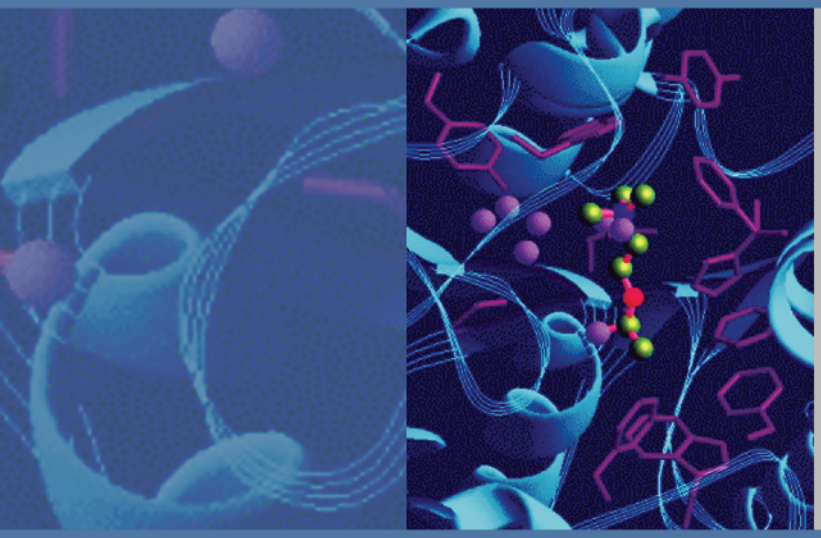

# ChromQuest 5.0

Chromatography Data System

## Administrator Guide

CHROM-97251 Revision A March 2008

Thermo SCIENTIFIC

Software Version: ChromQuest 5.0

**For Research Use Only. Not regulated for medical or veterinary diagnostic use by U.S. Federal Drug Administration or other competent authorities.**

# Contents

# Preface

## About This Guide

Welcome to ChromQuest 5.0. The ChromQuest™ chromatography data system is a member of the Thermo Scientific family of LC data systems.

This *ChromQuest Administrator Guide* describes the administrative tasks that you must perform after you install the ChromQuest data system.

For information on configuring a SpectraSYSTEM LC or a Surveyor™ Plus LC, refer to the *ChromQuest User Guide for the SpectraSystem LC* or the *ChromQuest User Guide for the Surveyor LC*, respectively.

The ChromQuest SI data system for single instruments does not provide security or project management features.

## Related Documentation

In addition to this guide, Thermo Fisher Scientific provides the following documents for the ChromQuest and ChromQuest SI chromatography data systems:

- *ChromQuest 5.0 Installation Guide*
- *ChromQuest 5.0 User Guide*
- *ChromQuest 5.0 Reference Guide*
- *ChromQuest 5.0 Quick Reference Guide*

# Safety and Special Notices

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

Safety and special notices include the following:

**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.

# Contacting Us

There are several ways to contact Thermo Fisher Scientific for the information you need.

### ❖ To contact Technical Support

| | |
|---|---|
| Phone | 800-685-9535 |
| Fax | 561-688-8736 |
| E-mail | TechSupport.C+MS@thermofisher.com |
| Knowledge base | www.thermokb.com |

Find software updates and utilities to download at www.mssupport.thermo.com.

### ❖ To contact Customer Service for ordering information

| | |
|---|---|
| Phone | 800-532-4752 |
| Fax | 561-688-8731 |
| Web site | www.thermo.com/ms |

### ❖ To copy manuals from the Internet

Go to mssupport.thermo.com and click **Customer Manuals** in the left margin of the window.

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

- Fill out a reader survey online at www.thermo.com/lcms-techpubs.
- Send an e-mail message to the Technical Publications Editor at techpubs-lcms@thermofisher.com.

# Managing ChromQuest

You can install the ChromQuest enterprise in a variety of configurations to satisfy the needs of the your individual company:

- Single stand-alone data system computer with instruments attached
- Multiple stand-alone data system computers on a network without a domain controller (non-Windows® 2000/XP network)
- Data system computers on a Windows 2000/XP network using a domain controller
- Client/server mode with multiple networked ChromQuest interfaces and ChromQuest clients.

To maximize the security and efficiency of the data system, system administration functions are available for all configurations.

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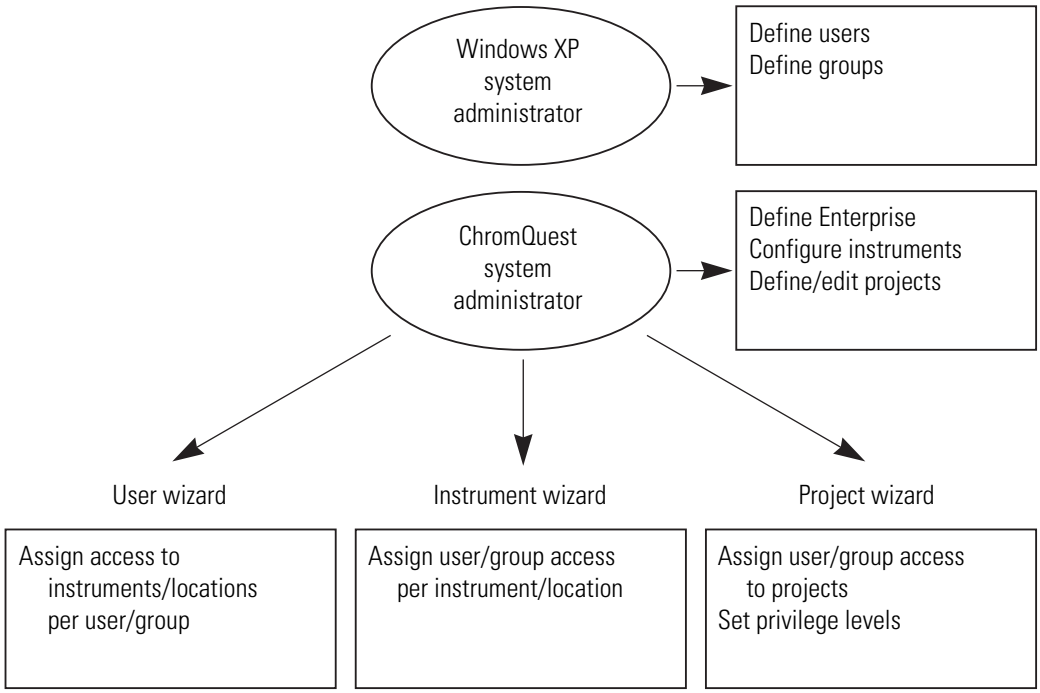
# Environments

When systems are networked using a Windows 2000/XP computer as a domain controller, the Windows XP system administrator grants security privileges to users and groups for resources that are shared on the network through the domain controller. The ChromQuest system administrator then configures the Enterprise, configures instruments, defines projects, and assigns users or groups access privileges to projects and instruments within the enterprise. Project definition and editing, and assignment of user and group access and privileges are accomplished using the System Administration Wizards. See Figure 1.

