folders" on page 54.		
d. Specify whether users are required to make comments.	"Viewing the Authorization Manager History Log" on page 59.		
e. Save the configuration settings.	"Saving the Security Settings" on page 61.		

Figure 4 and Figure 5 show flowcharts of the configuration process for domain users and local users, respectively.

Figure 4. Configuration tasks of the laboratory administrator and IT professional for domain users

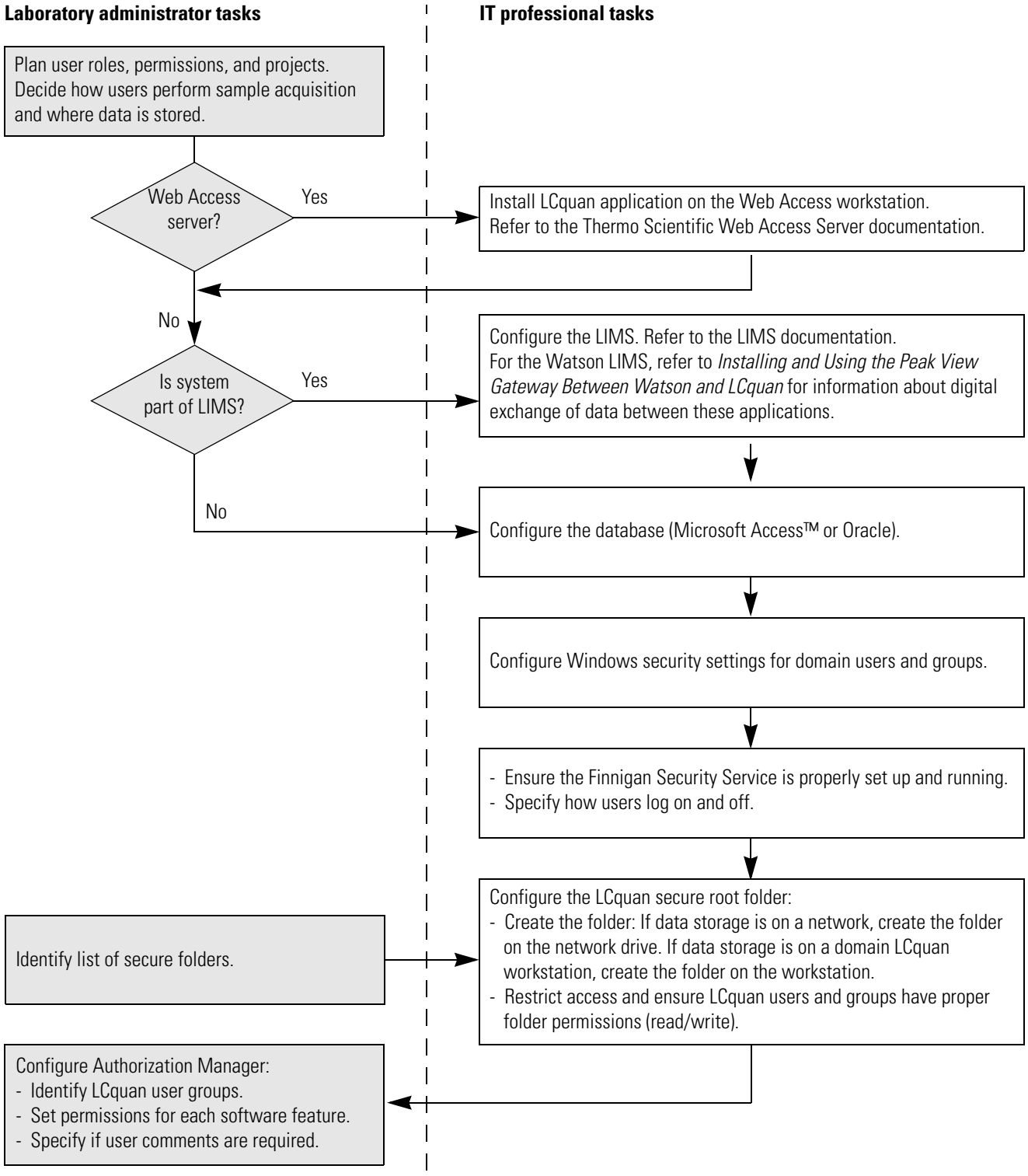
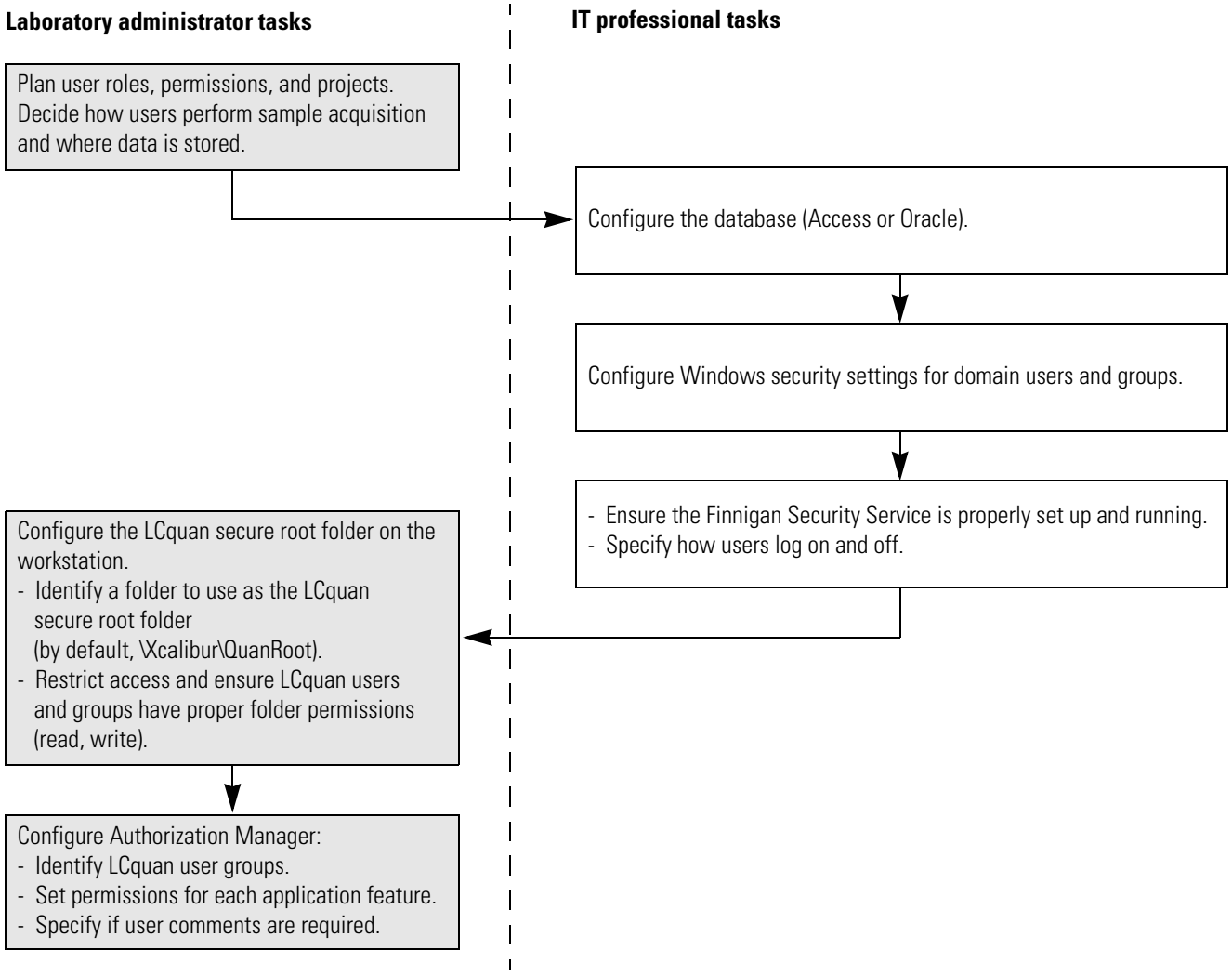


Figure 5. Configuration tasks of the laboratory administrator and IT professional for local users



Using the Database Configuration Manager

This chapter describes how to use the Database Configuration Manager to configure your compliance database. The compliance database keeps a record of auditable events and changes made to files that the Xcalibur data system creates and manages. Until you run the Database Configuration Manager, all applications run without auditing and might not be in compliance.

Contents

Using Microsoft and Oracle Databases

The LCquan application uses a Microsoft Access™ database to store each LCquan workbook audit trail. To store the Xcalibur Global audit trail, you can use either of the following:

- Oracle database on a network workstation or server (remote system)
- Microsoft Access database on a standalone or networked workstation or server

If the Watson LIMS is part of the workflow, refer to the Watson documentation for database setup instructions that are specific to the Watson LIMS.

To use an Oracle database, make sure that you complete the following tasks:

1. If the site does not have an Oracle server, version 11g or later, install an Oracle database on an accessible remote server. For more information, consult your Oracle database administrator.
2. Install the Oracle client software on your local system. For more information, consult your Oracle database administrator.
3. If you do not know the user name, password, and Oracle Net Service Name of your Oracle database, obtain this information from your Oracle database administrator.

IMPORTANT Ensure that no other Xcalibur applications are running at the same time as the Database Configuration manager. Auditing of Xcalibur applications cannot take place while running the Database Configuration manager.

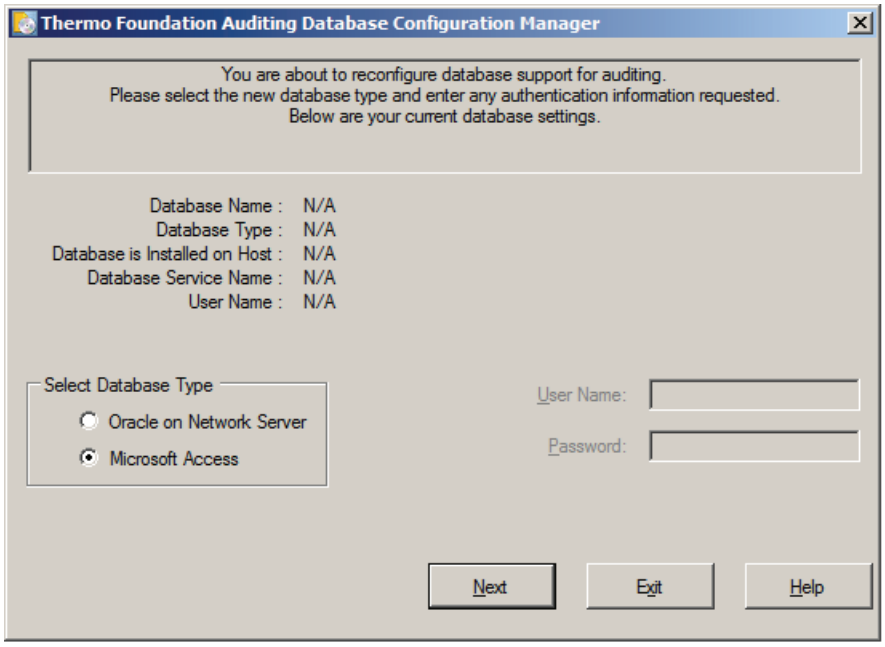
Configuring Your Auditing Database

This section describes how to use the Database Configuration manager to configure your auditing database.

❖ To configure your auditing database

1. From the Windows taskbar, choose **Start > All Programs > Thermo Foundation 2.0 > Database Configuration**.

   The Thermo Foundation Auditing Database Configuration Manager opens.



2. In the Select Database Type area, select the database type:

   - If you are using an Access database, select the **Microsoft Access** option and go to step 4.
   - If you are using an Oracle database, select the **Oracle on Network Server** option and go to step 3.

3. For an Oracle database, specify the Oracle database parameters:

   a. In the User Name box, type the database user name.

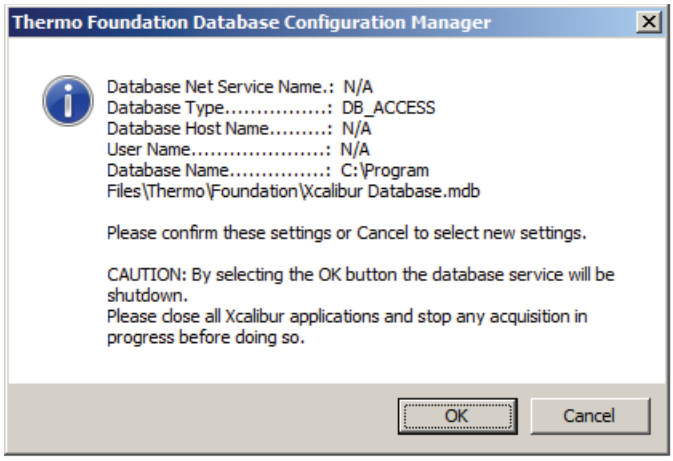
   b. In the Password box, type the database password.

   c. In the Oracle Net Service Name list, select the Oracle Net Service Name for your database.

   Note Be sure to use the Oracle user name and password provided by your Oracle database administrator.

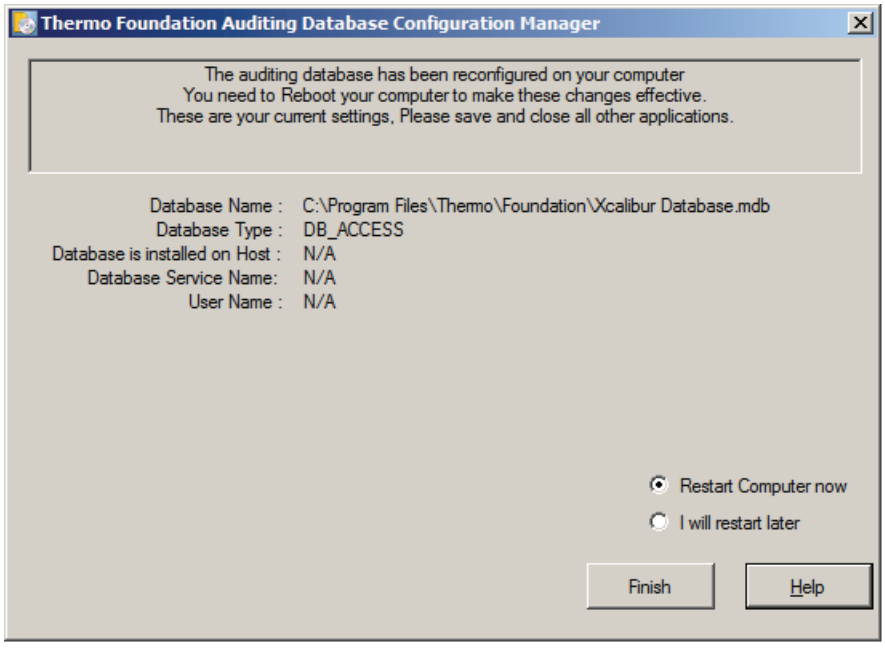
4. Click **Next**.

   The Thermo Foundation Database Configuration Manager dialog box opens.



5. Verify that the settings in the Thermo Foundation Auditing Database Configuration Manager dialog box are correct and click **OK**.

   The next page of the Thermo Foundation Auditing Database Configuration Manager opens.



6. Select a restart option:
   - To automatically restart the computer, select the **Restart Computer Now** option.
   - To manually restart the computer at a later time, select the **I Will Restart Later** option.

   Note The changes made in the Database Manager take effect after restarting the computer.

7. Click **Finish** to save your settings and close the Auditing Database Configuration Manager.

Establishing Secure File Operations

You must protect records to allow for their accurate and ready retrieval, and previously recorded information cannot be obscured by record changes. To comply with these requirements, you must store all electronic records in protected folders and you must establish standard operating procedures for precise and systematic record archiving.

Contents

Verifying the Properties of the Finnigan Security Server

The Finnigan Security Server has two main functions:

- User authentication—If you select authentication for certain events using the Foundation Authorization Manager, the Security Server verifies user names and passwords whenever they are entered.
- Secure file operations—You can set the Security Server to take ownership of the data folders and files. This security measure prevents users from deleting data they own.

When you install the application, the Security Server is installed and started. It is configured to start automatically every time the computer is restarted.

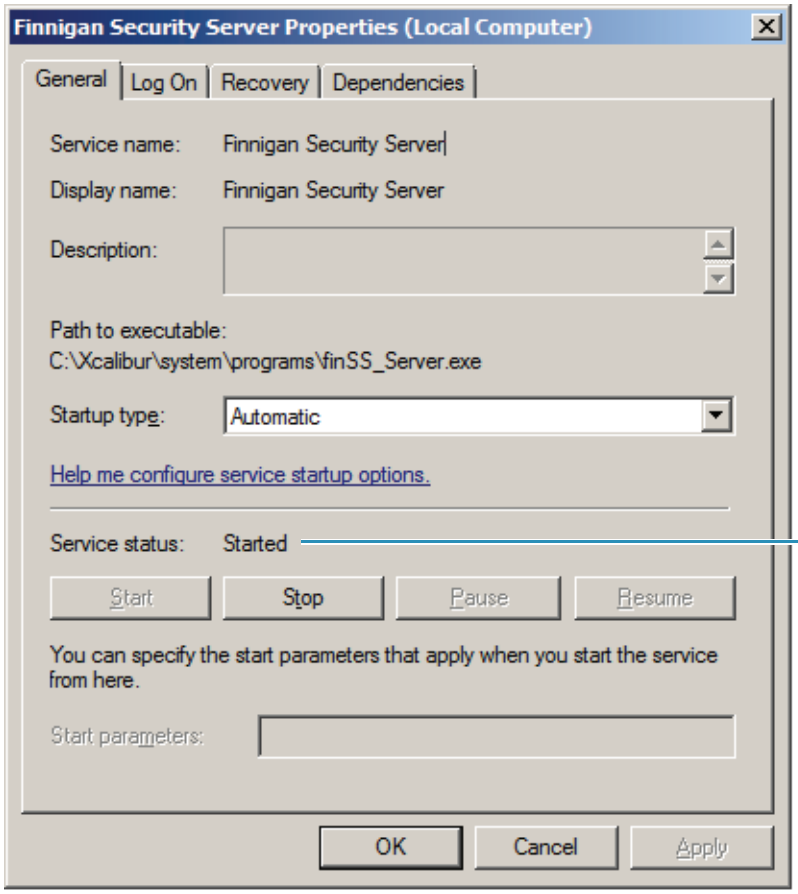
IMPORTANT You must prevent unauthorized users from stopping the Security Server. If the Security Server is stopped, the security features in the application do not function properly.