**Figure 1.** ChromQuest Windows 2000/XP environments




# System Administration Functions

The System Administration function includes setting up or modifying the system enterprise (locations and laboratories), and adding and configuring instruments. It also involves defining the access privileges that laboratory personnel have to specific areas of the data system.

This section contains the following topics:

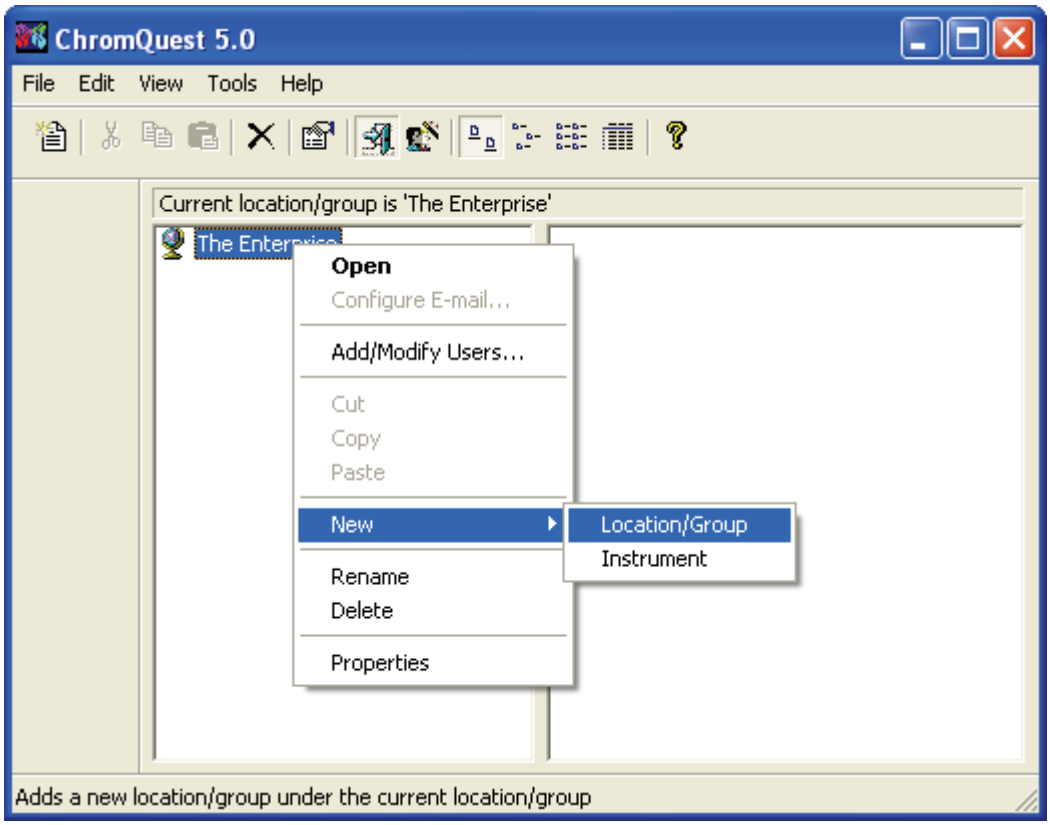
- Enterprise Configuration
- Enterprise Options
- System Administration Wizards

## Enterprise Configuration

The Enterprise consists of all the ChromQuest workstations, ChromQuest interfaces, and ChromQuest clients in your network. After you install the ChromQuest chromatography data system, configure the Enterprise that consists of the data system computers running ChromQuest. Configuring the Enterprise and the workstation computers within the Enterprise is described in detail in Chapter 5, "Configuring Instruments." Figure 2 shows the Main Menu window of the ChromQuest data system.

**Note** The ChromQuest SI data system controls a single instrument and does not provide the system administration features described in this chapter.

**Figure 2.** Main Menu window with a view of the Enterprise shortcut menu




## Enterprise Options

Once you have successfully logged on to the Enterprise, you have access to setting the workstation, Enterprise, general, and e-mail options.

# System Administration Wizards

There are three System Administration Wizards:

- The User Wizard
- The Instrument Wizard
- The Project Wizard

Administrating the Enterprise with these wizards is described in detail in Chapter 4, "Using the System Administration Wizards."

## The User Wizard

With the User Wizard you can do the following:

- Assign Administration functions to a user or group, including System Administration and Instrument Administration.
- Select instruments or locations available to a user or group.
- Add or delete users (only for non-domain workstations).

## The Instrument Wizard

With the Instrument Wizard you can do the following:

- Assign users or groups to an instrument on the domain.
- Assign users or groups to a location on the domain, granting access to all instruments in that location.

## The Project Wizard

With the Project Wizard you can do the following:

- Define new projects or editing existing projects. A project is comprised of a name, location, description, and defined locations for data, method, template, and sequence files.
- Select users and groups for a project.
- Set project privileges for each user (access to command functions such as method development or instrument control).
- Remove projects from active use.

System Administration capabilities can be assigned to as many users as required. The System Administration function is set as part of the User Wizard.

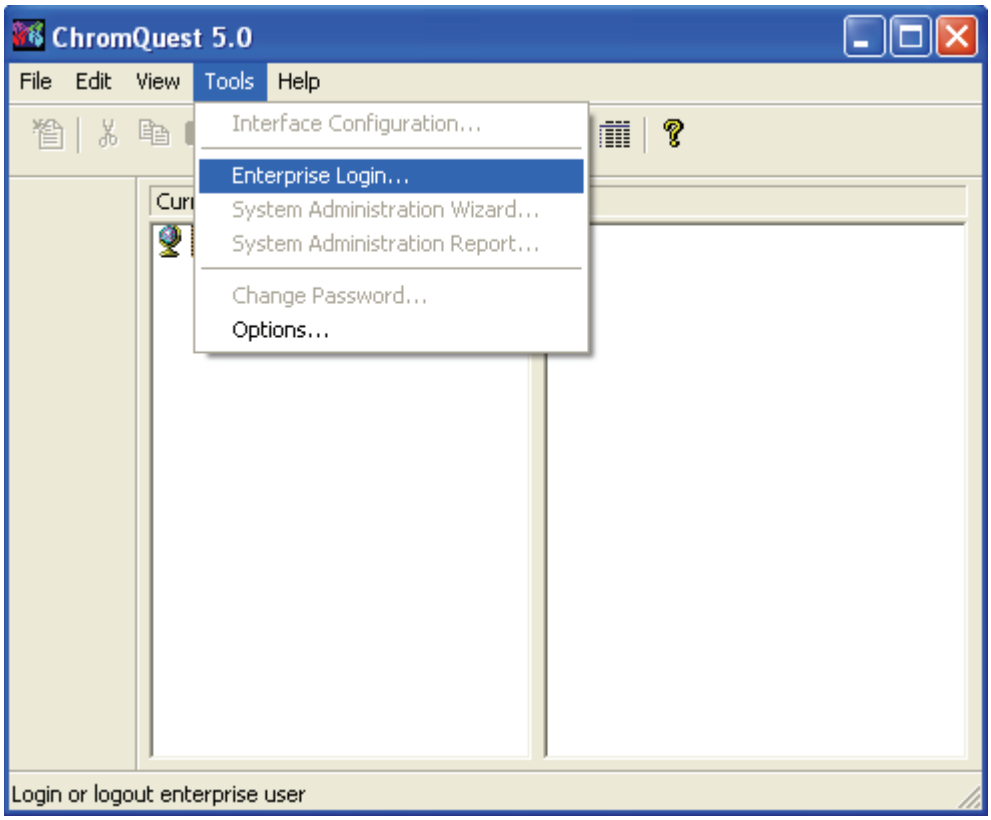
# Enabling the System Administration Functions