Only the system administrator who installed the application software and the Security Server, or someone who has administrative rights, can stop the server.

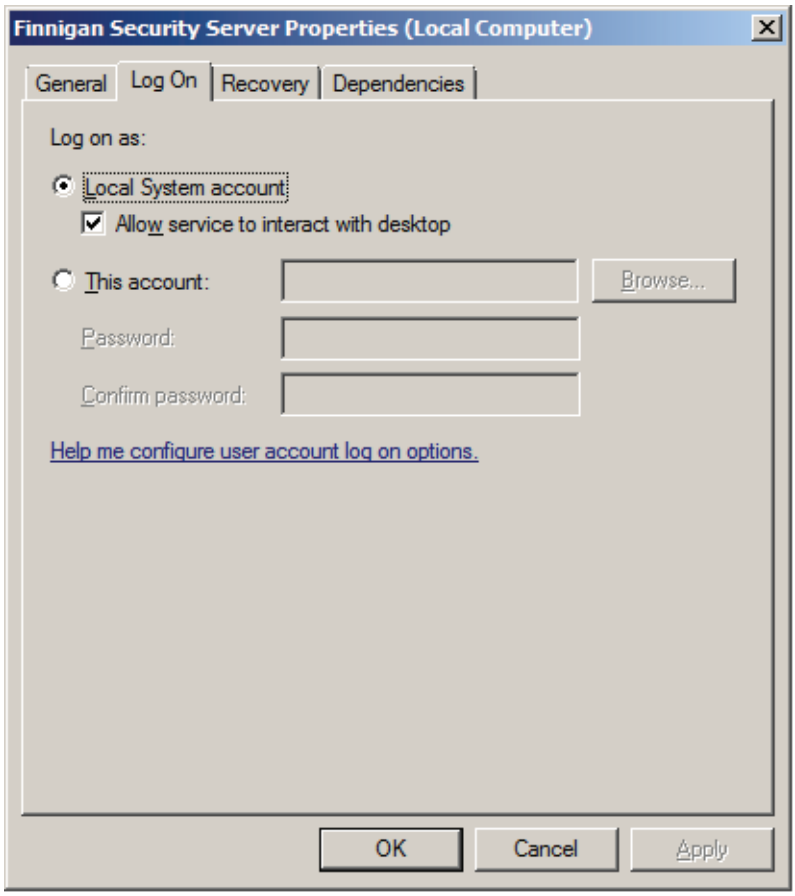
❖ To verify that the properties of the Security Server are set correctly

1. Open the Windows Services feature as follows:
   a. From the Windows taskbar, choose **Start > Control Panel > System and Security**.
   b. Click **Administrative Tools**.
   c. Double-click **Services**.
2. Right-click **Finnigan Security Server**, and choose **Properties** from the shortcut menu.

   The Finnigan Security Server Properties dialog box opens to the General page.
3. On the General page, set Startup Type to **Automatic**.
4. Ensure that the Service Status reads **Started**.



5. Click the **Log On** tab.



6. On the Log On page, select the **Local System Account** option.
7. Select the **Allow Service to Interact with Desktop** check box.
8. Click **OK** to close the Finnigan Security Server Properties dialog box.
9. Close the Services window, and then close the Administrative Tools window.

You have now confirmed that the Security Server is properly set up.

Verifying the Properties of Thermo Foundation DatabaseService

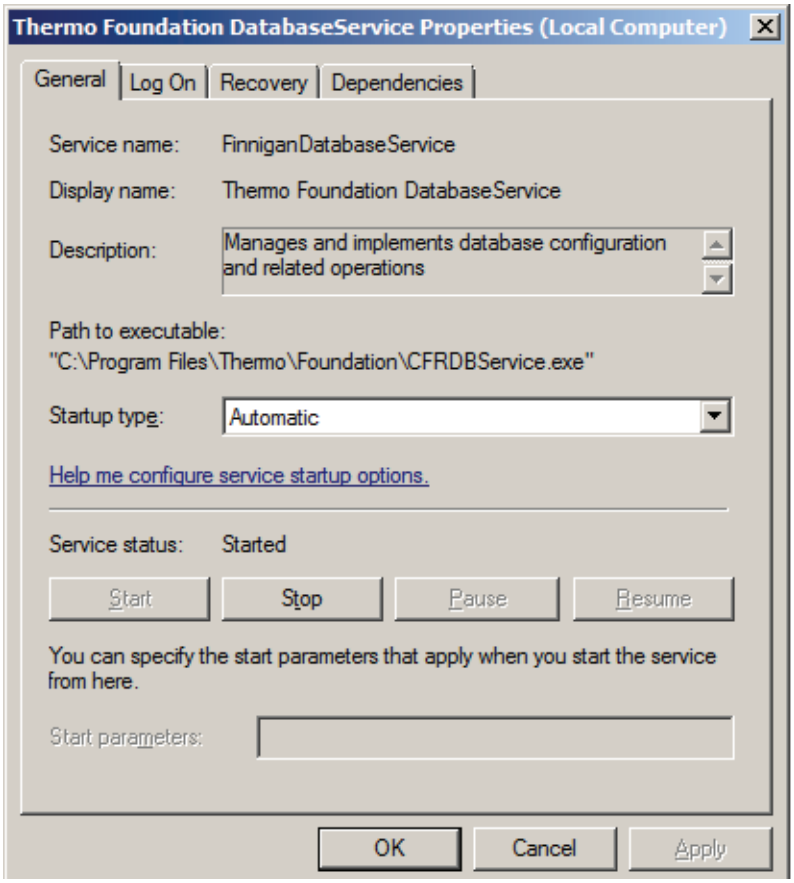
Using Thermo Foundation DatabaseService, Xcalibur applications can access the auditing database and make auditing entries.

Verify that the properties of the Foundation Database Service are correctly specified.

❖ To verify properties of Foundation DatabaseService

1. Open the Windows Services feature as follows:
   a. From the Windows taskbar, choose **Start > Control Panel > System and Security**.
   b. Click **Administrative Tools**.
   c. Double-click **Services**.
2. Verify properties for Foundation DatabaseService:
   a. Right-click **Thermo Foundation DatabaseService**, and choose **Properties** from the shortcut menu.

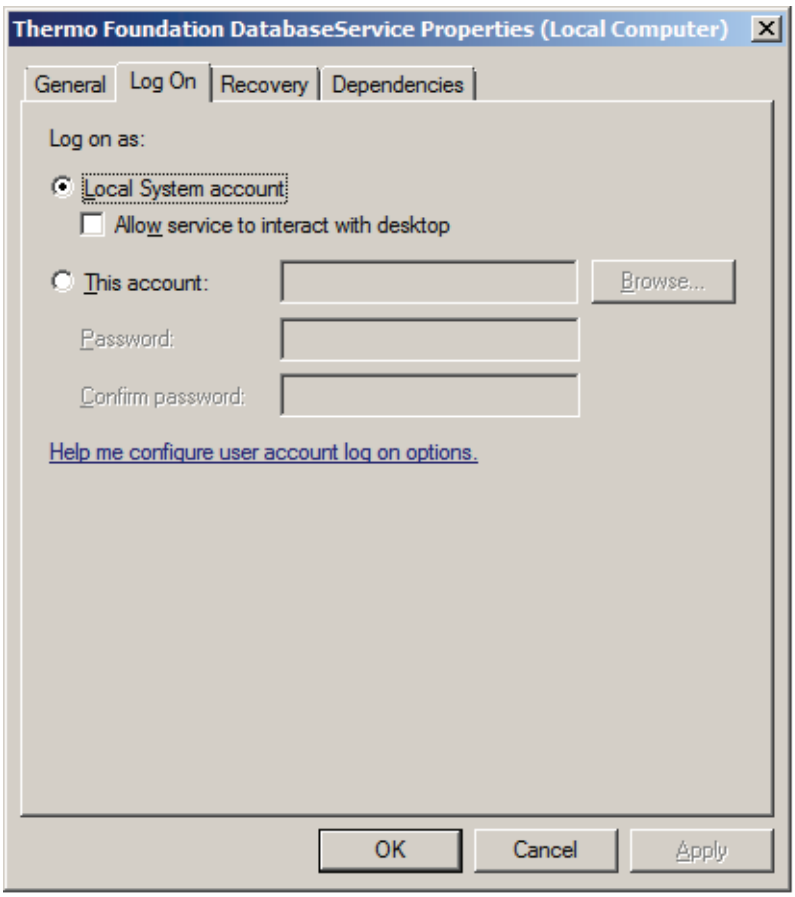
      The Thermo Foundation DatabaseService Properties dialog box opens to the General page.



b. Ensure that the Startup Type is set to **Automatic**.

c. Ensure that the Service Status reads **Started**.

d. Click the **Log On** tab.



e. Ensure that the **Local System Account** option is selected.

f. Ensure that the **Allow Service to Interact with Desktop** check box is cleared.

g. Click **OK** to close the Thermo Foundation DatabaseService Properties dialog box.

3. Close the Services window, and then close the Administrative Tools window.

You have now confirmed that the services are properly set.

Configuring Security Settings for Folders and Files

To ensure the security of your data, you must restrict access to the following folders and the files contained within them:

- Root folder or folders—Contain the LCquan projects. See "LCquan Folder Structure" on page 6. You cannot permit non-administrators to delete files within the root folder.
- Security folder—Contains the configuration files. Because the Foundation Authorization Manager reads the controlled feature information from the configuration files, you must prohibit non-administrators from accessing these files. The security folder is located in the following folder:

  C:\ProgramData\Thermo Scientific\INI

With the New Technology File System (NTFS—an advanced file system used within the Windows operating system), you can set the access permissions for folders and files for specific user groups. When you set up permissions, you specify the level of access for user groups. For example, you can do the following:

- Allow members of one user group to read the contents of a file.
- Allow members of another user group to make changes to the file.
- Prevent members of all other user groups from accessing the file.

New subfolders and files inherit folder permissions. You can make existing subfolders and files inherit new permissions that have been applied to the parent folder by using the Properties dialog box for the folder. (See "Preparing a Root Folder" on page 23.)

After you set the appropriate permissions, an unauthorized user cannot maliciously or accidentally alter previously recorded information using utilities such as Windows Explorer.

This section contains the following topics:

Configuring Security Settings for the Root Folder

You must create a root folder or folders for your data and configure the proper security settings for each folder. To do this, use the Security tab of the Properties dialog box to add users and groups and set the permissions for each.

In the procedures that follow, add an administrative user (or administrative group) and the group Everyone to the Permission Entries list. Then, grant the administrator full access to the folder and grant limited access to everyone else.

Tip To further restrict access to folders and files, you can grant access to specific user groups only. To do this, first set up appropriate user groups, as described in "Adding Windows Users and Groups" on page 28, and then perform the procedures that follow, using your specific user groups instead of the group Everyone.

Continue with the following topics:

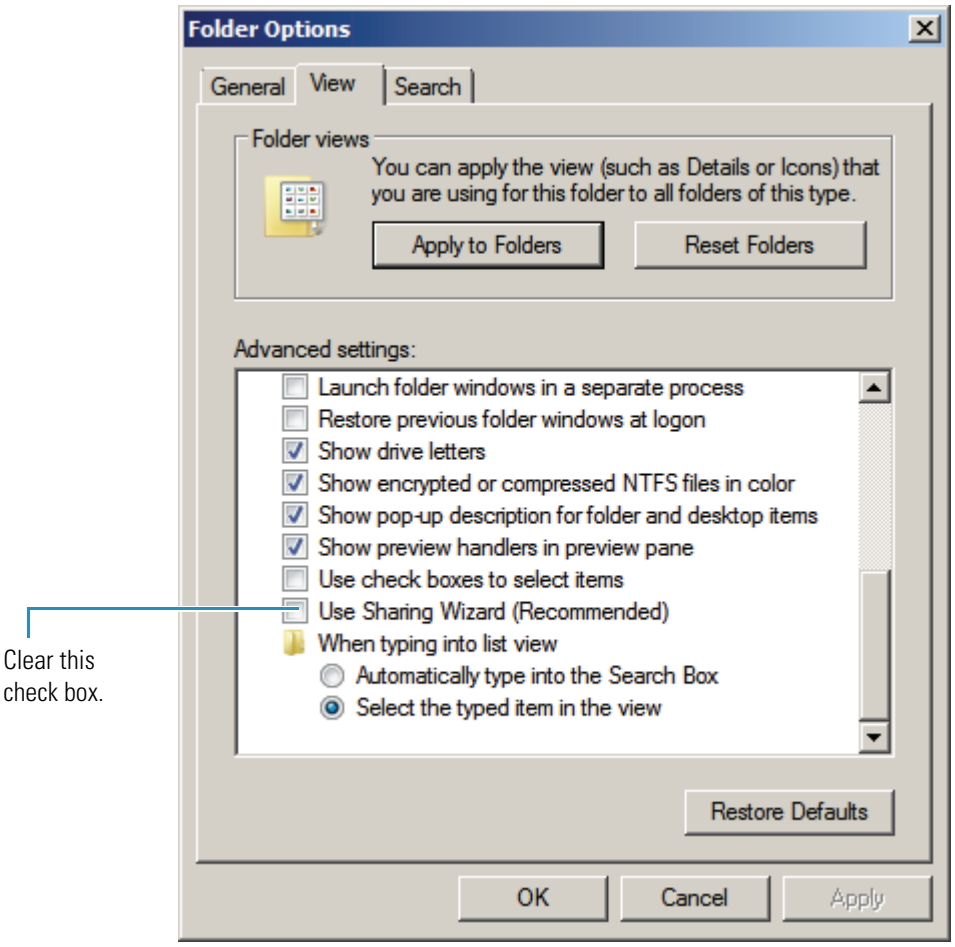
Preparing a Root Folder

To prepare a root folder, first turn off Use Simple File Sharing in folders. You can then create a root folder for storing all your projects.

❖ To turn off Use Simple File Sharing

1. Log on to the system as a user with administrative privileges.
2. From the Windows taskbar, choose **Start > All Programs > Accessories > Windows Explorer**.
3. Choose **Organize > Folder and Search Options**, and then click the **View** tab.

4. In the Advanced Settings list, at the bottom, clear the **Use Sharing Wizard** check box.



5. Click **OK** to save the change and close the Folder Options dialog box.

❖ To create or locate a folder to use as the root folder for storing all projects

1. Create or use any folder (except the Xcalibur folder).

   In this example, the folder is named Study.

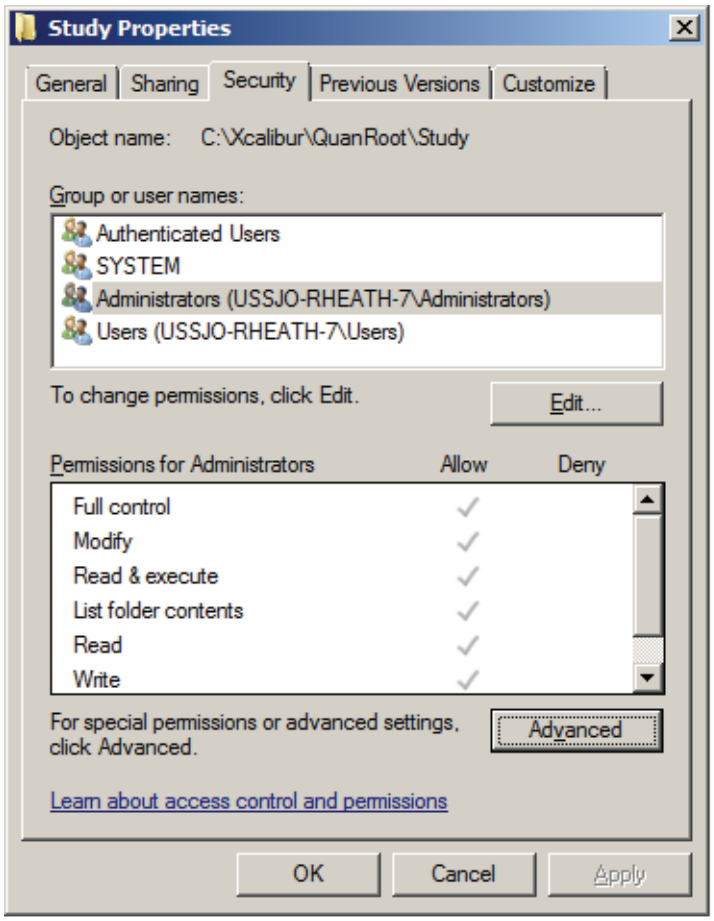
   For example, you can use the QuanRoot folder (located in the Xcalibur folder) as the root folder for LCquan projects. This folder is created on your system when you load the LCquan software.

   IMPORTANT Do not use the Xcalibur folder as your root folder. If you change the permission settings for this folder, Xcalibur applications will not run correctly. Instead, create a new folder or use another existing folder as your root folder.

2. Right-click the folder and choose **Properties** from the shortcut menu.

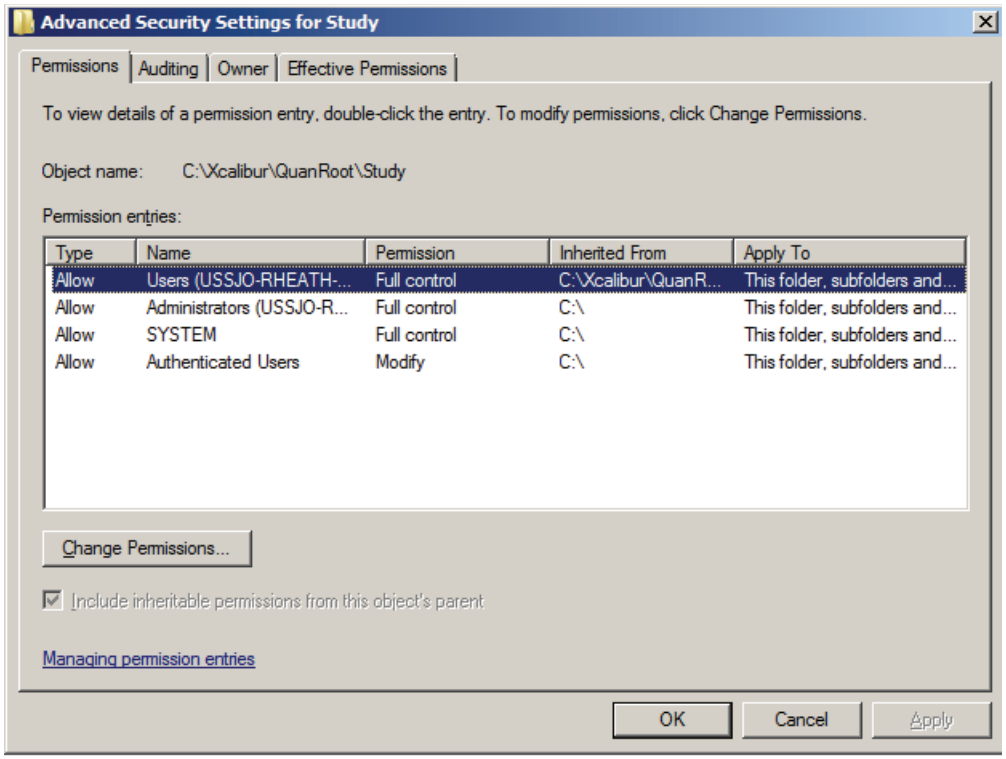
   The Properties dialog box for the folder opens.

3. Click the **Security** tab.



4. Click **Advanced**.

The Permissions page of the Advanced Security Settings dialog box opens.

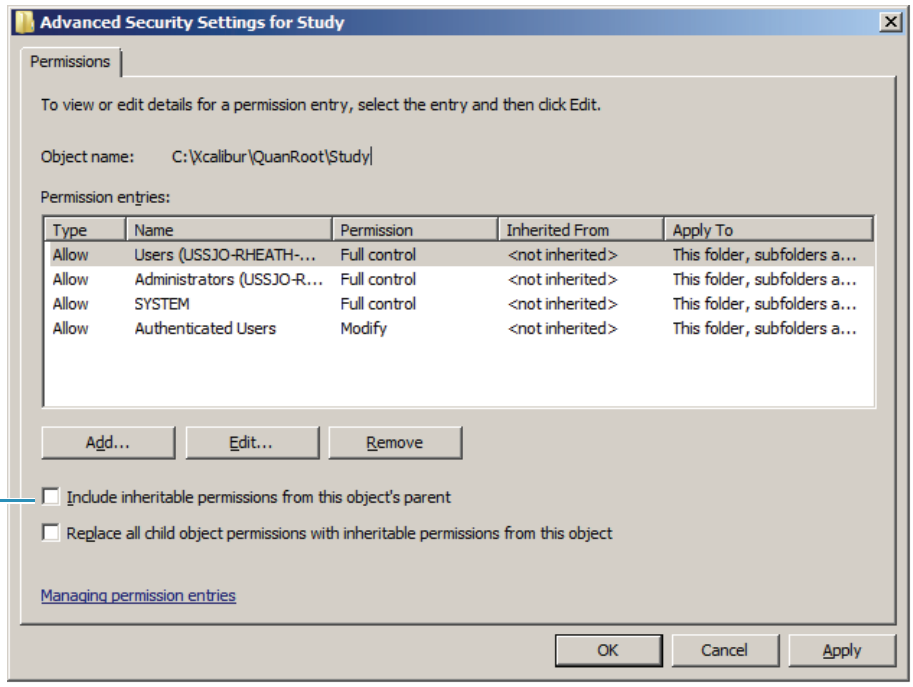


IMPORTANT When you create a new root folder, the permissions from the parent folder automatically propagate to the new folder, indicated by:

- Shaded check boxes in the Permissions list
- In the Advanced Security Settings dialog box, selection of the check box labeled "Inherit from parent the permission entries that apply to child objects. Include these with entries explicitly defined here."

IMPORTANT Normally, you do not want to allow your secure root folder to inherit permissions from the parent folder. Prevent this inheritance by clearing the Inherit From Parent… check box in the next steps. Then correct the permissions in the topic "Setting Permissions" on page 31.

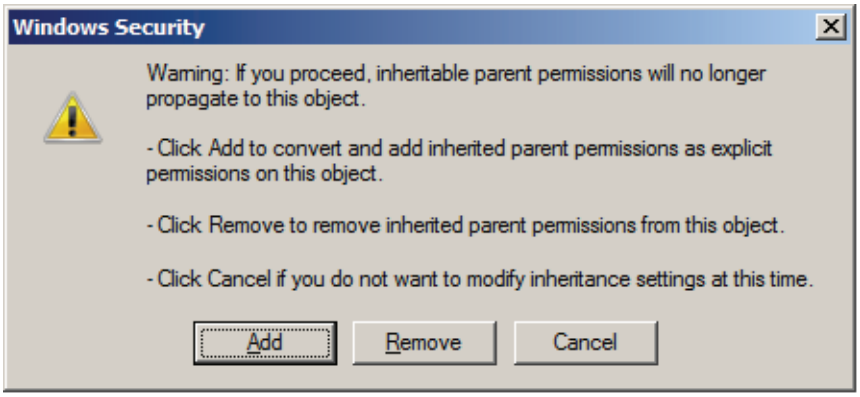
5. Click **Change Permissions** to display the permission entries.



Clear this check box.

6. Clear the **Include Inheritable Permissions…** check box.

   The Windows Security dialog box opens.



7. To copy the inherited permissions to the new folder, click **Add**.

8. Click **OK** to close the Advanced Security Settings dialog box.

   You will correct the permission settings later.

   Note After you clear the Inherit From Parent… check box and copy the inherited permissions to the new folder, the new root folder no longer inherits permissions from the parent folder. If someone then changes the permission settings of the parent folder, the permission settings of the new root folder do not change. However, any subfolders created under the new root folder still inherit the permissions from the root folder.

9. On the Security page of the Properties dialog box, examine the Group or User Names list and notice which groups or users appear in the list.

   You want only the group Everyone and your administrator name (or the name of the administrator group) to appear in this list.

   - If either is missing from the list, go to the next topic "Adding Windows Users and Groups."
   - If both appear in the list, and additional groups or users also appear in the list, go to "Removing Unnecessary Users" on page 30.
   - If both appear in the list, and no additional groups or users appear in the list, go to "Setting Permissions" on page 31.

Adding Windows Users and Groups

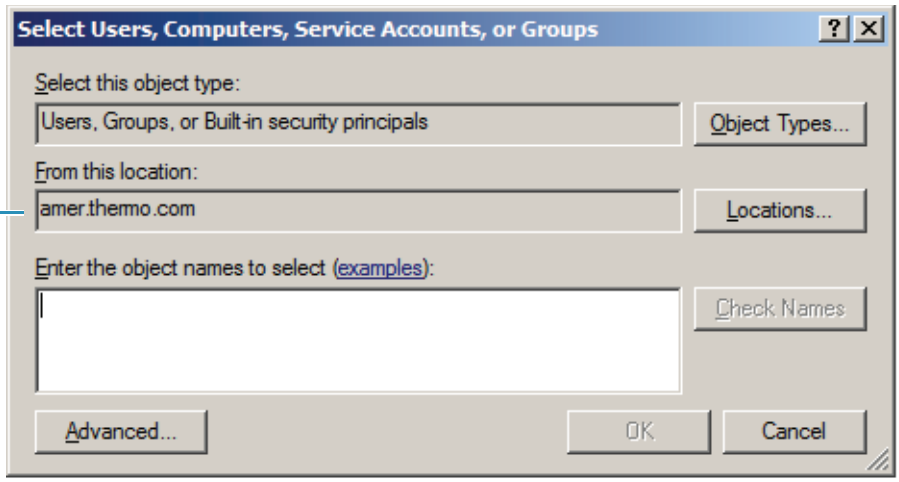
In preparation for setting permission levels for the folder, you might need to add users and groups to the Group or User Names box on the Security page.

IMPORTANT Each Windows user account must be associated with a user ID, password, and full description. These items are required for the system to store the auditing information in the designated database.

❖ To add users and groups

1. On the Security page of the Properties dialog box, click **Edit** and then **Add**.

   The Select Users, Computers, Service Accounts, or Groups dialog box opens.



Network name (if domain users on network)
–or–
workstation name (if local users on standalone workstation)

2. Ensure that the Select This Object Type box contains the object types that you require (Users, Groups, or Built-in security principals).

   To change the list of objects, click **Object Types**. In the Object Types dialog box, edit the list of objects (for example, Users and Administrator) and click **OK**.

3. Ensure that the From This Location box lists the root location that contains your users and groups.

   To change the location, click **Locations**. In the Locations dialog box, specify a new location and click **OK**.

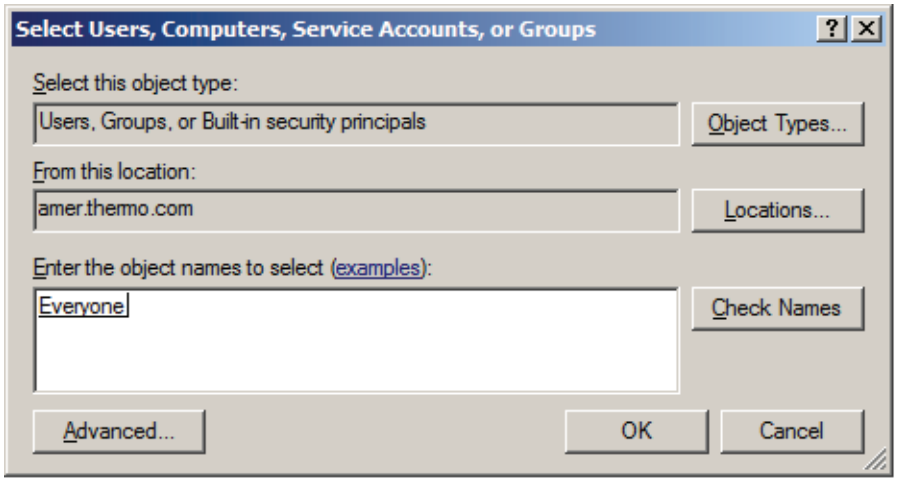
4. In the Enter the Object Names to Select box, type the names of the users or groups that you want to add:

   - If the group Everyone is missing from the Permission Entries list on the Security tab, type **Everyone**.
   - If your administrator name (or the name of the administrator group) is missing from the Permission Entries list on the Security page, type the appropriate user name or group name.

   Tip You can enter multiple object names at the same time by separating the names with a semicolon.

5. To search for the specified users or groups, click **Check Names**.

   All similar or matching object names that were found appear underlined in the Enter the Object Names to Select box.



6. In the Enter the Object Names to Select box, ensure that only the correct object name or names appear and click **OK**.
7. In the Properties dialog box, click the **Security** tab.

   Ensure that only the following entries appear in the Permission Entries box:

   - Administrators (administrator name)
   - Everyone

   If no additional groups or users appear, go to Setting Permissions.

   If additional groups or users appear, you must remove them. Go to Removing Unnecessary Users.

Removing Unnecessary Users

You must remove unnecessary users or groups from the Group or User Names box on the Security page.

❖ To remove the names

1. On the Security page of the Properties dialog box, click **Edit**.

   The Permissions dialog box opens.

2. In the Group or User Names box, select the name of the unnecessary user or group and click **Remove**.
3. Repeat this step to remove any other unnecessary users or groups.

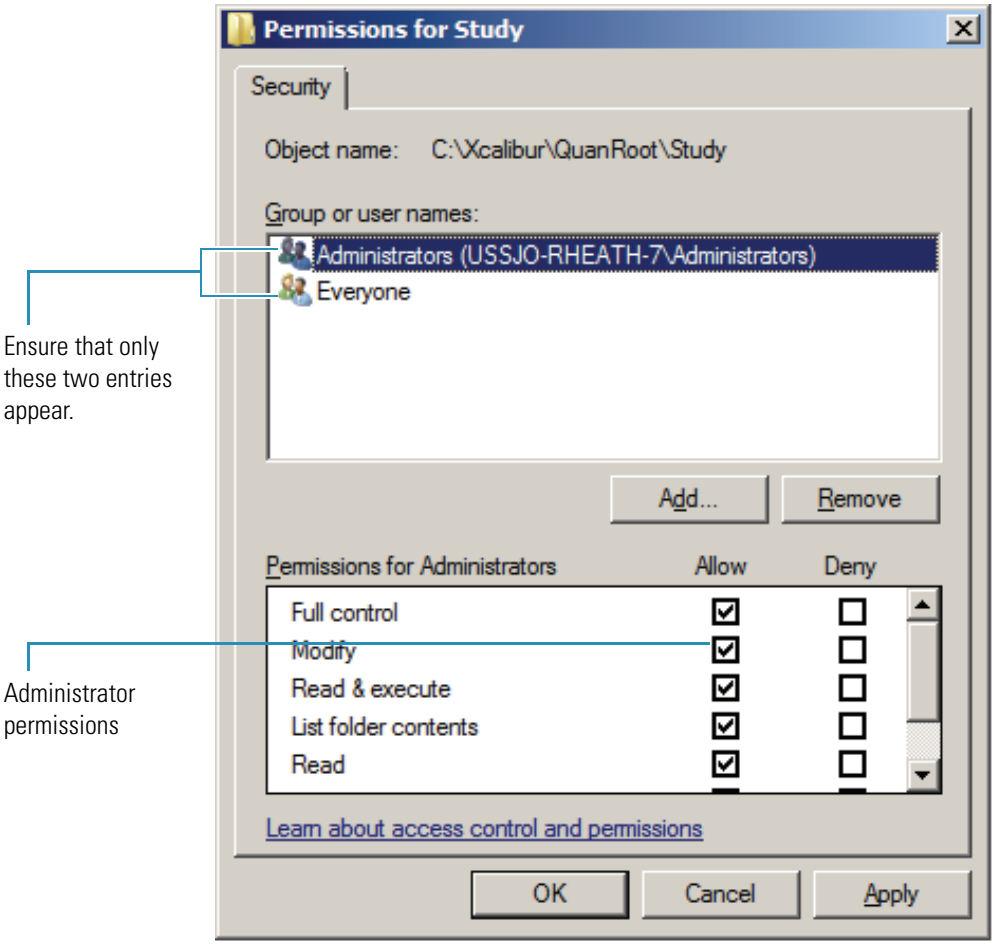
Setting Permissions

After the correct users and groups are in the Group or User Names box on the Security page of the Properties dialog box, set the permissions.

❖ To set the permissions

1. In the Group or User Names box, select the administrator (or the administrator group).
2. In the Permissions for Administrators list, select the **Allow** check box for Full Control.

   All the other check boxes in the Allow column are automatically selected.



IMPORTANT Groups or users who are granted Full Control for a folder can delete files and subfolders within that folder, regardless of the permissions protecting the files and subfolders.

3. In the Group or User Names box, select **Everyone**.

4. In the Permissions for Administrators list, select **Allow** for each of the following:
   - Read & Execute
   - List Folder Contents
   - Read
   - Write
5. Clear the **Allow** check box for all other actions in the list, then click **OK**.

   Note Setting these permissions ensures that none of the files in the folder can be deleted by using Windows Explorer.
6. Ensure that the inheritance setting is correct as follows:
   a. Click **Advanced**.

      The Advanced Security Settings dialog box opens.
   b. Click **Change Permissions**.
   c. Ensure that the **Include Inheritable Permissions…** check box is cleared.
   d. Click **OK**.
7. In the Advanced Security Settings dialog box, click **OK**.
8. In the Properties dialog box, click **OK**.

You have configured the security settings for the root folder. You are now ready to configure the security settings for the Security folder.

Configuring Settings for the Security Folder

The procedure for configuring the security folder is similar to that for configuring the root folder. For the security folder, you must grant full access rights only to the administrator and read-only access rights to everyone else.

For additional information about any step, see "Configuring Security Settings for the Root Folder" on page 23.