To access the System Administration functions from the Main Menu window, the login security feature must be enabled.

### ❖ To log in to the Enterprise

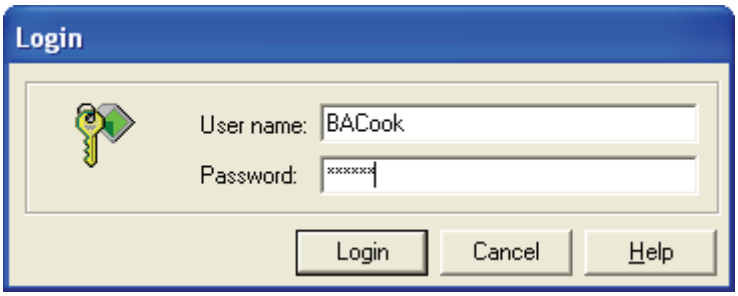
1. Choose **Tools > Enterprise Login**. Or, click the **Enterprise Login** or **Logout** icon on the command toolbar. Figure 3 shows the Tools menu.

**Figure 3.** View of the Tools menu




The Login dialog box appears. See Figure 4.

**Figure 4.** Login dialog box



2. To log in, do the following:

   a. In the User name box, type your assigned user name.

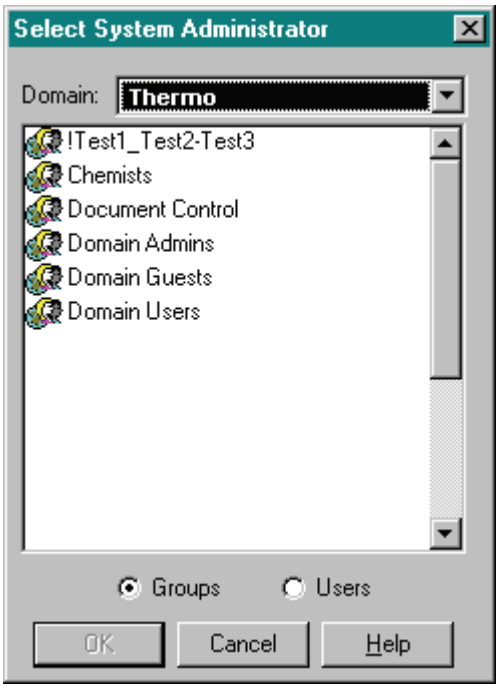
   b. In the Password box, type your password.

   c. In the Domain controller box, select the Windows 2000/XP domain you are using. If your system does not use a domain controller, the Domain controller box does not appear in the Login dialog box.

   Once you have logged on, the System Administration functions and buttons on the menu bar become active.

   The first time you run the software after installation, you are presented with a dialog box where you must designate the System Administrator.

**Figure 5.** Select System Administrator dialog box




3. To select a single administrator, do the following:

   a. Select the correct domain, and then select the **Users** option to view the users of the domain.

   b. Select a user from the list, and then click **OK** to establish this user as the System Administrator.

**Note** You can give system administration capabilities to additional users through the System Administration User Wizard.

# Specifying the Enterprise Options

Once you have enabled the System Administration mode and have successfully logged into the system, you can specify the workstation, Enterprise, general, and e-mail options.

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## Specifying the Workstation Options

To specify the workstation options, perform these tasks:



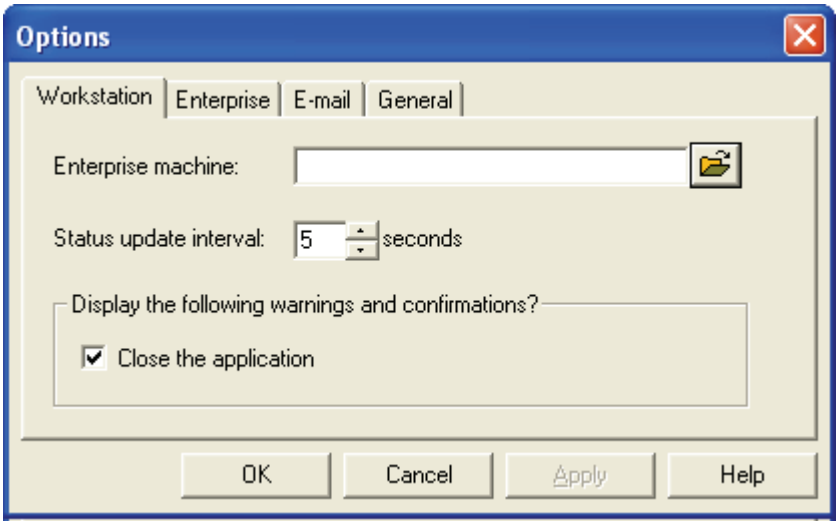
### Selecting the Enterprise Machine

To use a network domain to supply user lists, you must designate the network computer that supplies the network information. If you specified an Enterprise machine when you installed ChromQuest, the name of this computer appears by default in the Enterprise machine box on the Workstation page of the Options dialog box. You must also install ChromQuest on the Enterprise machine.

❖ **To change the Enterprise machine**

1. In the Main Menu window, choose **Tools > Options**. The Options dialog box appears. See Figure 6.

**Figure 6.** Options dialog box




2. Click the **Workstation** tab.
3. On the Workstation page, type the name of the computer in the Enterprise machine box or browse to and select the computer from a list of Enterprise machines.

   The Enterprise machine must be the same for all clients and servers in the enterprise.

## Changing the Status Update Interval

When you choose **View > Details** in the Main Menu window, ChromQuest displays the status of each instrument; for example, Idle, Available, or In Use.