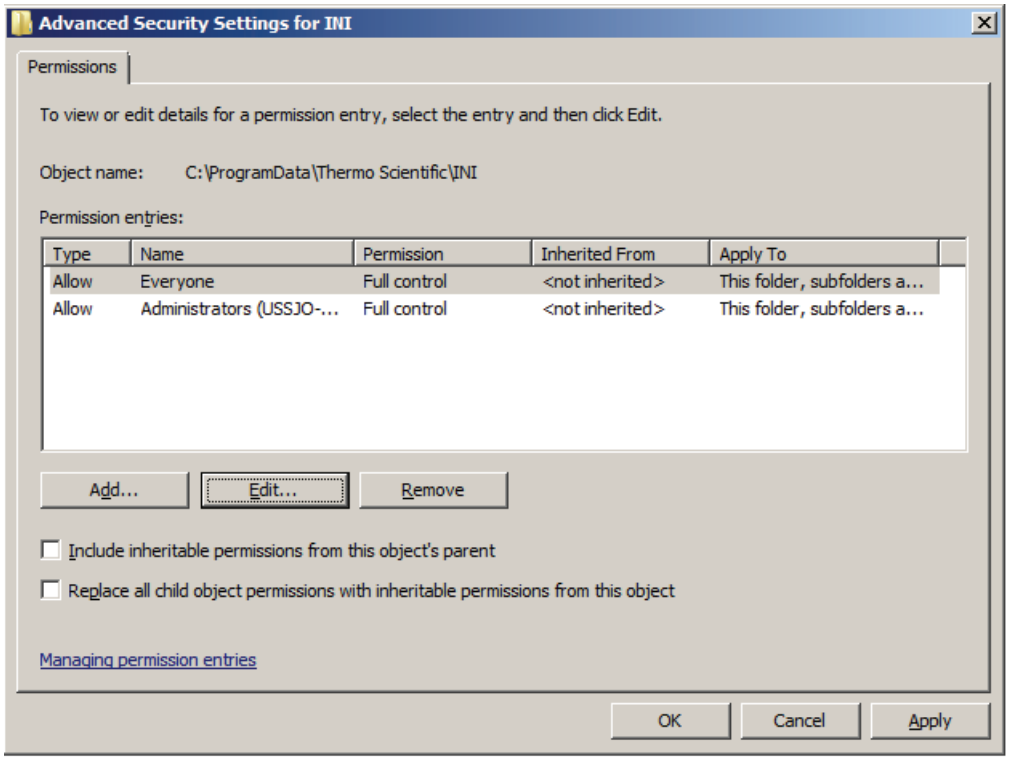
❖ To configure the Security folder

1. Use Windows Explorer to locate the Security folder.

   The folder path is as follows:

   C:\ProgramData\Thermo Scientific\INI
2. Right-click the **INI** folder and choose **Properties** from the shortcut menu to open the Properties dialog box.

3. Click the **Security** tab.
4. Click **Advanced** to open the Advanced Security Settings dialog box for the Security folder.
5. Click **Change Permissions**.
6. Clear the **Include Inheritable Permissions from This Object's Parent** check box.
7. When the Windows Security dialog box opens, click **Add**.
8. Ensure that the Permission Entries box contains only your administrator name (or the administrator group) and the group Everyone.
   - If Administrator (or the Administrator group) does not appear in the list, add it.
   - If the group Everyone does not appear in the list, add it.
   - If any other users or groups appear in the list, select and remove them.



9. Set the permissions for the folder:
   a. In the Permission Entries box, select **Administrator**.
   b. Click **Edit**.
   c. In the Permissions list, select the **Allow** check box for Full Control.

      All the other Allow check boxes are automatically selected.
   d. Click **OK**.

e. In the Permission Entries box, select **Everyone**.

f. Click **Edit**.

g. In the Permissions list, select the **Allow** check box for Read and clear the **Allow** check box for all the other options.

h. In the Advanced Security Settings dialog box, ensure that the **Inherit From Parent…** check box is cleared.

i. Click **OK** twice to close the Advanced Security Settings dialog box.

10. Click **OK** to save the permission assignments and close the Properties dialog box.

You have configured the security settings for the Security folder.

Configuring Security Settings for the Database Registry Key

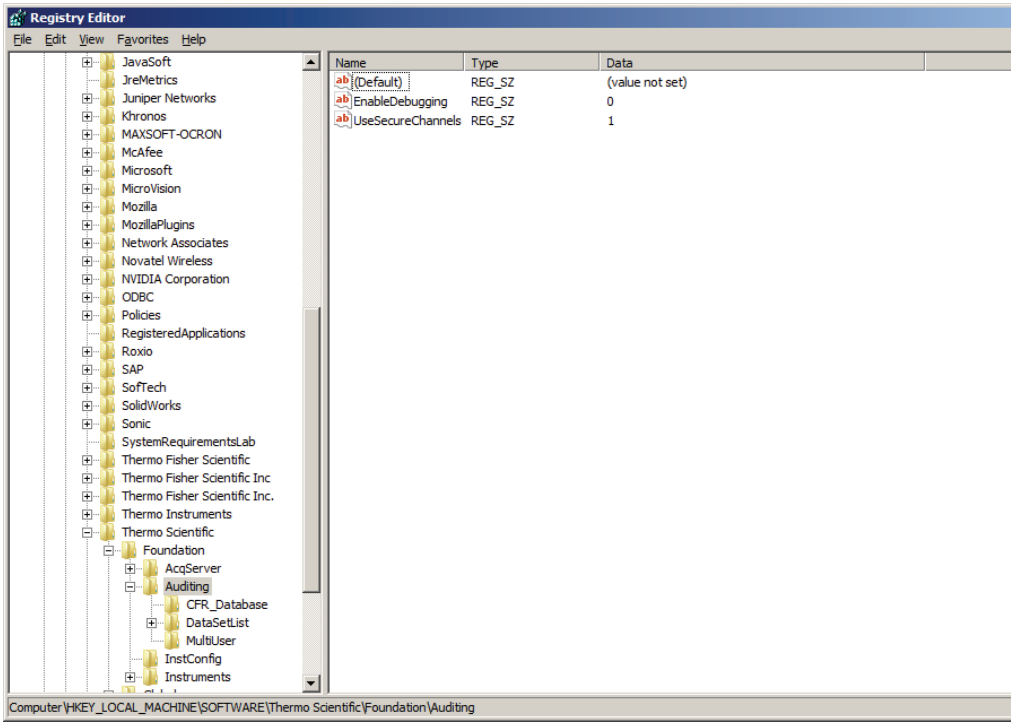
When you run the Database Configuration tool for the first time, the tool creates a Windows registry key that stores information about the database. To ensure the security of the auditing database, set the security settings for this registry key so that only the workstation administrator can make changes to the key.

Note You must configure the database registry key whenever you create a new global database.

❖ To configure the security settings for the database registry key

1. From the Windows taskbar, choose **Start > Run** to open the Run dialog box.
2. In the Run dialog box, type **regedit** and click **OK**.

   The Registry Editor dialog box opens.



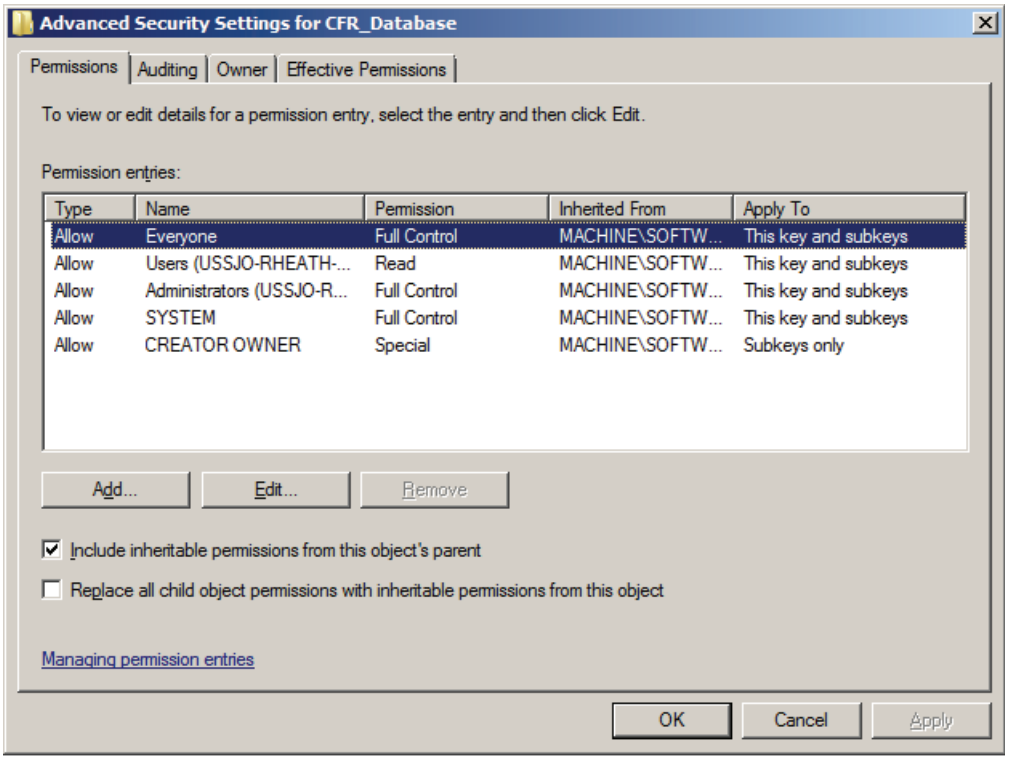
3. In the left pane of the Registry Editor dialog box, locate the folder:

   Computer\HKEY_LOCAL_MACHINE\SOFTWARE
   \Thermo Scientific\Foundation\Auditing\CFR_Database

4. Right-click the **CFR_Database** folder and choose **Permissions** from the shortcut menu to open the Permissions dialog box for this registry key.

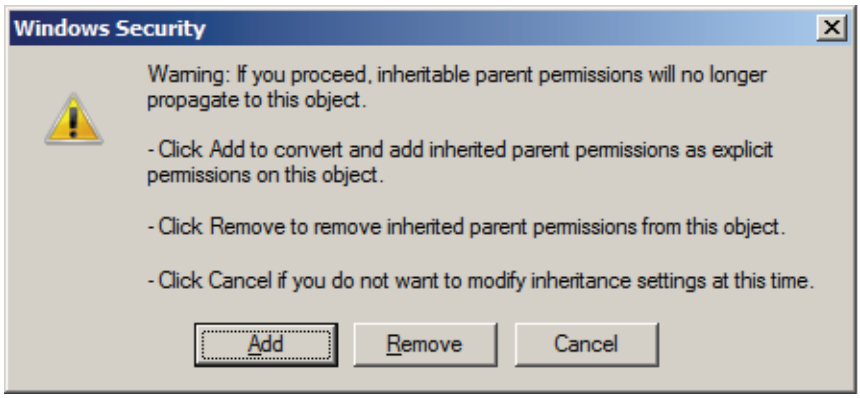
5. Click **Advanced**.

   The Advanced Security Settings dialog box opens.



6. Clear the **Include Inheritable Permissions from This Object's Parent** check box.

   The Windows Security dialog box opens.



7. Click **Add** to copy the inherited parent permissions to the CFR_Database registry key.
8. Click **OK** to close the Advanced Security Settings dialog box.

9. On the Security page of the Permissions dialog box, examine what groups or users appear in the Group_or_User_Names box.

   You want only your administrator name (or the administrator group) and the group Everyone to appear in this box.

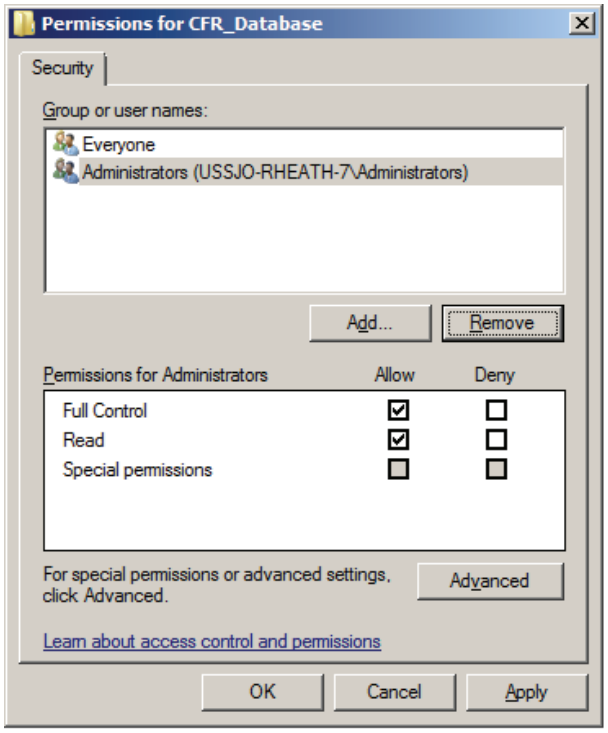
   - If your administrator name (or the administrator group) does not appear in the box, add it. (See "Adding Windows Users and Groups" on page 28.)
   - If the group Everyone does not appear in the box, add it. (See "Adding Windows Users and Groups" on page 28.)
   - If other users or groups appear in the box, remove them. (See "Removing Unnecessary Users" on page 30.)

10. Set the permissions for the registry key:

    a. In the Group or User Names box, select your administrator name (or the administrator group).

    b. In the Permissions list, select the **Allow** check box for Full Control.

       The Read check box in the Allow column is automatically selected.



    c. In the Group or User Names box, select **Everyone**.

    d. In the Permissions list, select the **Allow** check box for Read, and clear the **Allow** check box for all other actions in the list.

11. Click **OK**.
12. Choose **File > Exit** to close the Registry Editor.

Specifying the Way Users Log On and Off

This section describes the following:

Turning Off Fast User Switching for Local Workstations

Starting with Windows 7, you can switch between users without actually logging off from the computer. You can turn off this feature, called Fast User Switching, so that the current user must log off before another user logs on.

Turning off Fast User Switching is important because if it is allowed, two users could log on at the same time, which can cause strange behavior when they try to control their mass spectrometer. The acquisition service can only handle one user logged in at a time. Thermo Fisher Scientific recommends that all labs turn off Fast User Switching, regardless of whether secure file operations is important to the user or not.

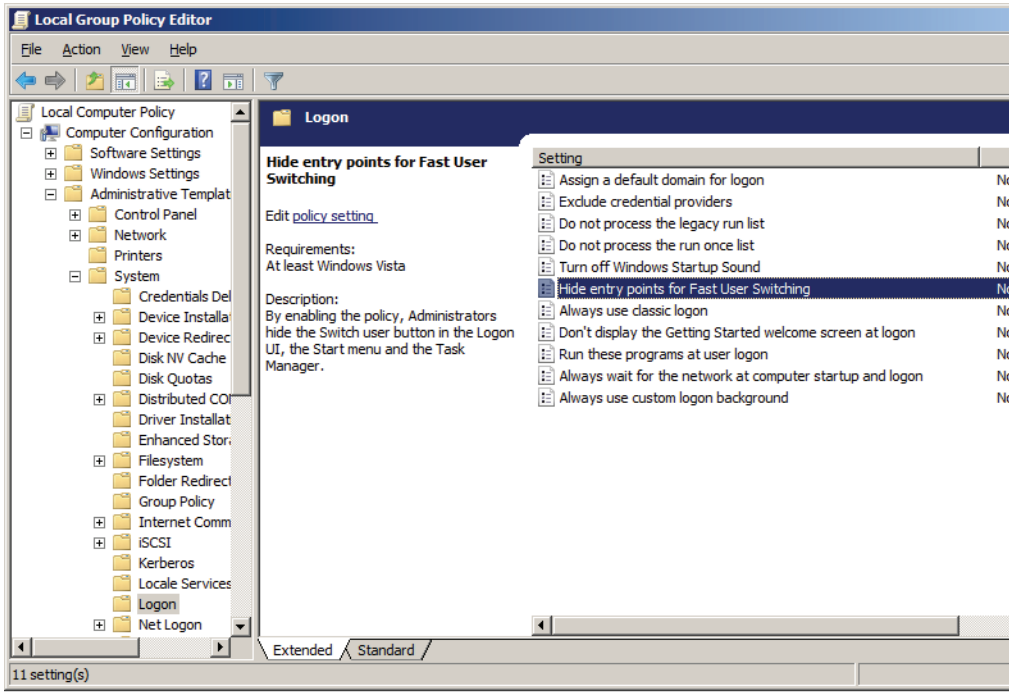
To maintain secure file operations, turn off the Fast User Switching feature on all computers.

❖ To turn off Fast User Switching

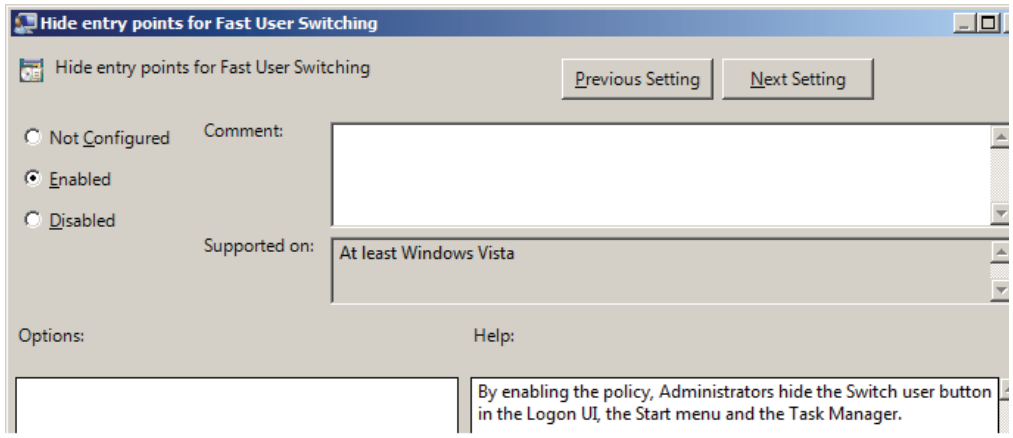
1. From the Windows taskbar, choose **Start**.
2. In the search box, type **gpedit.msc**.
3. Click **gpedit.msc** in the Programs list.

   The Local Group Policy Editor opens.

4. In the Local Computer Policy pane, choose **Computer Configuration > Administrative Templates > System > Logon** to display the Logon options.