❖ **To specify how often ChromQuest updates the instrument status display**

In the Status update interval box on the Workstation page (see Figure 6), type or select the number of seconds you want to have between status updates.

## Displaying Warnings and Confirmations

❖ **To view warnings and confirmations when you close the applications**

Select the **Close the application** check box on the Workstation page. (see Figure 6).

# Specifying the Enterprise Options

To specify the Enterprise options, perform these tasks:

- Selecting the Instrument Control Mode
- Enabling Instrument Login and Project Management

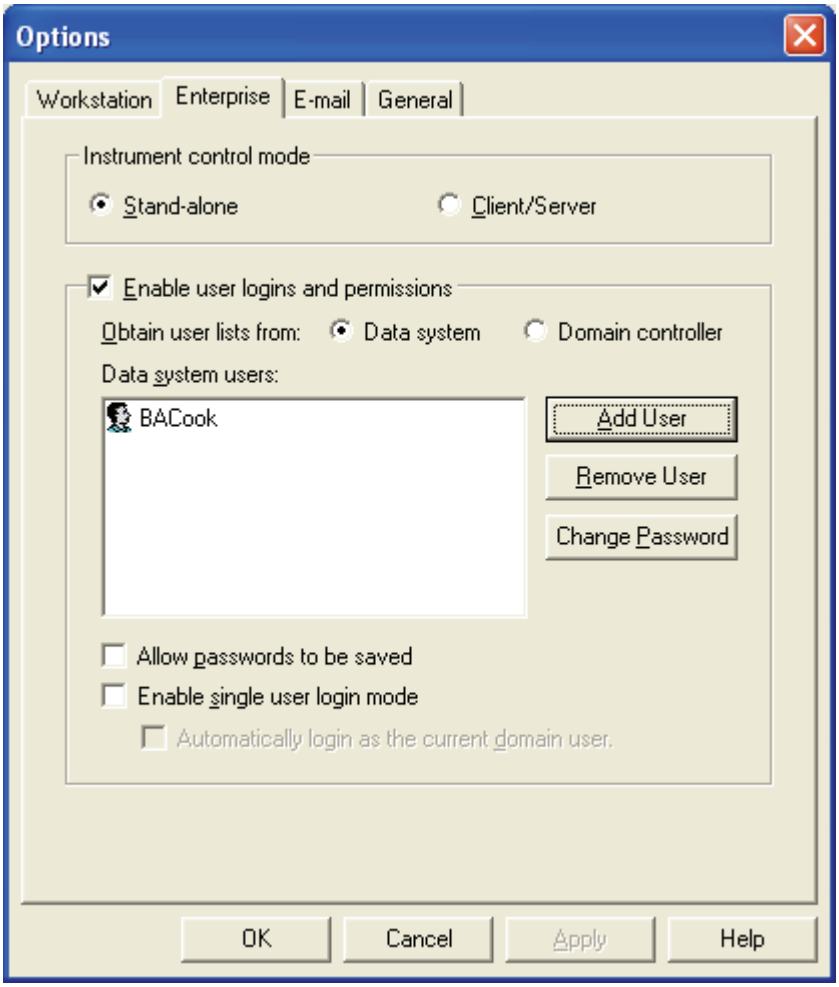
## Selecting the Instrument Control Mode

You can use ChromQuest in the stand-alone mode or the client/server mode.

### ❖ To select the instrument control mode

1. In the Main Menu window (see Figure 2), choose **Tools > Options**. The Options dialog box appears.
2. Click the **Enterprise** tab. The Enterprise page appears. See Figure 7.

**Figure 7.** Enterprise page of the Options dialog box



3. Select the instrument control mode:
   - To select the stand-alone mode, select the **Stand-Alone** option.
   - To select the client/server mode, select the **Client/Server** option.

## Enabling Instrument Login and Project Management

If the Enable user logins and permissions check box on the Enterprise page of the Options dialog box is cleared, ChromQuest users are not required to log in when accessing instrument or administration functions. Normally, this check box is selected, except in single-user labs or where instrument or project access security is not an issue.

### ❖ To enable the security functions for logon and project management

1. In the Main Menu window (see Figure 2), choose **Tools > Options**. The Options dialog box appears.
2. Click the **Enterprise** tab. The Enterprise page appears. See Figure 7 on page 9.
3. Select the **Enable Instrument Login and Project Management** check box.
4. Do one of the following:
   - To obtain the user list from the data system computer, go to "Obtaining the User List from the Data System Computer."
   - To obtain the user list from the domain controller, go to "Obtaining the User List from the Domain Controller," on page 12.
5. To allow users to log in without passwords after an initial login, select the **Allow Passwords to be Saved** check box.

   When users log in for the first time, ChromQuest saves their passwords and does not require them to enter their passwords for subsequent logins. Because users are not required to use passwords after their initial login, system security is decreased.
6. To allow users to log in to the entire Enterprise, select the **Enable Single User Login Mode** check box. After users log into one instrument, for each subsequent instrument they open, ChromQuest only requires them to select a project from the Select Project dialog box.

## Obtaining the User List from the Data System Computer

Use this option if you are running a stand-alone workstation (not networked) or you are not using a domain controller for your network.

### ❖ To add users to the data system computer

1. Select the **Data system** option.

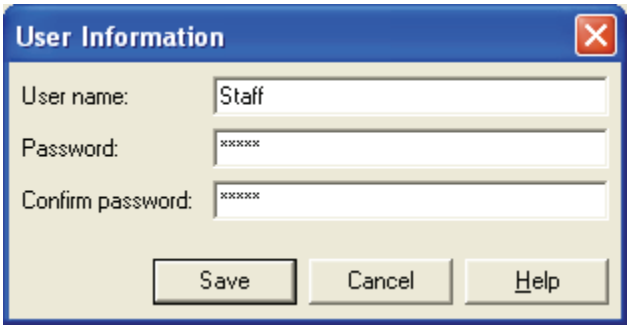
   A list of currently defined users for your workstation appears in the Data system users box.

2. To add a user, do the following:

   a. Click **Add User.**

      The User Information dialog box appears. See Figure 8.

      **Figure 8.** User Information dialog box

   b. In the User name box, type a name for the user.

   c. In the Password and Confirm password boxes, type a password for the user.

   d. Click **Save**.

3. To delete a user, select the user name from the list and click **Delete User**.

4. Return to step 5 on page 10.

## Obtaining the User List from the Domain Controller

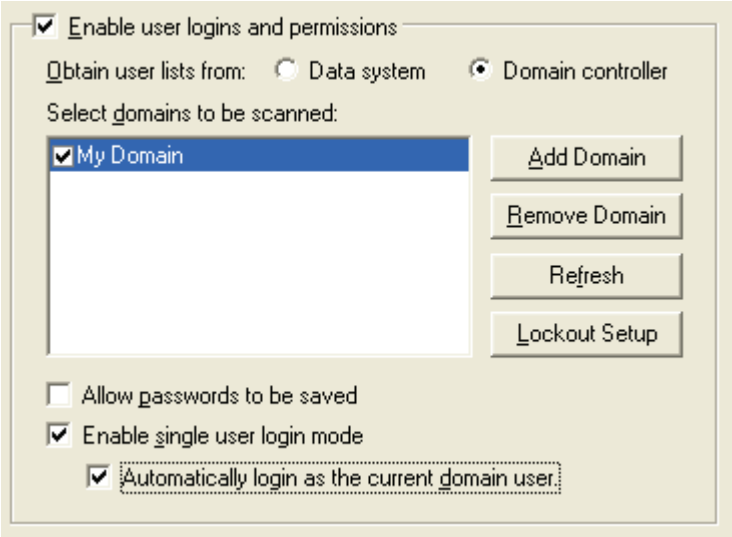
Use this option if the workstation is connected to a Windows XP network with a domain controller.

### ❖ To obtain the user list from the domain controller

1. Select the **Domain Controller** option.

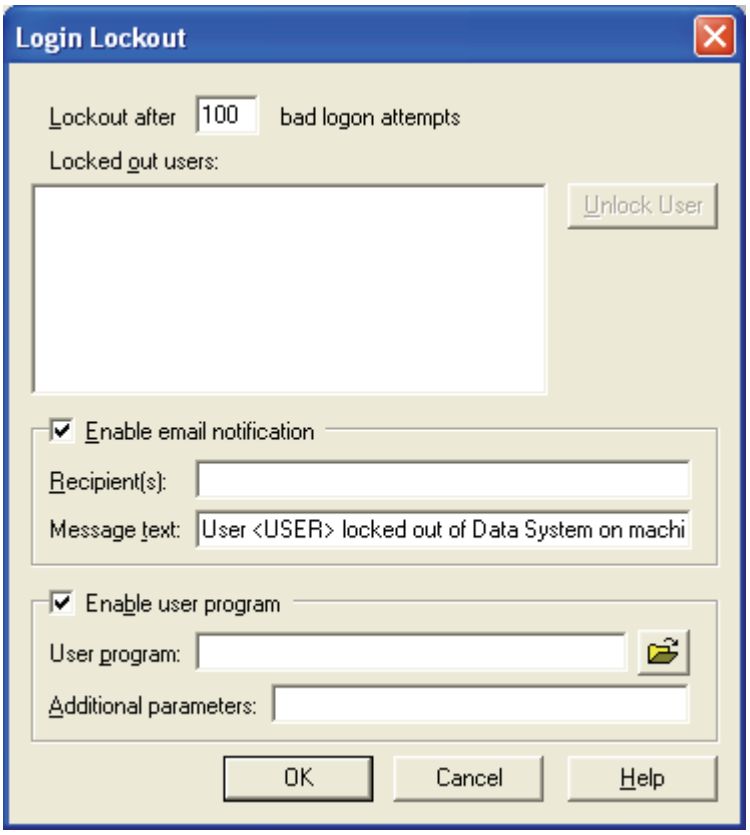
   A list of currently defined domains for your workstation appears in the Select domains to be scanned box.

   **Figure 9.** Domain controller options

2. Select the check boxes next to the domains you want to scan for users or user groups.
3. To modify the list of domains to be scanned, do the following:
   - Click **Remove Domain** to delete a domain from the list after highlighting it with the mouse.
   - Click **Add Domain** to add a domain to the list. The Domain Information dialog box appears. Type a name in the Domain name box and click **Save**.
   - Click **Refresh** to update the list of current domains.
4. To modify the number of bad logon attempts that a user can make before being locked out of ChromQuest, do the following:
   a. Click **Lockout Setup**. The Login Lockout dialog box appears (see Figure 10).

**Figure 10.** Login Lockout dialog box




b. In the Lockout after bad logon attempts box, type the maximum number of login attempts you want users to be able to make before ChromQuest locks them out.

5. To be notified by e-mail when ChromQuest locks users out of the system, do the following:

   a. Select the **Enable E-mail notification** check box.

   b. In the Recipients box, type the e-mail addresses of the people or departments to be notified. You can enter multiple e-mail addresses by separating them with a semicolon.

   c. In the Message text box, type the text that appears in the e-mail message.

      The default message for e-mail notification is as follows: User <USER> locked out of Data System on machine <MACHINE> due to failed login. This string is also used for the subject line of the e-mail generated. You cannot modify the subject line.

   d. Install a MAPI or SMTP-compatible e-mail address on the server. See "Specifying E-Mail Options" on page 14.

   e. Select the and E-Mail notifications must be enabled on the e-mail tab of the Options dialog.

6. To launch a user program when a login lockout occurs, do the following:
   a. Select the **Enable user program** check box.
   b. In the User program box, type the UNC path and the filename of the user program or browse to the user program and select it. The user program runs on the Enterprise machine.
   c. In the Additional parameters box, type any additional parameters required by the program.

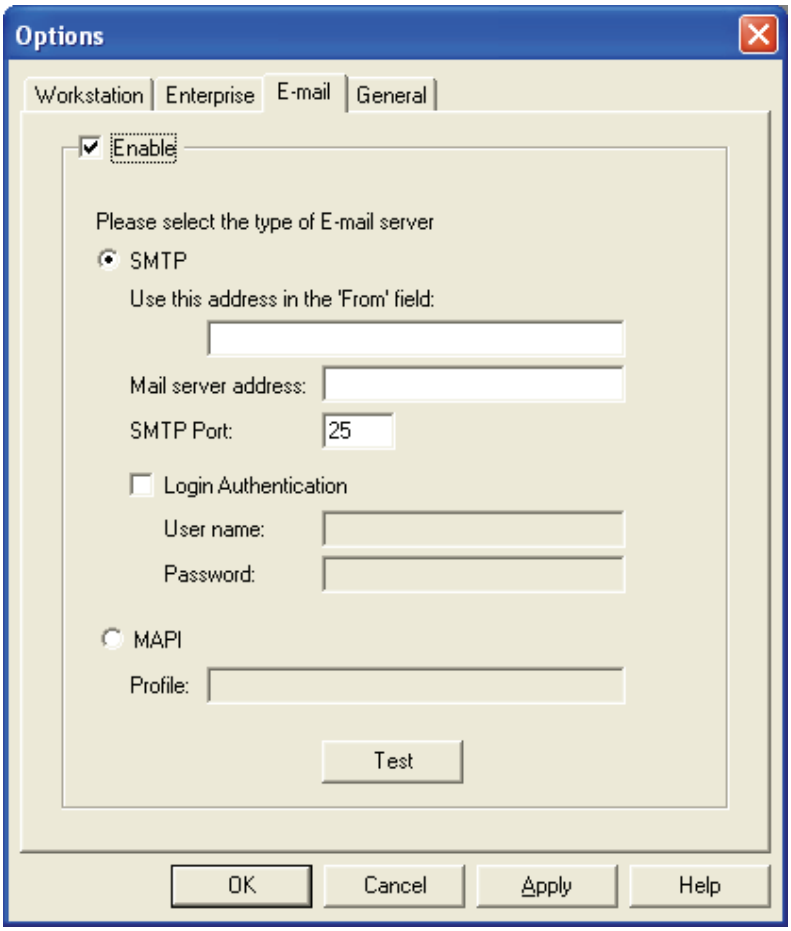
# Specifying E-Mail Options

Use the E-mail page of the Options dialog box to set up the e-mail protocol for ChromQuest.