5. Double-click **Hide Entry Points for Fast User Switching**.



6. Select the **Enabled** option, and then click **OK**.

7. Close the User Accounts dialog box and close the Control Panel.

Automatic Logoff

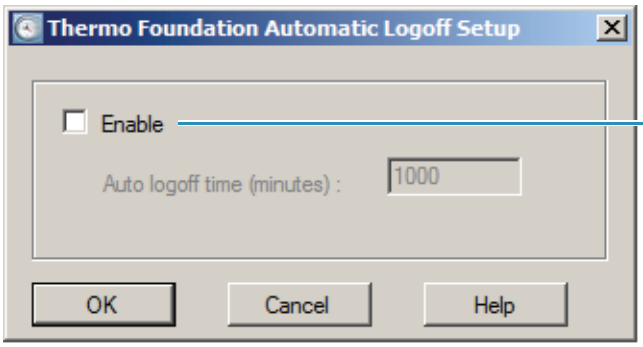
Automatic logoff cannot occur if a password-protected screen saver precedes it. Automatic logoff can occur if the screen saver is not password-protected, but you are not notified when it occurs.

IMPORTANT Thermo Fisher Scientific recommends that you enable automatic logoff to help ensure file integrity and access controls.

❖ To enable or disable automatic logoff

1. Choose **Start > All Programs > Thermo Foundation 2.0 > AutoLogoff**.

   The Thermo Foundation Automatic Logoff Setup dialog box opens.



2. Do one of the following:

   - To turn on the feature, select the **Enable** check box and type a value (1–1000) in the Auto Logoff Time (minutes) box to specify how long the system waits before logging off the current user.
   - To turn off the feature, clear the **Enable** check box.

3. Click **OK**.

If the Windows screen saver is set to appear on the computer at an earlier time than the Auto Logoff time, the automatic logoff still occurs at the specified time, even though the user cannot see evidence of the logoff because the screen saver is active.

Removing and Archiving Files

You must have proper procedures in place for long-term archiving and retrieving of electronic records—including raw data, processed data, and metadata. You must also have a procedure for ensuring that retrieved records can be read. Generally, this requires you to convert records to a new format or to keep and maintain the tools for reading the records in their current format.

To archive files, use third-party software designed for this purpose. In addition, to protect the archived data, develop and implement standard operating procedures for archiving files and security procedures to protect the archived data.

Defining Secure User Groups and Permissions

As the laboratory administrator, you control access to the Xcalibur data system and certain application features by using Thermo Foundation Authorization Manager to define secure user groups and grant these groups appropriate permission levels. Every member of a secure user group has the same permissions. Only those users in a designated secure user group can perform authorized actions. All others are prohibited access.

Follow these procedures to use the Foundation Authorization Manager to configure the secure groups and set permissions for controlled features in the Xcalibur data system.

Contents

Using the Authorization Manager

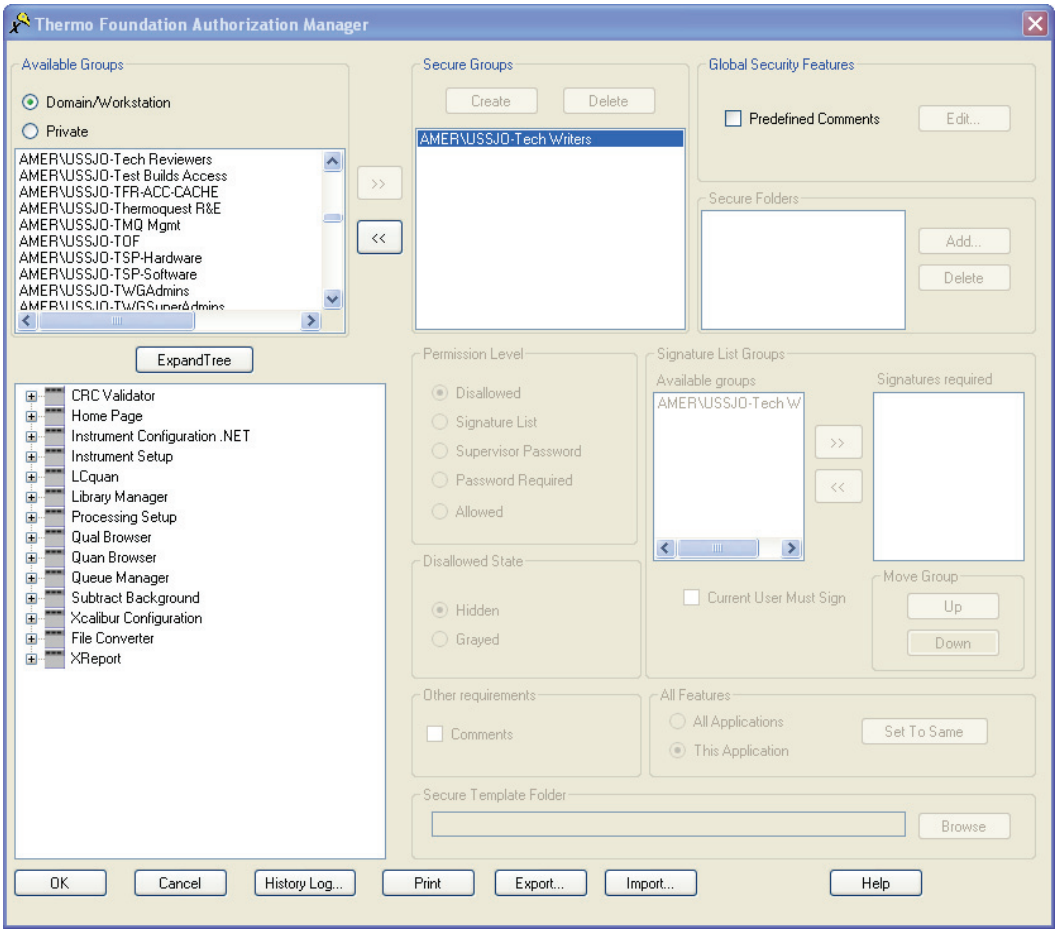
With Thermo Foundation Authorization Manager and the security features of the Windows operating system, define user groups and set permission levels for these groups. The Authorization Manager ensures that only individuals who have some level of responsibility for the records can access them.

❖ To start the Authorization Manager

From the Windows taskbar, choose **Start > All Programs >Thermo Foundation 2.0 > Authorization Manager**.

The Thermo Foundation Authorization Manager opens.

Figure 6. Thermo Foundation Authorization Manager



Setting Up Secure User Groups

To set up the secure user groups in Thermo Foundation Authorization Manager, you can use either preexisting Windows user groups or create your own private groups in the Authorization Manager.

The LCquan application places no limit on the number of user groups you can define. For simplicity, if all users are to have the same privileges, you can define a single user group.

IMPORTANT

- You must define secure user groups; otherwise, the LCquan system is not secure. If no secure groups are defined, all users can access all features of the software.
- A single user can belong to more than one user group. If the groups have different permission levels, the most lenient permission level applies to the user.

Defining User Groups

❖ To define user groups

1. In the Authorization Manager, select the appropriate Available Groups option to specify the type of user group:

   - To use preexisting Windows user groups, select the **Domain/Workstation** option. Contact your domain administrator to create or change logon groups.

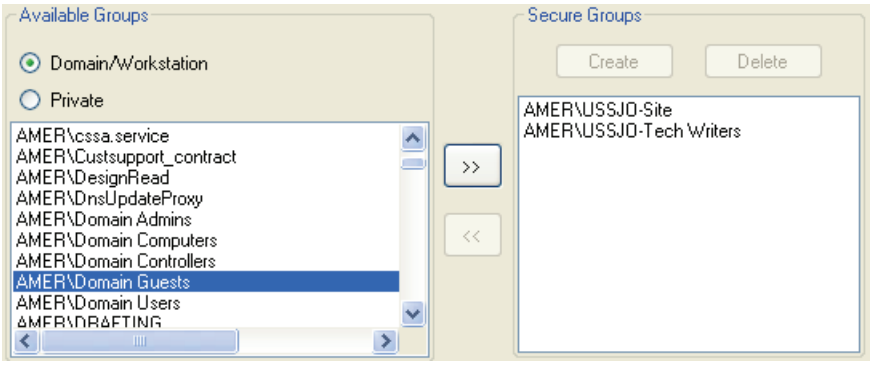
     Continue to step 2.

   - To use (or create) a local user group, select the **Private** option. The lab administrator can create private groups.

     Skip to step 3.

2. To define secure domain/workstation user groups, select a group in the Available Groups list and click the right arrow.

   The group name appears in the Secure Groups box.

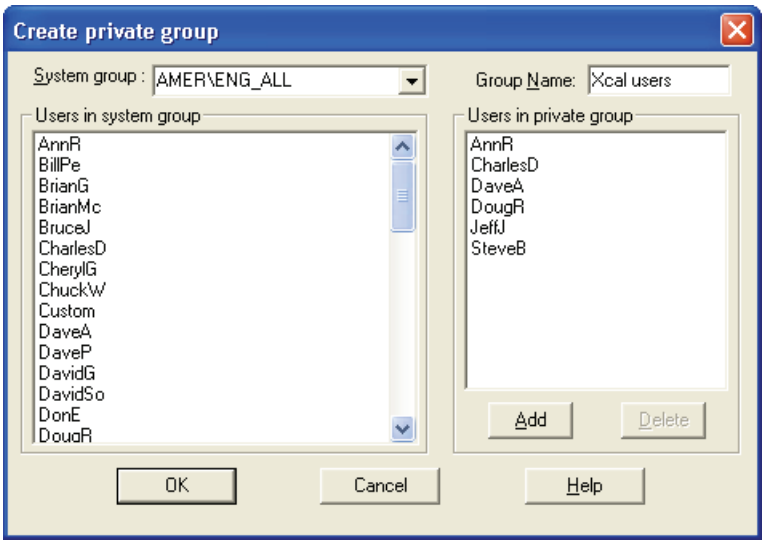


Repeat this step to define more secure groups. When you are finished creating groups, go to "Editing User Groups" on page 47.

3. To define secure private groups, do the following:

   a. In the Secure Groups area, click **Create**.

      The Create Private Group dialog box opens.



   b. In the Group Name box, type a name for the group.

   c. In the System Group list, select a domain.

      The domain user accounts are displayed in the Users in System Group list.

   d. In the Users in System Group list, select a user account and click **Add**.

      The user account appears in the Private Group box.

   e. To add users in other domains to the private group, repeat steps c and d.

   f. Click **OK**.

      The new private group appears in the Secure Groups box.

   g. To create additional private groups, repeat steps a through f.

Note Private groups are necessary only if the required groups are not available as Windows user groups.

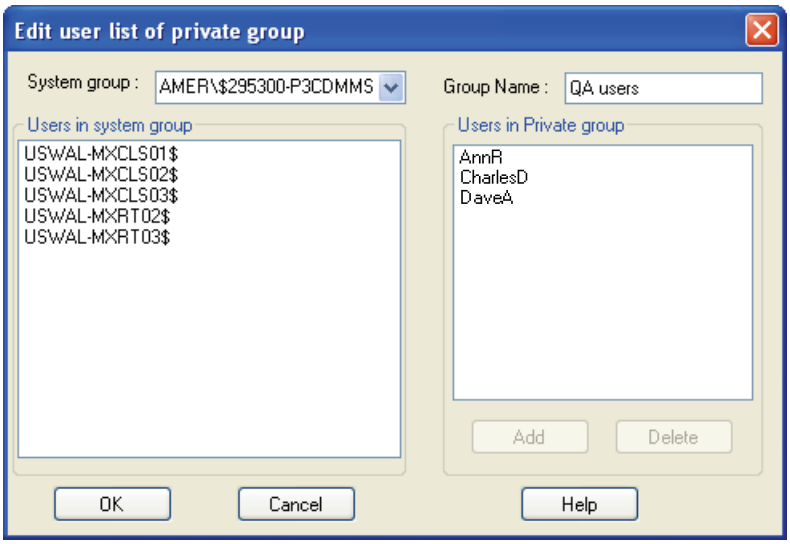
Editing User Groups

After you define a secure user group, you can view and (for private groups only) edit the members of the group.

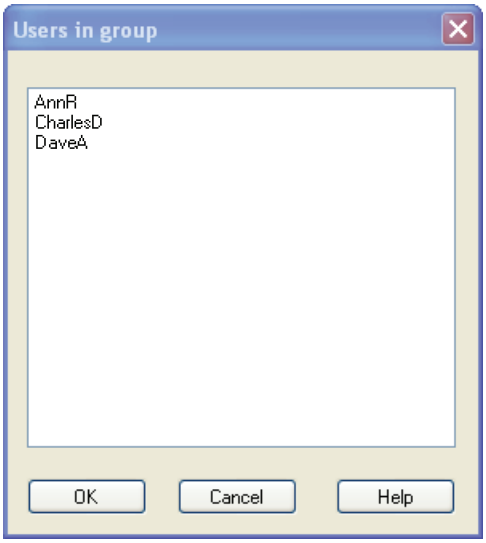
❖ To view and edit the members of a group

In the Secure Groups box, right-click the user group and choose **Members** from the shortcut menu.

- If the group is a private group, the Edit User List of Private Group dialog box opens. To add or remove names from the user group, click **Add** or **Delete**.



- If the group is a domain/workstation logon group, the Users in Group dialog box opens. Because membership in these groups is controlled by the domain administrator, the lists are read-only. To make changes to domain/workstation logon groups, contact your domain administrator.



Setting Permissions

For each secure user group, you can set the permission levels for certain features in the software. You set permissions in the Permission Level section of the Thermo Foundation Authorization Manager.

The following table lists the available permission levels. All new secure user groups, whether domain/workstation groups or private groups, have all features set to Disallowed.

Table 2. Permission levels

Permission Level	Description
Disallowed	Not permitted. You can specify whether the user interface control for the disallowed operation is hidden or grayed out.
Signature List	Enter the names and passwords of everyone on the required signature list to perform the authorized action. In the Signature List Groups area, you specify the groups whose signatures are required. A representative from each group on the required signature list must enter the user ID and password before the action is authorized. A user who belongs to more than one group on the required signature list can sign on behalf of each group by entering his or her user ID and password for each group.
Supervisor Password	Enter the supervisor name and password to perform the action. Anyone who has permission to perform the Allowed or Password Required actions can sign as a supervisor.
Password Required	The user must enter a password before continuing to perform the authorized action.
Allowed	No restrictions.

You can set permission levels by doing the following:

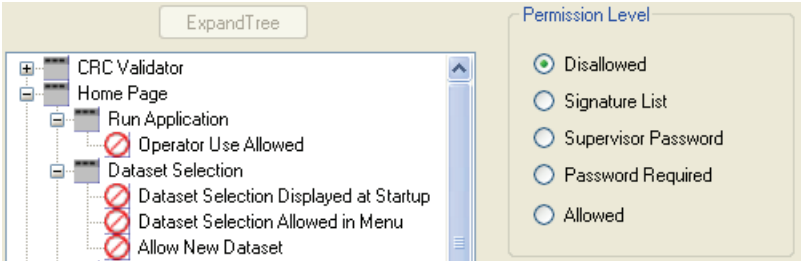
- Changing the Permission Level of a Feature
- Setting All Permissions
- Inheriting Permissions
- Exporting and Importing Permissions

Changing the Permission Level of a Feature

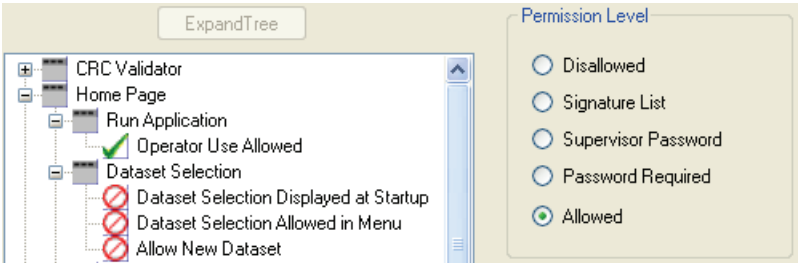
This section provides a general procedure for changing the permission level for most features.

❖ **To change the permission level of a feature**

1. In the Authorization Manager, select a user group from the Secure Groups box.
2. In the controlled features list to the lower left of the Authorization Manager, select the name of your software application.
3. To show the entire list of controlled features for the application, click **Expand Tree**.



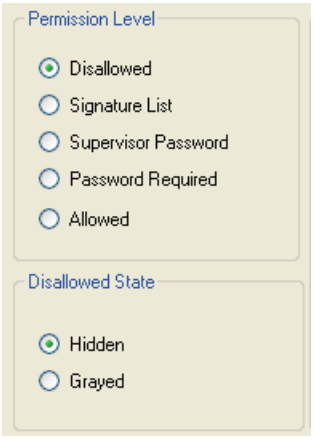
4. From the list, select a feature and select one of the following Permission Level options:
   - Disallowed
   - Signature List
   - Supervisor Password
   - Password Required
   - Allowed



Note You can set permissions only for individual features, such as Allow New Dataset. You cannot set permissions for groups, such as Dataset Selection. When you select a feature, the Permission Level options for that feature are available.

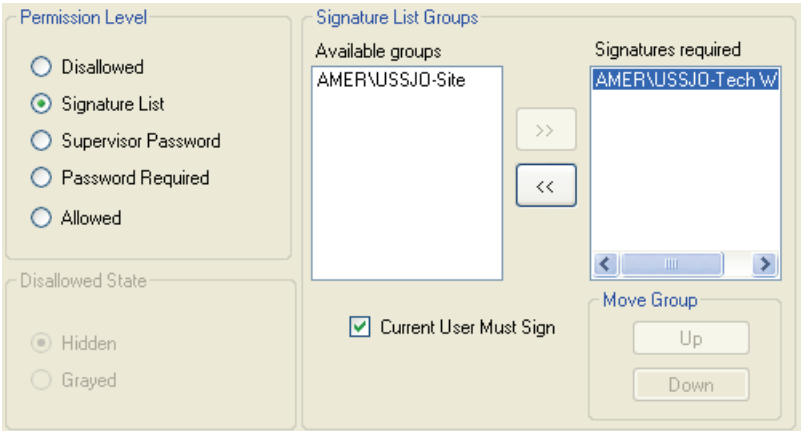
Tip Right-click a feature to select the permission level from the shortcut menu.

5. If you selected Permission Level: Disallowed, select how the user interface appears for the disallowed state.



   - To hide the unavailable control, select the **Hidden** option.
   - To gray out the unavailable control, select the **Grayed** option.

6. If you set the permission level to Signature List, use the Signature List Groups–Available Groups area to define the signature list groups:



   a. In the Available Groups box, select a user group and click the right arrow. The group appears in the Signatures Required box.

   b. To add other groups to the Signatures Required list, repeat step a.

   c. To require that the current user of the application be placed on the signature list, select the **Current User Must Sign** check box.

   d. To rearrange the order of the groups in the Signatures Required box, select a group and click the Move Group buttons: **Up** or **Down**.

Note When a user uses a feature with a permission level of Signature List, a series of password dialog boxes appears, one dialog box for each signature (name and password of a member of the designated group).

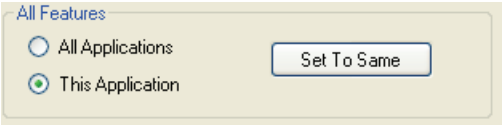
The order of the groups in the Signature List Groups: Available Groups box defines the display order of the password dialog boxes.

7. If you want the users to enter a comment when they perform an action, select the **Comments** check box in the Other Requirements area.

This option is available for all permission settings except **Disallowed**. When a user enters a comment, it appears in the audit log for the software.

8. Set the permission levels for any or all remaining features as follows:

   - To set the permission level of an individual feature, repeat steps 4 to 7.
   - To set the permission levels of the other features in the currently selected application to the same permission level you just set, select the **This Application** option and click **Set To Same**.



   - If you want to set the permission levels of all the features in all the applications to the same permission level you just set, select the **All Applications** option and click **Set To Same**.

     The Permission Level setting, the Disallow State setting (if applicable), and the Comments setting are copied to all the other features.

9. To set the permission levels for other user groups in the Secure Groups list, repeat steps 1 through 8.

Note The Authorization Manager retains permission level settings if you move a user group out of the Secure Groups box and into the Available Groups box. If you move the group back into the Secure Groups box, the permission settings remain intact; however, if you delete a user group from the Secure Groups box, all permission settings are lost.

Setting All Permissions

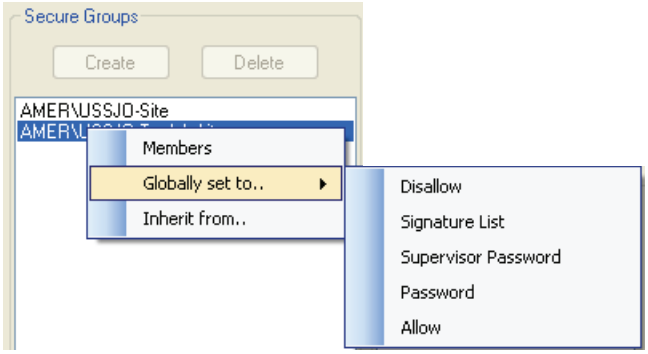
You can set every feature to the same permission level in one of two ways.

❖ **To set features to the same permission level**

- After you set the permission level for one feature, click the **All Applications** option and click **Set To Same**.

  –or–

- Right-click the user group name in the Secure Groups box and choose **Globally Set To >** ***permission level*** from the shortcut menu.

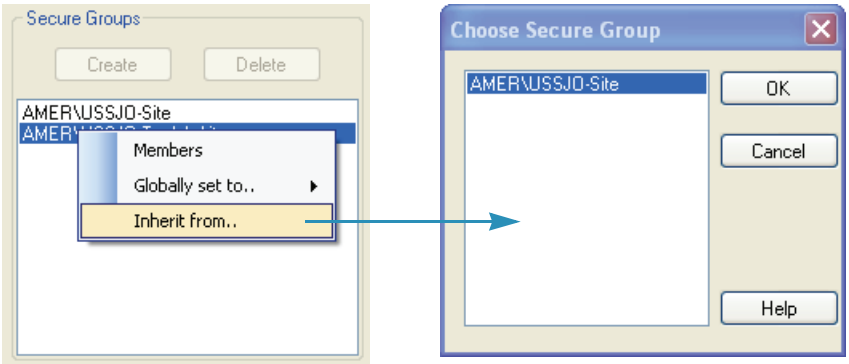


Inheriting Permissions

You can copy a complete set of permission levels from one secure user group to another secure user group.

❖ **To copy permission levels from one secure user group to another secure user group**

1. In the Secure Groups box, select the user group to receive the set of permission levels.
2. Right-click the selected group and choose **Inherit From** from the shortcut menu.



The Choose Secure Group dialog box opens and displays a list of the secure groups (minus the currently selected group).

3. Select the group whose permission levels you want to copy and click **OK**.

Both user groups now have the same set of permission levels.

Exporting and Importing Permissions

You can import the permission list that contains the user groups and permissions from another computer. Doing this saves time if you have more than one computer in your lab and you want to allow users access to all computers. Instead of setting up identical user groups on each computer, you can import the permission list from a computer that has the user groups and access permissions that you require.

Note To maintain the security of the permission list, you must export it to a secure location. The Security folder (with proper security settings) on the current computer is an ideal location.

❖ To export and import the permission list

1. On the system where the correct users and permission levels are set, start the Thermo Foundation Authorization Manager.
2. In the Foundation Authorization Manager, click **Export**.

   The Save As dialog box opens.
3. Save the permission list in the Security folder as a file with the file extension .eperm.

   (The path for the security folder is \Xcalibur\system\security. The default file name is permissions.eperm.)
4. Copy the file into the Security folder on the new system.
5. On the new system, start Thermo Foundation Authorization Manager and click **Import.**

   The Open dialog box opens.
6. Select the permission list file (*filename.eperm*) and click **Open**.

   The user groups and permission levels appear in the Foundation Authorization Manager.
7. Confirm that the user groups and permissions are correct and click **OK** to save the settings and close Thermo Foundation Authorization Manager.

Defining the List of Secure Folders

All electronic records must be in protected folders. To ensure the LCquan root folder is protected, do not permit users to change the root folder to an unprotected folder.

IMPORTANT If you have not configured the security settings to protect your root folders, do so before setting the root folder feature permissions. See Chapter 3, "Establishing Secure File Operations."

The Foundation Authorization Manager list of controlled features includes the following two features for each application:

- Allow Arbitrary Selection of Root Folder—Allows users to change the root folder to any folder that they choose. You must ensure that the Allow Arbitrary Selection of Root Folder feature is set to Disallowed.
- Allow Change of Root Folder—Allows users to change the root folder to another secure folder. You can set the Allow Change of Root Folder feature to any permission level. If you set the permission level to anything other than Disallowed, you must define a list of secure folders from which the user can select a new root folder.

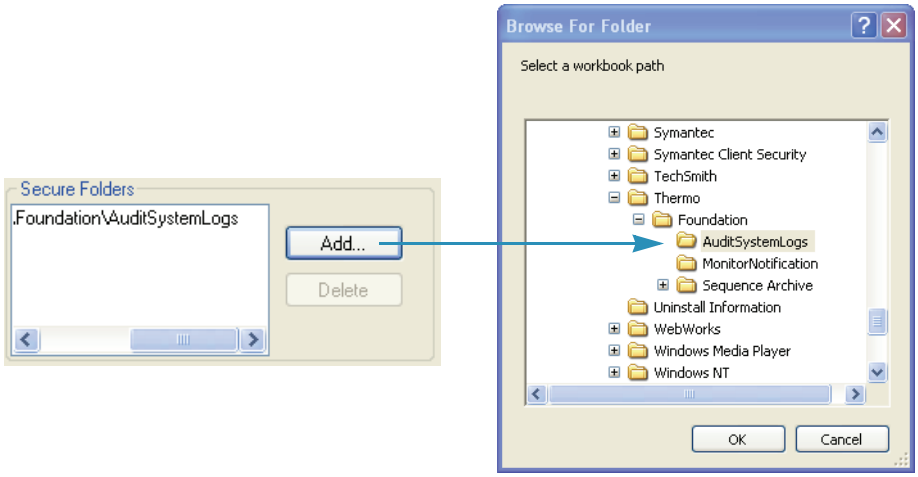
Tip To display these two features in the Foundation Authorization Manager, double-click **LCquan** in the controlled features list and double-click **Root Folder**.

❖ To define the list of secure folders

1. In the Secure Folders box, click **Add**.

   The Browse For Folder dialog box opens.

   Tip Define secure folders by using fully qualified path names. Use of mapped drive paths might result in network disconnection upon auto-logoff.



2. Select the secure folder that you want to add to the Secure Folders box and click **OK** to close the dialog box.

   The folder appears in the list in the Secure Folders box.

3. Repeat steps 1 and 2 for each folder that you want to add to the Secure Folders box.

After the permission levels and the Secure Folders box have been correctly set up, a user cannot change the root folder to a folder that is not secure. The user must select the new folder from the Secure Folders box from within the application. The secure folders information is saved as part of the configuration in a protected folder. For more information, see "Saving the Security Settings" on page 61.

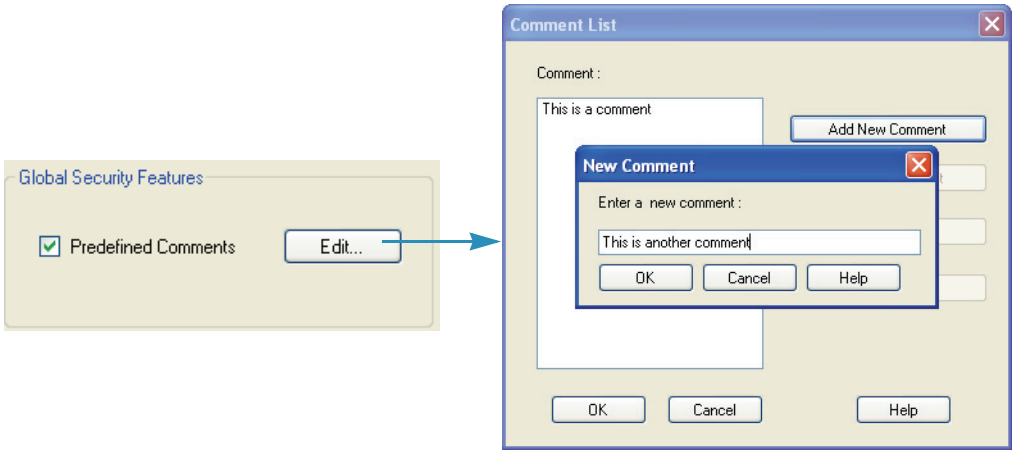
Requiring User Comments

For details about how to require users to enter comments when they perform a controlled action, see "Changing the Permission Level of a Feature" on page 49. When a user enters a comment, it appears in the audit log for the application. (This option is available for all permission settings except Disallowed.)

❖ To restrict users comments to a predetermined list of comments

1. Select the **Predefined Comments** check box in the Global Security Features area and click **Edit**.

   The Comment List dialog box opens.



2. Click **Add New Comment**.

   The New Comment dialog box opens.

3. Enter the comment and click **OK**.

   The new comment appears in the Comment box.

4. Repeat steps 2 and 3 for each new comment that you want to enter.

   The Comment box displays the predefined comments in the order that you entered them in. You can rearrange the order of the comments by clicking Move Up or Move Down, or delete a comment by selecting it and clicking Remove Comment.

5. When you are finished, click **OK**.

IMPORTANT The use of predefined comments precludes the use of free text comments.

Setting Up Secure Reports

You can limit a user group's authorization for creating LCquan quantitation reports to the secure XReport templates that you specify. After you configure the secure XReport templates feature, the user groups with this permission level can use only the templates from the specified secure templates folder. Users are limited to saving only, and the file format is limited to PDF files. In the LCquan Review Reports view, the options to print reports and create new XReport templates are not available.

About the Secure Reports

Users create secure reports when they use the secure XReport templates in the secure templates folder. The secure reports have the following characteristics:

- The only option available for creating a secure report is to save the report as a PDF file. The PDF document properties allow for printing only.

  The application changes any other preexisting report formats in the given workbook to PDF and tracks the changes in the audit trail.

- A watermark design appears on the background of each page of a secure report.
- A unique serial number appends to the footer of each page:

  workbookName_timestamp_*n*

  where *n* is a counter for the number of reports printed from a workbook.

The serial number increments for each report generated from a given LCquan workbook. If user groups with different security privileges create reports from the same workbook, both the secure and non-secure reports are included in the total count of reports when assigning the serial number.

Setting Up a Secure Template Folder

Secure XReport templates are available in the designated secure templates folder. You can specify only one secure templates folder. Templates that are not in the secure templates folder are not available to the user, even if the templates were previously available in another workbook.

Use the following guidelines when setting up a secure templates folder:

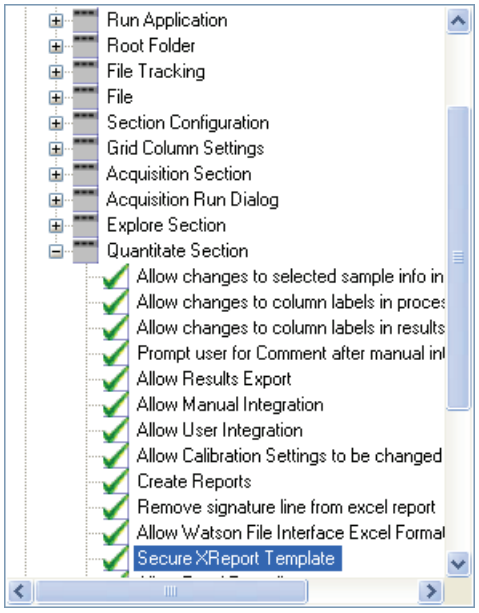
- To prevent users from adding any unapproved templates to the folder, assign read-only access to the folder.
- For a locked workbook, make sure to designate the folder that already contains the templates for the locked workbook.
- Ensure the secure template folder contains only the approved XReport template files (.xrt).

Configuring Secure Reports

❖ **To configure secure reports**

1. In the Foundation Authorization Manager, select a user group from the Secure Groups area.
2. In the list of controlled features (lower left side), select **LCquan** and click **Expand Tree**.
3. In the Quantitative Section, select **Secure XReport Template**.

Figure 7. LCquan Quantitate Section controlled features



4. In the Permission Level area, select **Allowed**.

   For the Secure XReport Template feature, Allowed is the most restrictive setting.

5. In the Secure Template Folder area, click **Browse**.

6. In the Browse for Folder dialog box, select the folder that contains the secure templates and click **OK**.

Locking the Workbook After Creating Reports

You can have the LCquan application automatically lock the workbook (not a copy of the workbook) after you create a report. A locked workbook (and its associated files) is a workbook that cannot be overwritten. You cannot save any changes made to a locked workbook, and you cannot acquire data in a locked workbook. You can create new reports, but the application does not save the report selections. When you open a locked workbook, [Locked] is displayed in the title bar next to the workbook name and in the status bar.

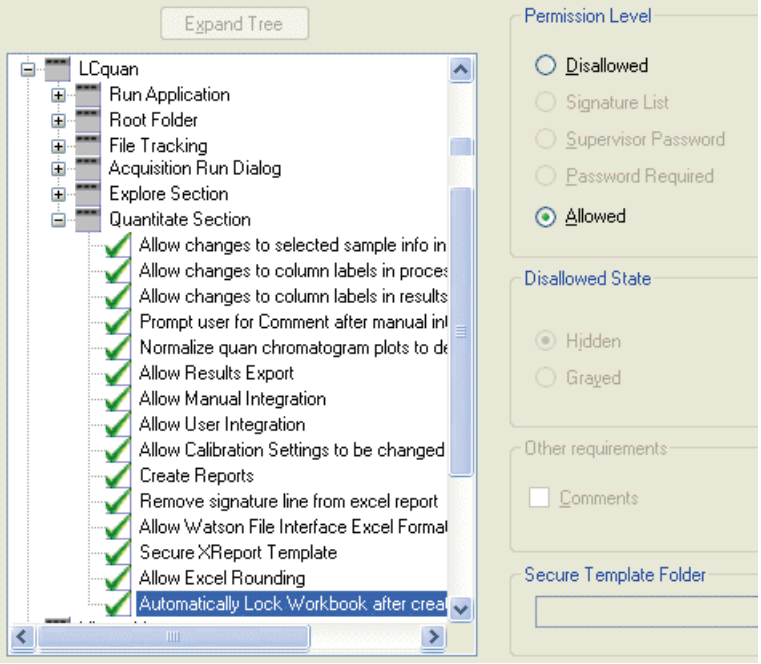
❖ To automatically lock the workbook after you create a report

1. Choose **Start > All Programs > Thermo Foundation > Authorization Manager** to open the Authorization Manager.
2. In the Authorization Manager, do the following:
   a. Select a user group in the Secure Groups list.
   b. Click **Expand Tree** to show the entire list of controlled features for the application (see Figure 8).
   c. From the list, click the plus sign before the LCquan folder.
   d. Click the plus sign before the Quantitate Section folder.
   e. Select **Automatically Lock Workbook after Creating Reports**.

      The Permission Level options become available.

   f. Select the **Allowed** option, and click **OK**.