❖ **To specify the e-mail options for the ChromQuest data system**

1. In the Main Menu window (see Figure 2), choose **Tools > Options**. The Options dialog box appears. See Figure 6.
2. Click the **E-mail** tab. The E-mail page appears. See Figure 11.

**Figure 11.** E-mail page of the Options dialog box



3. Select the **Enable** check box.

   When the Enable check box is clear, ChromQuest does not send e-mails.

4. Select the type of E-mail server used by your network, SMTP or MAPI.

5. If SMTP is to be used for

   - SMTP (Simple Mail Transfer Protocol)

     An SMTP server is a server that sits on a network port and receives connections. An SMTP session involves the identification of the client (usually a machine running an e-mail program), and the transmission of e-mail headers and content. When a session ends, the SMTP server starts the process of sending the mail over the network.

     Select the **SMTP** option if SMTP is to be used for e-mail.

     – Use this address in the 'From' field

       Enter an e-mail address of a valid user.

     – Mail server address

       This box is used to specify the SMTP compliant e-mail address of the local mail server to whom the e-mail notification should be sent. This field can be a valid TCP/IP address or a URL name understood by the network.

     – SMTP Port

       This field is used to specify the TCP/IP port number used for SMTP mail.

     – Login Authentication

       Select this check box to enable login authentication. Enter your user name and password for login authentication.

   - MAPI (Messaging Application Programming Interface)

     MAPI is a system built into Microsoft™ Windows™ that enables different e-mail applications to work together to distribute mail. As long as both applications are MAPI-enabled, they can share mail messages with each other.

     Select the **MAPI** option if MAPI is to be used for e-mail.

     – Profile box

       This box is used to specify the MAPI Profile to be used for sending e-mail.

   - Test

     Clicking this button causes the system to attempt to connect to the e-mail server and test the port (for SMTP) or checks if the profile exists on the server (for MAPI). This function displays a message box indicating the success or failure of the connection attempt.

E-mail notifications from ChromQuest (version 4.0 or higher) are done through a Messaging Application Programming Interface (MAPI) on the Enterprise machine. To set this up, you must know how to install the e-mail software and connect to the appropriate network server for the organization. The specific settings are different for all organizations so it is generally necessary to consult with a network administrator.

### ❖ To set up e-mail notification

1. Verify or install e-mail software that supports the MAPI.

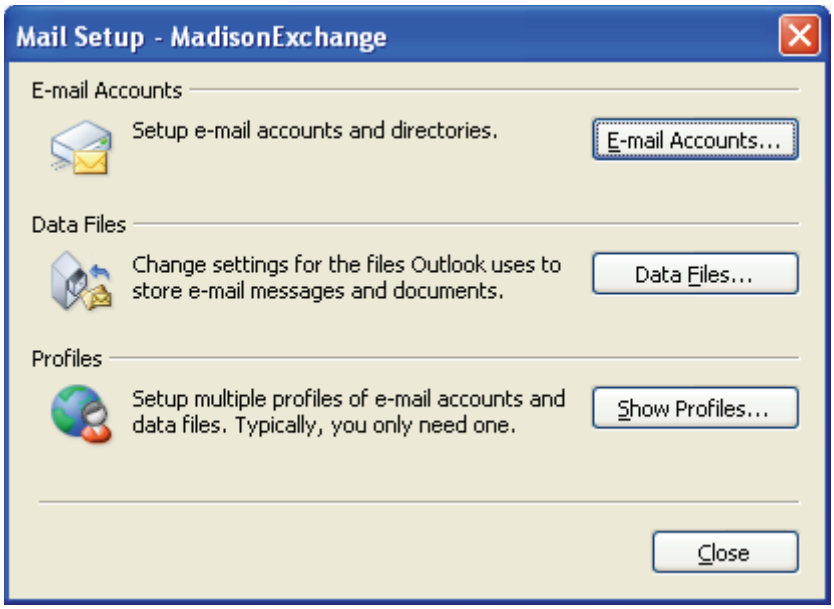
   Windows Messaging Mail and Microsoft Outlook support MAPI but Microsoft Outlook Express does not. If you use Microsoft Outlook, it must be configured for "Corporate or Workgroup." The "Internet only" configuration does not support MAPI.

   For Windows 2000, a separate MAPI-compatible e-mail program must be installed, as one is not included with the operating system.

2. Send e-mail directly from the e-mail program on the Enterprise machine and verify it is received as expected. If this is not working, ChromQuest cannot send e-mail.

3. From the Windows XP Control Panel, double-click **Mail**. The Mail Setup dialog box appears. See Figure 12.

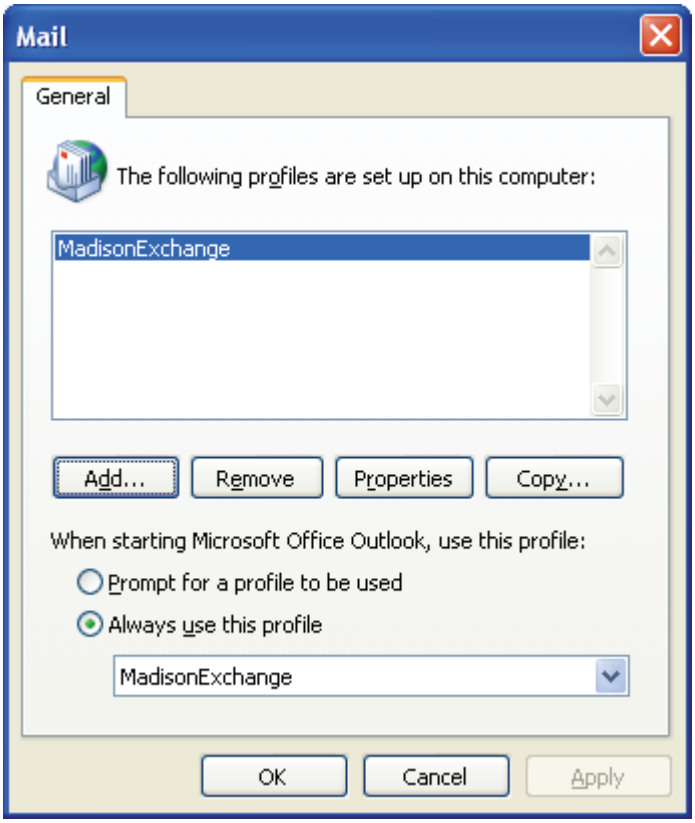
   **Figure 12.** Mail Setup dialog box




4. Click **Show Profiles**.

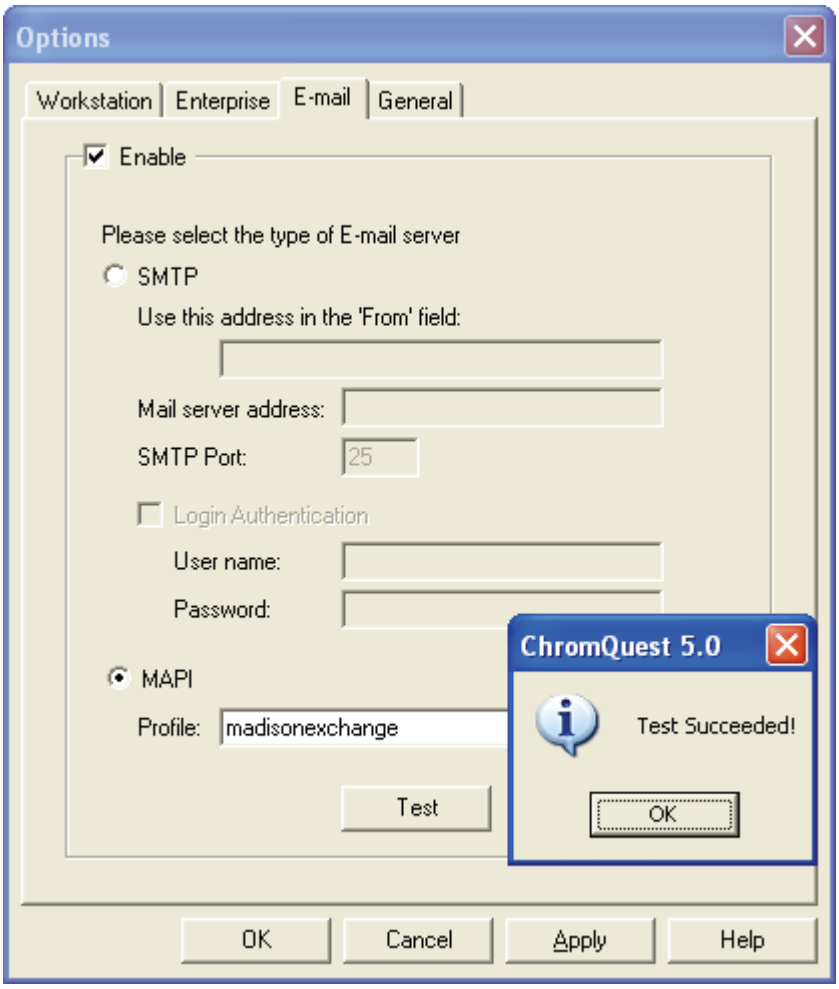
   The Mail dialog box appears. See Figure 13.

**Figure 13.** Mail dialog box




5. On the E-mail page, click **Test** to verify the MAPI profile setting. See Figure 14.

**Figure 14.** E-mail page




6. Click **OK** to close the message dialog box.
7. In the Login Lockout window (**Tools > Options > Enterprise** page with the Domain Controller option selected) in ChromQuest, enter the profile name.

**Note** Be sure the e-mail software is set up so that there is no password or other response required to send e-mail.

# General Options

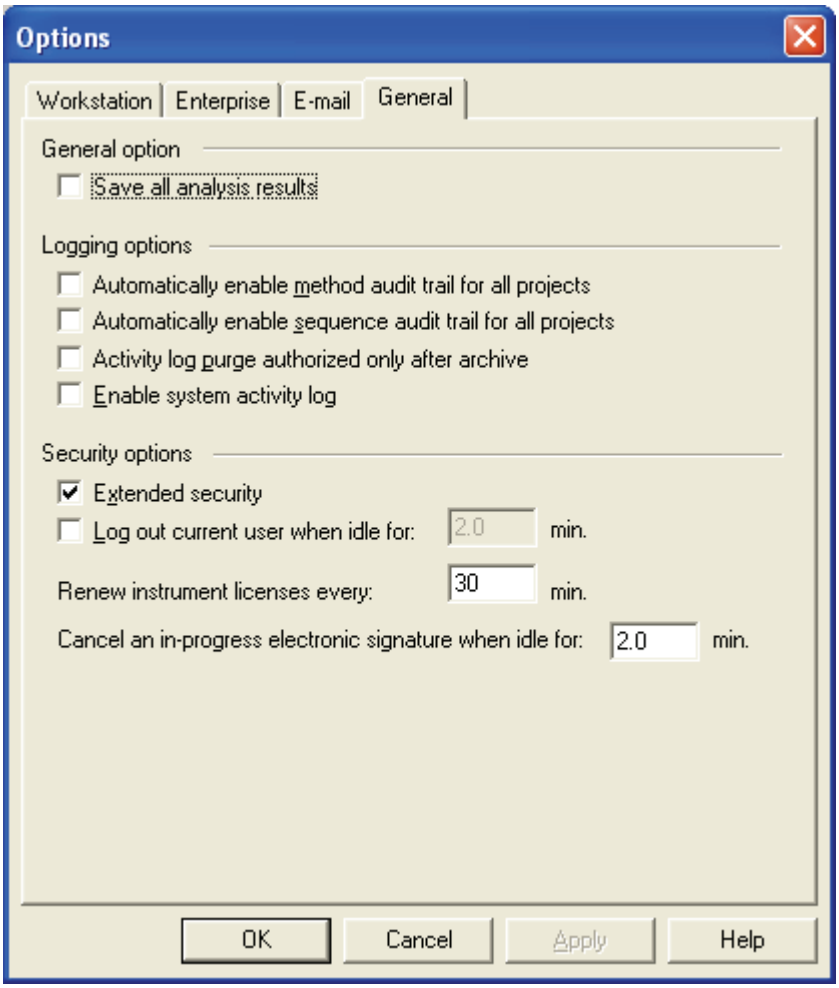
Use the General page of the Options dialog box to specify the logging options, security options, and whether the ChromQuest data system saves all the analysis results or just the original and most recent analysis results.