Figure 8. LCquan Quantitate Section controlled features



Viewing the Authorization Manager History Log

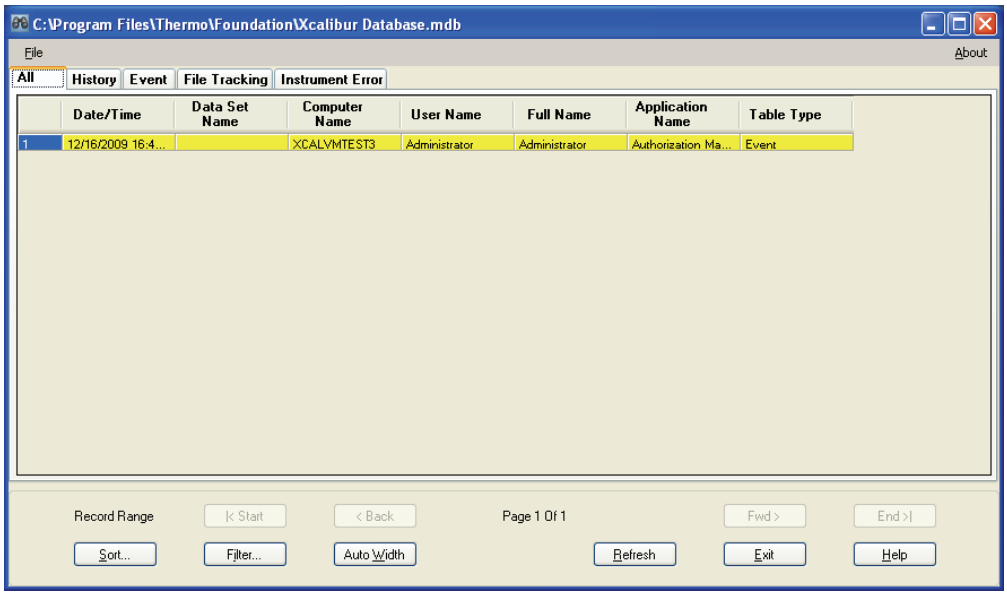
Thermo Foundation Authorization Manager automatically maintains a history log to record all changes made to the security settings. The log records the following events:

- The creation of a private group
- The addition or deletion of members from a group
- A change in group permissions
- A switch between private and domain/workstation groups
- The manipulation of the signature list

❖ To display the history log

In Thermo Foundation Authorization Manager, click **History Log**.

The audit view window opens, showing the history log for the Authorization Manager.



Each entry in the history log contains the time and date, and the user ID and full name. You can sort and filter the entries in the history log by field (for example, you can sort and filter by date and time). You can also print the log.

Printing the Security Settings

You can print a report of the security settings for each secure user group. The report contains a listing of the members of the group, the controlled features information for each application, and the names of any secure folders for each application (for example, see Figure 9).

❖ To print the security settings

1. In Thermo Foundation Authorization Manager, click **Print**.

   The Print dialog box opens.

2. Select the print options, and click **OK**.

Figure 9. Sample Security Settings printout

```
Xcalibur Security Settings for secure group : AMER\USSJO-Site
Thursday, June 05, 2008 12:48:05 PM
User dana.powers
Computer USSJO-LGUZZE-PC
Xcalibur Version 3.0


Members
_____________________________________________________________________________________________________________
nick.chavez
don.mcmichael

Application                    Secure Folders
_____________________________________________________________________________________________________________
CRC Validator                  [none]
Home Page                      [none]
Instrument Configuration .NET  [none]
Instrument Setup               [none]
LCquan                         C:\Program Files\Thermo\Foundation\AuditSystemLogs
Library Manager                [none]
Processing Setup               [none]
Qual Browser                   [none]
Quan Browser                   [none]
Queue Manager                  [none]
Subtract Background            [none]
Xcalibur Configuration         [none]
File Converter                 [none]
XReport                        [none]

Application                     Feature                                    Permission  Comment  Disallowed  Signature
                                                                           Required?   State    List
_____________________________________________________________________________________________________________
CRC Validator                   Run Application|Operator Use Allowed       DisAllowed  n/a      Hidden      n/a
Home Page                       Run Application|Operator Use Allowed       DisAllowed  n/a      Hidden      n/a
Home Page                       Dataset Selection|Dataset Selection Displayed.. DisAllowed  n/a      Hidden      n/a
Home Page                       Dataset Selection|Dataset Selection Allowed i.. DisAllowed  n/a      Hidden      n/a
Home Page                       Dataset Selection|Allow New Dataset        DisAllowed  n/a      Hidden      n/a
Home Page                       Analysis|Start Analysis                    DisAllowed  n/a      Hidden      n/a
Home Page                       Analysis|Stop  Analysis                    DisAllowed  n/a      Hidden      n/a
Home Page                       Analysis|Pause Analysis                    DisAllowed  n/a      Hidden      n/a
Home Page                       Devices|Devices On                         DisAllowed  n/a      Hidden      n/a
Home Page                       Devices|Devices StandBy                    DisAllowed  n/a      Hidden      n/a
```

Saving the Security Settings

After you have defined your user groups, set the appropriate permission levels, and specified the type of application auditing, click **OK** to save your settings and exit the Authorization Manager.

The controlled features information is saved in a configuration file in the following folder:

C:\ProgramData\Thermo Scientific\INI

You must properly set the security for this folder to prohibit access by nonadministrators. If you have not already done this, go to Chapter 3, “Establishing Secure File Operations.”

Auditing

This chapter describes how to use the Audit Viewer utility for auditing functions. You can display all auditable events and changes made to files created or managed by the LCquan application, view a history of what has been done during data acquisition and data processing to produce results, and get information about all events that have occurred within the application.

Contents

Accessing the Auditing Databases

The LCquan application writes to the Global Auditing database and maintains the LCquan workbook databases to assist in regulatory compliance—though it does not ensure it. The Global Auditing database stores LCquan start and stop events. All other LCquan events are stored in the LCquan workbook databases.

IMPORTANT Before you can access the Global Auditing database, you must configure the database in the Auditing Database Configuration Manager. For instructions, see Chapter 2, "Using the Database Configuration Manager."

IMPORTANT Each Windows user account must be associated with a user ID, password, and full description. The system requires these items to store the auditing information in the designated database.

You can access either of the following types of databases using Audit Viewer:

- The Global Auditing database, which keeps a log of auditable events for all the Xcalibur-related data files and applications it recognizes. The Xcalibur-related data files include the raw files that you acquire in the LCquan application.
- The LCquan workbook database, which keeps a log of auditable events associated with the current workbook, including the entries that have not been saved to the database. Each workbook database also includes a log about the raw files that are acquired as part of the workbook.

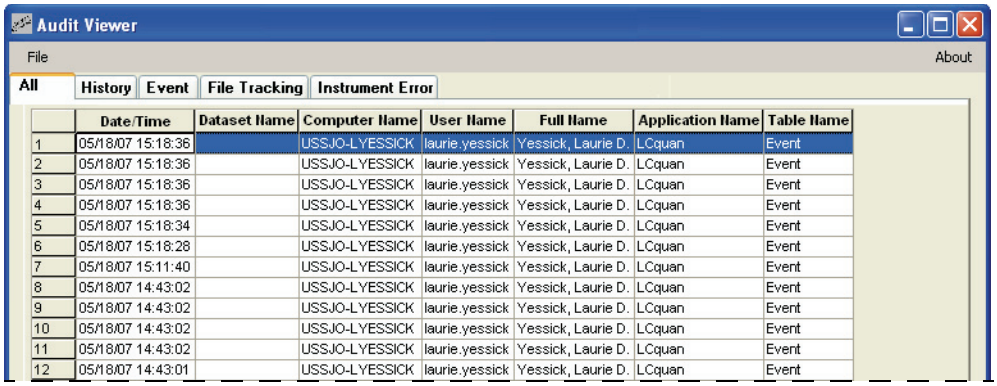
Accessing the Global Auditing Database

You can access the Global Auditing database when you start Audit Viewer from the Windows desktop.

❖ **To start Audit Viewer from your Windows taskbar**

Choose **Start > All Programs > Thermo Foundation 2.0 > Audit Viewer**.

The Audit Viewer opens.



	Date/Time	Dataset Name	Computer Name	User Name	Full Name	Application Name	Table Name
1	05/18/07 15:18:36		USSJO-LYESSICK	laurie.yessick	Yessick, Laurie D.	LCquan	Event
2	05/18/07 15:18:36		USSJO-LYESSICK	laurie.yessick	Yessick, Laurie D.	LCquan	Event
3	05/18/07 15:18:36		USSJO-LYESSICK	laurie.yessick	Yessick, Laurie D.	LCquan	Event
4	05/18/07 15:18:36		USSJO-LYESSICK	laurie.yessick	Yessick, Laurie D.	LCquan	Event
5	05/18/07 15:18:34		USSJO-LYESSICK	laurie.yessick	Yessick, Laurie D.	LCquan	Event
6	05/18/07 15:18:28		USSJO-LYESSICK	laurie.yessick	Yessick, Laurie D.	LCquan	Event
7	05/18/07 15:11:40		USSJO-LYESSICK	laurie.yessick	Yessick, Laurie D.	LCquan	Event
8	05/18/07 14:43:02		USSJO-LYESSICK	laurie.yessick	Yessick, Laurie D.	LCquan	Event
9	05/18/07 14:43:02		USSJO-LYESSICK	laurie.yessick	Yessick, Laurie D.	LCquan	Event
10	05/18/07 14:43:02		USSJO-LYESSICK	laurie.yessick	Yessick, Laurie D.	LCquan	Event
11	05/18/07 14:43:02		USSJO-LYESSICK	laurie.yessick	Yessick, Laurie D.	LCquan	Event
12	05/18/07 14:43:01		USSJO-LYESSICK	laurie.yessick	Yessick, Laurie D.	LCquan	Event

Accessing an LCquan Workbook Database

Each LCquan workbook has its own database. When you start Audit Viewer from an LCquan workbook, Audit Viewer displays the saved and unsaved entries for the current workbook. The unsaved entries are highlighted in yellow in the Audit Viewer window.

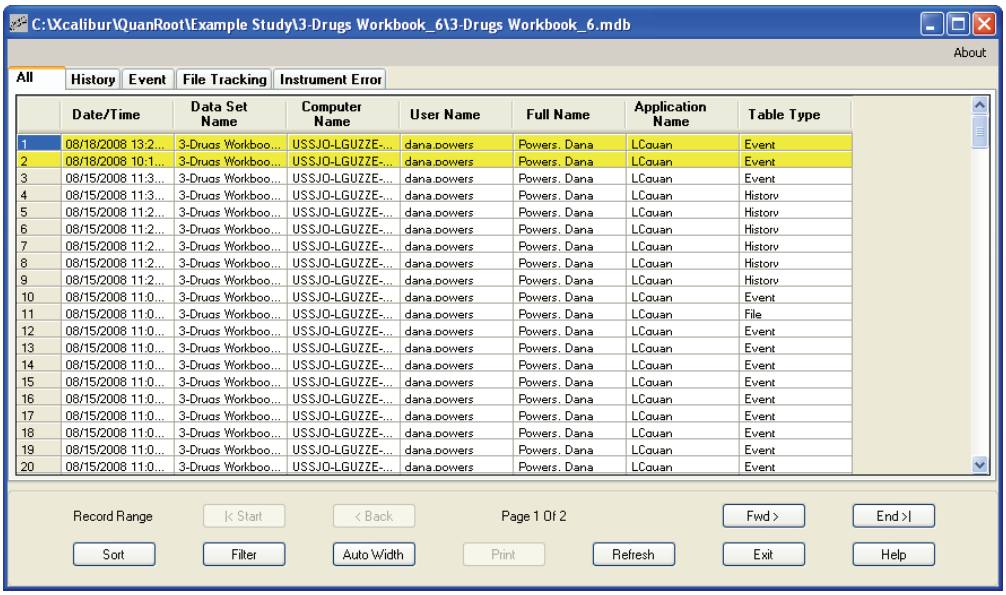
Note The Audit Viewer entries can also include unsaved changes from another workbook if the changes are still in memory.

❖ **To access the auditing database for a workbook**

1. Open the LCquan workbook.
2. From the LCquan interface, choose **File > Audit Trail**.

   The Audit Viewer opens and displays the entries for the open workbook. Unsaved entries are highlighted in yellow.

To access the auditing database for a different workbook, repeat steps 1 and 2. A second instance of Audit Viewer starts and displays the entries for that workbook.



Viewing the Audit Viewer Pages

The Audit Viewer window contains the following tabs, each with a different function:

- The All tab provides a summary of all entries for the current database.

  To display the Audit Viewer page associated with an entry on the All page, double-click the entry on the All page.

- The History tab provides a chronological listing of all the changes made to method files and result lists.
- The Event tab lists all user-initiated auditable events. All events that are subject to authorization control are auditable.

- The File Tracking tab provides the following type of information:
  - Global Auditing database: Lists the changes that are made by any program to the Xcalibur-created files.
  - LCquan workbook database: Lists the changes made within the application to any LCquan-owned files in the workbook, including the workbook file (.lqn), processing method (.pmd), instrument method (.meth), sequence (.sld), and any imported sample data files (.raw). The File Tracking page does not include the data files (.raw) acquired from within the LCquan workbook, which are tracked in the Global Auditing database.

    If any of the workbook files are modified outside the system, the LCquan application displays a file-tracking error message.

  Note The LCquan application does not save entries to the database until you save the workbook. The Audit Viewer headlights the unsaved entries in yellow.

- The Instrument Error tab lists significant events that occur to instruments that the Xcalibur data system creates or manages.

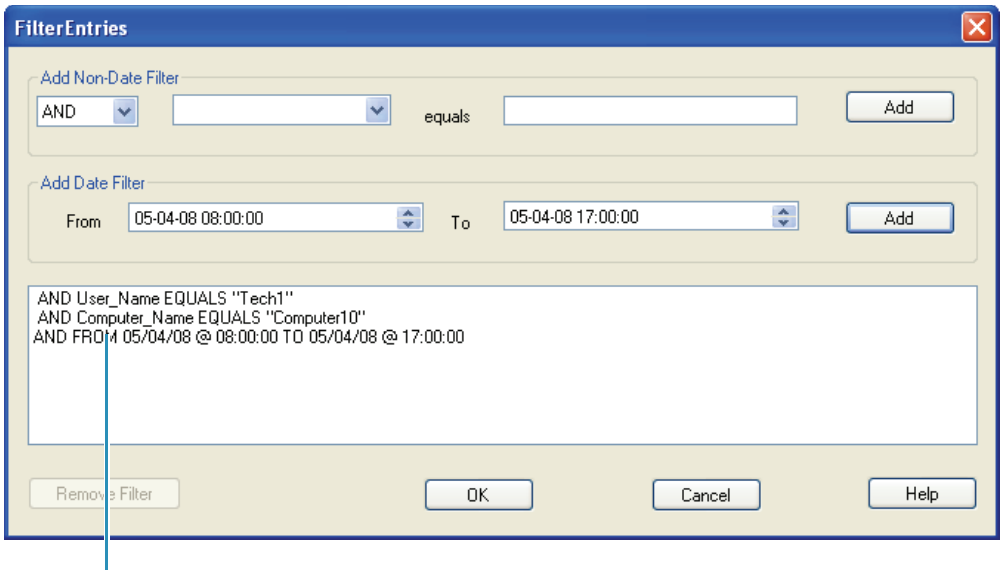
Filtering the Audit Viewer Entries

By applying a filter, you can display a subset of the entries in the Audit Viewer window. You can set up two types of filters: filters that are based on dates and filters that are not based on dates (non-date filters). You can use a combination of the two types of filters.

❖ To set up a non-date filter

1. In the Audit Viewer window, click **Filter**.

   The Filter Entries dialog box opens.



   Searches for records created by Tech1 on Computer10 between 8:00 A.M. and 5:00 P.M. on May 4, 2008.

2. In the Add Non-Date Filter area, select **AND** or **OR** from the first list.
   - AND filters for entries that match ALL the specified criteria.
   - OR filters for entries that match ANY of the criteria.
3. Specify a filter in the form of *Column Name* equals *string*.
   a. From the drop-down list, select a column to filter on.
   b. In the adjacent box, type the text string to match.
   c. Click **Add**.

      The filter criteria appear in the space below.
4. To add additional filters, repeat steps 2 and 3.

   If you select an OR filter, records must match only one of the filters. If you selected an AND match, records must match ALL the specified filters.

> **Note** The non-date filter accepts partial matches. For example, if you have a user name of `john.doe`, then a filter string of `john` or `doe` will match entries for that user name.

❖ **To set up a date filter**

1. In the Add Date Filter area, select or type the beginning date and time in the From box.
2. Enter the ending date and time in the To box.
3. Click **Add**.

❖ **To remove a filter**

1. In the Filter Entries dialog box, select the filter statement.
2. Click **Remove Filter**.

❖ **To search for filter criteria**

When you have defined all your filters, click **OK**.

The Audit Viewer window displays the results on the All page.

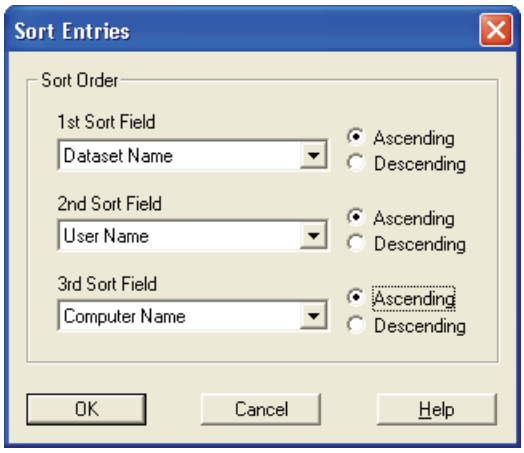
Sorting the Audit Viewer Entries

You can sort entries by the column headings on each of the Audit Viewer pages.

❖ **To sort entries on an Audit Viewer page**

1. In the Audit Viewer window, click the tab of the page you want to view.
2. Click **Sort**.

   The Sort Entries dialog box opens.



3. In the 1st Sort Field list, select a column heading and select the **Ascending** or **Descending** option.

   Repeat this step for the 2nd Sort Field and 3rd Sort Field.

4. Click **OK**.

   The Audit Viewer page displays the entries in the specified sort order.

Printing the Audit Viewer Entries

The printing options vary depending on whether you are printing the audit trail for the Global Auditing Database or a workbook database. For a workbook database, you must save all displayed records on the Audit Viewer page before you can print the entries.

❖ To print the audit trail for the Global Auditing database

1. From the Windows desktop, choose **Start > All Programs > Thermo Foundation 2.0 > Audit Viewer**.
2. In the Audit Viewer, click the tab of the page you want to print.
3. Click **Print**.
4. In the Print Options dialog box, select your printing options and click **OK**.

❖ To print the audit trail for an LCquan workbook database

1. In the LCquan window, choose **File > Audit Trail**.

   If you already saved workbook entries, go to step 3.

   If the workbook contains unsaved entries, a View Audit Trail message appears prompting you to save the workbook before continuing.

2. In the View Audit Trail dialog box, do one of the following:

   - To save the workbook entries, click **Yes**.

     The Xcalibur data system logs the automatic save in the audit trail and starts Audit Viewer.

   - To start Audit Viewer without saving the workbook, click **No**.

   Note If you select the Don't tell me about this again check box, the application automatically applies the last requested behavior (Save or Not Save) each time you start Audit Viewer when the workbook contains unsaved entries. To restore the message, choose **Options > Enable Warnings**.

3. In the Audit Viewer, click the tab of the page that you want to print.

4. Make sure the displayed page contains only saved entries. The rows of unsaved entries are highlighted in yellow.

   If you have a mix of saved and unsaved entries, you can do one of the following:

   - In the LCquan Workbook window, choose **File > Save** to save the LCquan workbook. In the Audit Viewer window, click **Refresh**.
   - In the Audit Viewer window, click **Filter**, and then add filter rules so that only the saved records appear on the page you want to print. For details about adding filter rules, see "Filtering the Audit Viewer Entries" on page 66.

5. Click **Print**.

6. In the Print Options dialog box, select printing options and click **OK**.

Permission Level Settings in the LCquan Application

This appendix discusses the different LCquan permission levels and how they interact.

Certain permission level settings override other settings. In addition, some features are unavailable—regardless of their permission level settings—if a workbook is locked or has been opened in review mode.

The Permission Level Settings table lists the LCquan features that you can configure in the Foundation Authorization Manager.

Table 3. Permission Level Settings (Sheet 1 of 6)

LCquan feature	Description
Run Application	
Operator Use Allowed	If you set this feature to Disallowed, the user cannot open the application. As a result, the permission level settings for the other features are irrelevant. If a user whose permission is set to Disallowed tries to access the system, the LCquan application makes an entry in the Global Auditing Database history log.
Root Folder	
Allow Change of Root Folder	If you enable this feature (set it to Signature List, Supervisor Password, Password Required, or Allowed), define a list of secure folders where the user can select a new root folder.
Allow Arbitrary Selection of Root Folder	If you set this feature to Allowed, the user can select any folder to be the root folder of the workbook.
File Tracking	
Allow Opening of Workbooks with Filetracking Errors	If you set this feature to Allowed, the user can open workbooks with file errors, such as workbooks with missing files or files that were modified outside of the LCquan application.

Table 3. Permission Level Settings (Sheet 2 of 6)

LCquan feature	Description
Allow Opening of Workbooks Already Marked as Opened	If you set this permission to Allowed, the user can open workbooks that the application flags as opened. When a user opens an LCquan workbook, the application flags the workbook as opened to prevent the workbook from being opened by multiple instances of the application. If the application is forced to close abnormally, the flag might not be removed even though the workbook is no longer open. To open the workbook, set this permission to Allow. The next time the workbook is closed, the open flag is removed.
File	
Save	If you set this permission to Disallowed, the user can lock the workbook only if it has not been changed. If it has been changed, the user cannot lock the workbook.
Save As	If you set this permission to Disallowed, the user cannot use the Save As command.
Create New Workbook	(No special information or interactions.)
Create Locked Version of Workbook	If you set this permission to Disallowed, the user does not have the option to lock a workbook.
Section Configuration	
Show Instrument Setup Section	If you set this permission to Disallowed, the user cannot display the Instrument Setup Section nor can the user make changes to the Instrument Methods.
Show Acquisition Section	If you set this permission to Disallowed, the user cannot create or modify an acquisition sequence nor can the user acquire data.
Show Explore Section	If you set this permission to Disallowed, the user cannot explore new quantitation methods.
Show Quantitate Section	If you set this permission to Disallowed, the user cannot: • Create or change a processing method. • Create or modify processing sequences. • Survey and review all the results. • Create reports from this section and process the data to produce quantitative results.

Table 3. Permission Level Settings (Sheet 3 of 6)

LCquan feature	Description
Grid Column Settings	
Allow Changes to Column setup info	If you set this permission to Disallowed, the user cannot change the number and arrangements of columns in the Results table.
Acquisition Section	
Start Acquisition Dialog	If you set this permission to Disallowed, the user cannot open the Run Sequence dialog box from the Acquisition view.
Allow Changes to Selected Sample Info in Acquisition Sequence	If you set this permission to Disallowed, the user cannot make changes to the sample information, such as Sample Name, Comment, Study, Client, Laboratory, and so on, in the acquisition sequence.
Allow Changes to Column Labels in Acquisition Sequence	If you set this permission to Disallowed, the user cannot make changes to the column labels in the acquisition sequence.
Prevent Raw File Time-Stamping When Doing Remote Workbook Acquisitions	If you set this permission to Disallowed, the LCquan application time-stamps the raw files during a remote acquisition. **Important** The LCquan application can overwrite raw files of the same name if you turn off time-stamping.
Acquisition Run Dialog	
OK Button	If you set this permission to Disallowed, the user can view the Run Sequence dialog box but cannot start a data acquisition because the OK button is unavailable in the Run Sequence dialog box.
Explore Section	
Allow Import of Peak Lists	If you set this permission to Disallowed, the user cannot import a Peak Name List.
Allow Export of Peak Lists	If you set this permission to Disallowed, the user cannot export a Peak Name List.

Table 3. Permission Level Settings (Sheet 4 of 6)

LCquan feature	Description
Quantitate Section	
Allow Changes to Selected Sample Info in Processing Sequence	If you set this permission to Disallowed, the user cannot make changes to the sample information, such as Sample Name, Comment, Study, Client, Laboratory, and so on, in the processing sequence.
Allow Changes to Column Labels in Processing Sequence	If you set this permission to Disallowed, the user cannot change the column labels in the processing sequence.
Allow Changes to Column Labels in Results	If you set this permission to Disallowed, the user cannot change the column labels on the Survey or Review All pages of the LCquan Quantitate section.
Prompt User for Comments after Manual Integration	If you set this permission to Allowed, the user must enter a comment before proceeding with a manual integration. Whenever the user performs a manual integration, the Chromatogram Comment dialog box opens and prompts the user for a comment before proceeding.
Normalize Quan Chromatogram Plots to Detected Peak	If you set this permission to Disallowed, the LCquan application normalizes the chromatogram plot so that the highest peak is 100%. If you set this permission to Allowed, the application normalizes the chromatogram plot so that the detected peak is 100%.
Allow Results Export	If you set this permission to Disallowed, the user cannot export results.
Allow Manual Integration	If you set this permission to Disallowed, the user cannot manually adjust the peak integration.
Allow User Integration	If you set this permission to Disallowed, the user cannot adjust the peak integration settings for an individual peak.
Allow Calibration Settings to Be Changed	If you set this permission to Disallowed, the user cannot change the Calibration settings of a particular component.
Create Reports	If you set this permission to Allowed, the user can create two types of reports: • Microsoft Excel™ Workbook with data and results • XReport report

Table 3. Permission Level Settings (Sheet 5 of 6)

LCquan feature	Description
Remove Signature Line From Excel Report	(Required for the Watson file interface) An Allow setting removes the signature line from the exported quantitation reports so that the Watson system can import the exported Excel spreadsheet via the file interface. See "Recommended Settings for Excel Reports" on page 79 in Appendix C, "Watson Interface."
Allow Watson File Interface Excel Format Reports	(Recommended for the Watson file interface) An Allow setting fixes the format of the Acq Date column entries in the exported quantitation reports so that the Watson file system can correctly import the acquisition date and time. See "Recommended Settings for Excel Reports" on page 79 in Appendix C, "Watson Interface."
Secure XReport Template	The Allowed setting prevents the user from creating quantitation reports with XReport other than reports that use the secure XReport templates. After you specify a secure template folder, users can save secure reports only as PDF files using the templates from the specified folder. For details, see "Setting Up Secure Reports" on page 56 in Chapter 4, "Defining Secure User Groups and Permissions."

Table 3. Permission Level Settings (Sheet 6 of 6)

LCquan feature	Description
Allow Excel Rounding	The Allowed setting restricts the number of decimal places in the exported Excel reports. The values for Area, Height, Response, ISTD Area, ISTD Height, and ISTD Response are restricted to zero decimals. All other values are limited to three decimals. The Allowed setting changes the behavior in the LCquan Column Arrangement dialog box for Excel reports, preventing the user from changing the precision. Any previous value settings are overridden with a restricted number of decimals and the values are not editable. The Allow setting does not affect the behavior of the LCquan grid views, the exported results, or the reports generated using XReport.
	Important Before the Excel rounding feature takes effect for the Watson digital interface, you must start and exit the LCquan application at least one time. See "Recommended Settings for Excel Reports" on page 79.
Automatically Lock Workbook After Creating Reports	The Allowed setting automatically locks the workbook (not a copy of the workbook) after you create a report. A locked workbook (and its associated files) is a workbook that cannot be overwritten. You cannot save any changes made to a locked workbook, and you cannot acquire data in a locked workbook. You can create new reports, but the LCquan application does not save the report selections. When you open a locked workbook, it displays [Locked] in the title bar next to the workbook name and in the status bar.

Oracle Database

For information about installing and configuring the Oracle Server and Client software, version 11g or later, refer to the Oracle manuals.

Consult with your Oracle database administrator and your Thermo Fisher Scientific service representative for advice and instructions about how to install this software for your application.

Watson Interface

This appendix describes Thermo Foundation Authorization Manager settings for the Watson interface.

Note To use the digital gateways, you must install the Xcalibur and LCquan XDK components.

Contents

Recommended Settings for Excel Reports

For the Watson file interface, set the following features in Thermo Foundation Authorization Manager to ensure that you can correctly import Excel reports from the LCquan application:

- Remove Signature Line from Excel Reports—This setting removes the signature line from the exported quantitation reports.
- Allow Watson File Interface Excel Format Reports—This setting corrects the format of the acquisition date and time entries in the exported quantitation reports.

Rounding the Decimal Places

For the Watson digital interface, you can ensure consistency in the number of decimal places displayed in the Excel reports that the LCquan application exports. To do this, use the Allow Excel Rounding feature.

If you specify Excel rounding, the exported values are restricted to three decimal places consistently in the Excel reports. However, if you use this feature, the Excel reports do not include a full precision value.

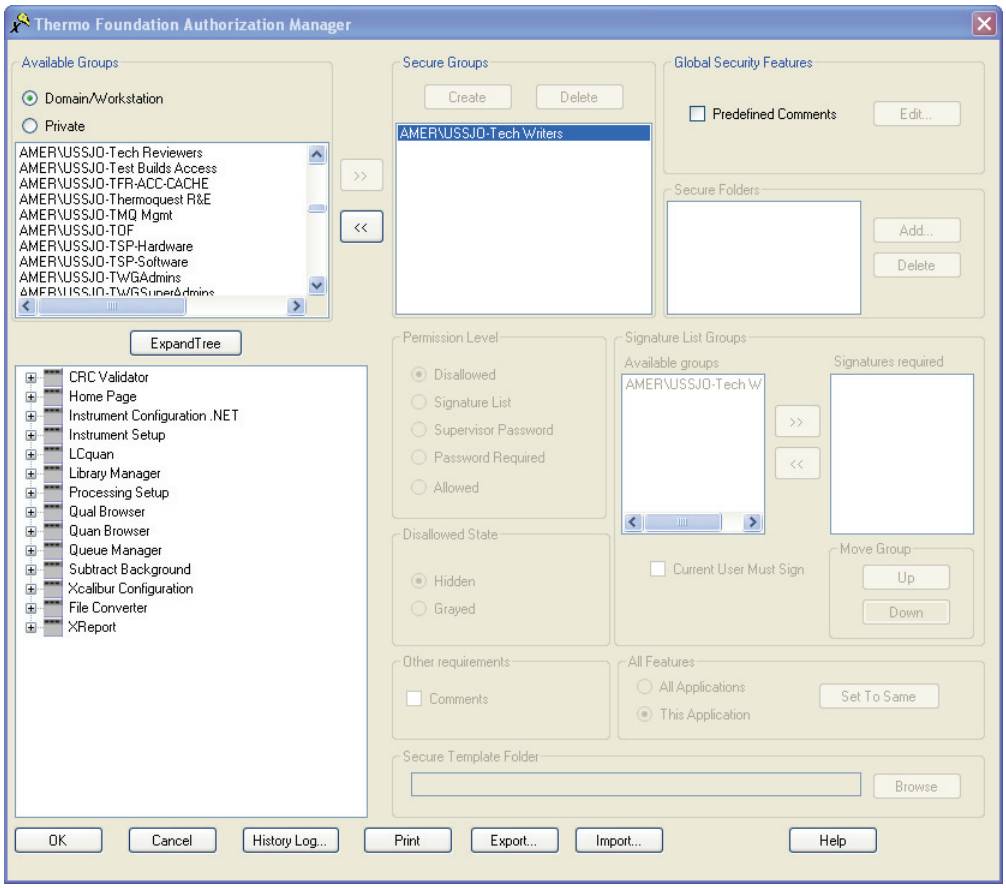
To use the Excel rounding feature, set the permission level to **Allowed** in the Foundation Authorization Manager (Setting the Excel Features). Before the Excel rounding feature takes effect for the Watson digital interface, you must start and exit the LCquan application.

Setting the Excel Features

❖ To set the Excel features for LCquan reports

1. From the Windows taskbar, choose **Start > All Programs > Thermo Foundation 2.0 > Authorization Manager**.

   Thermo Foundation Authorization Manager opens.

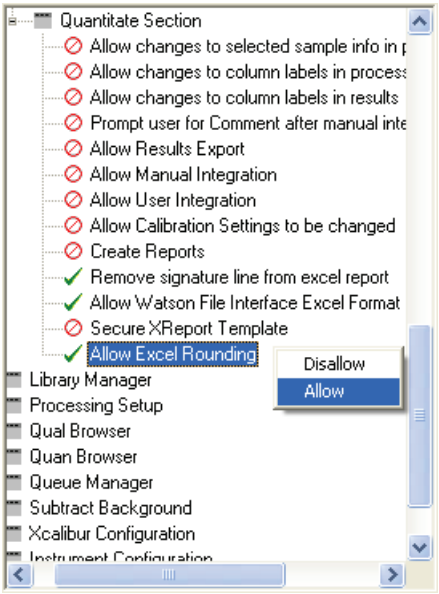


2. In the Secure Groups area, select the group.

3. In the controlled features list (lower left side), select **LCquan**, and click **Expand Tree**.

   The LCquan list of controlled features appears (see Figure 10).

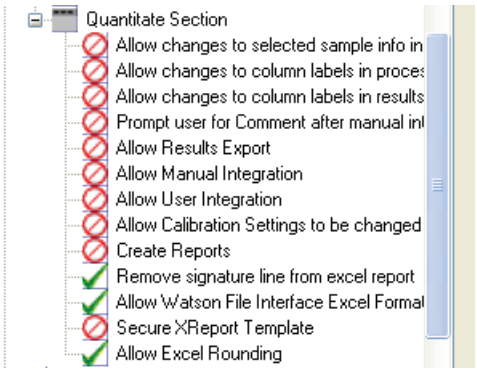
   Figure 10. LCquan quantitate section features list



4. Under Quantitate Section, right-click the feature and choose **Allow** from the shortcut menu for each of the following:

   - Remove signature line from Excel report
   - Allow Watson file interface Excel format
   - Allow Excel Rounding

   Figure 11. LCquan quantitate section features list



   A check mark appears next to each allowed feature.

5. Click **OK** to apply the changes and close the Foundation Authorization Manager.

About the Watson Digital Interface

The following fields are exported to the Watson application using the digital interface for each sample/analyte combination:

- Peak area
- Peak height
- Retention time

See "Rounding the Decimal Places" on page 79.

To use the digital interface with Watson 7.2 or later, refer to *Installing and Using the Peak View Gateway Between Watson and LCquan* for instructions.

IT Considerations

To ensure that both the Xcalibur and LCquan applications work properly, review these IT issues.

Contents

Avoid Antivirus Scanning During Data Acquisition

Schedule utilities that actively scan the hard drive—such as antivirus, defragmenting, and backup utilities—to run at times other than during data acquisition. These utilities can monopolize computer resources, interfere with data acquisition, or cause loss of communication with the instrument.

These directories are typically used during data acquisition:

- C:\Users*user name*\AppData\Local\Temp
- C:\Xcalibur\methods *or* the directory where the instrument method (.meth) and processing method (.pmd) files are stored
- C:\Xcalibur\Quanroot *or* the directory where raw files (.raw) are stored
- C:\Xcalibur\system\programs\

Do Not Delete the Xcalibur System Account

With sequential user logon, a user can log on, start an acquisition, and then log out. When Foundation is installed, a user account—Xcalibur System—is created under the Administrators group. This account runs in the background during data acquisition. Do not delete this account.

Ensure that a Firewall Exception Exists for the Instrument

Firewall settings must include an exception for the instrument in use. If the firewall exception is not configured, the computer is unable to communicate with the instrument. During installation, instrument software now automatically configures the required exception for the Microsoft Windows firewall.

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