## Specifying Whether ChromQuest Saves All the Analysis Results

❖ **To specify that ChromQuest saves all the analysis results**

1. In the Main Menu window (see Figure 2), choose **Tools > Options**. The Options dialog box appears.
2. Click the **General** tab. The General page appears. See Figure 15.

**Figure 15.** General page



3. To specify ChromQuest saves all the analysis results for a data file to the data file, select the Save all analysis results check box.

   Every time an analysis is made on a data file, the results are saved in the data file. The results are tagged with the user name and date of analysis. This makes it possible to open a specific result from the Open Data dialog box, using the Open with Results option. If this check box is not selected, only the original and most recent results are saved in the data file.

## Specifying the Logging Options

The logging options control how the audit trail and activity logs are handled.

- Automatically enable method audit trail for all projects

  When this check box is selected, the method audit trail is enabled whenever a method is saved.

- Automatically enable sequence audit trail for all projects

  When this check box is selected, the sequence audit trail is enabled whenever a sequence is saved.

- Activity log purge authorized only after archive

  When this check box is selected, the instrument activity log must be archived before it can be purged.

- Enable system activity log

  When this check box is selected, the system activity log is enabled. Once this is enabled, it cannot be turned off.

### ❖ To access the system activity log

In the Main Menu window, choose **File > System Activity Log**.

### ❖ To archive the system activity log

Choose **File > System Activity Log > Archive** from the Main menu. A dialog box appears where you can select the location for the archive file. A default name is assigned with the .logarc extension. This file can be viewed using the Archived Log Viewer that can be run from the Chromatography program group in Windows.

## Specifying the Security Options

In the Security options area of the General page, you have the following options:

- Extended security

  When this check box is selected, a checksum is calculated whenever a data file is closed. When the file is subsequently opened, its checksum is verified first. If the check fails (the calculated checksum for the file does not match the one previously calculated for the file) the file cannot be opened, and an error is posted in the instrument activity log. Checksum verification is enterprise-wide.

  **Note** Extended security does not affect Windows 2000/XP security settings in non-networked environments (Stand-alone).

  In addition, the Extended Security function provides additional security to the enterprise in the following ways:

  – All system administrators have full access to everything.

  – All non-system administrators have read/execute rights to project directories for which they have rights.

  – All non-system administrators have read/write/execute rights to project subfolders for which they have rights. This means that users in the project without system administrator rights cannot create subdirectories or files under the project directory, and they cannot rename or delete files under the project subfolders. Directories can still be created in project subfolders, but only through ChromQuest.

- Log out current user when idle for

  When this check box is selected, enter a number of minutes. If no mouse or keyboard activity is detected during the specified number of minutes in system administration mode, the system:

  – Cancels any open dialog boxes

  – Cancels any wizard in progress

  – Log outs of Administrative Mode

- Renew instrument licenses every

  Renewal of instrument licenses prevents license problems which might be caused by unexpected disconnection of the server in the client/server mode. The default for this value is 30 minutes, but when recovering from a network problem, you can temporarily set the value to 1 minute.

- Cancel an in-progress electronic signature when idle for

  If an electronic signature is in progress, it is cancelled if there is no input for the specified number of minutes.

# Setting Up E-Mail

The ChromQuest data system includes the ability to automatically send e-mail notifications when system events occur. E-mail notifications can be global or instrument specific.

**Note** If you are unfamiliar with the e-mail configuration of your network, consult your network administrator to complete this setup.

**Contents**



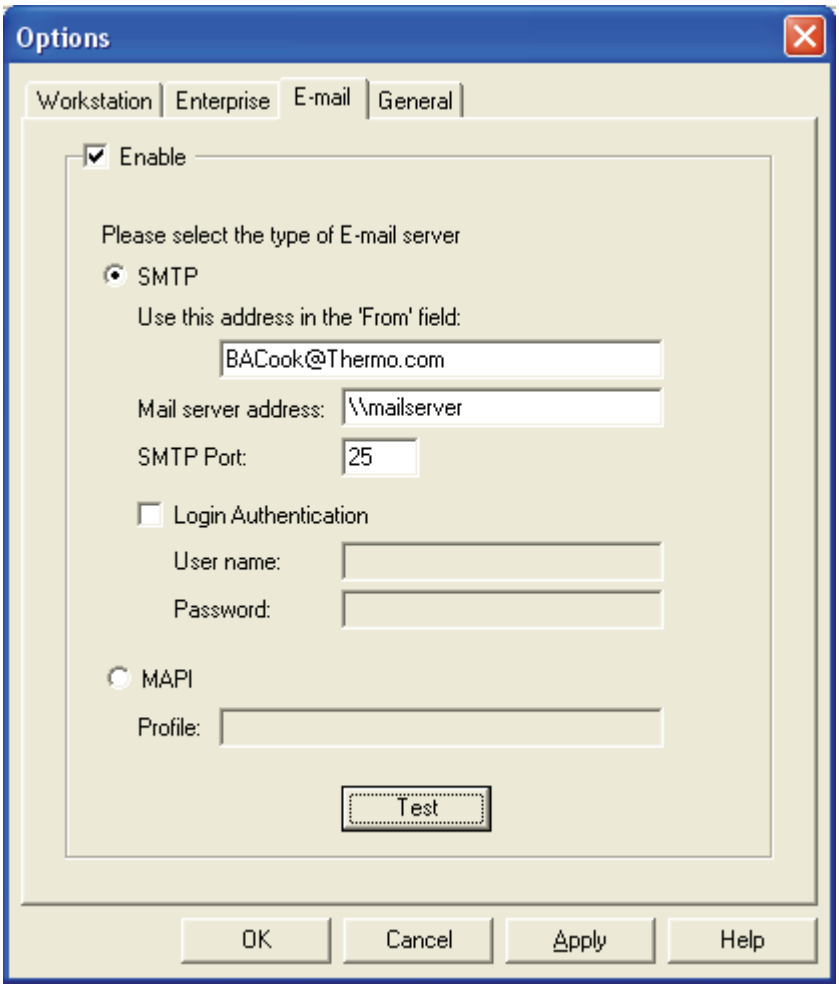
## Setting Up the E-Mail Option

❖ **To set up the e-mail notification feature**

1. Start ChromQuest and log on as a user with system administration privileges.
2. From the Main menu, choose **Tools > Options** to open the Options dialog box.
3. Click the **E-mail** tab to open the E-mail page. See Figure 16.
4. On the E-mail page, select the e-mail interface that is supported by your network: SMTP or MAPI. Then enter the appropriate parameters. For more information, refer to ChromQuest Help.
5. Click **Test**.

   This causes the system to attempt to connect to the e-mail server and test the port (for SMTP) or checks if the profile exists on the server (for MAPI). This function displays a message box indicating the success or failure of the connection attempt.

**Figure 16.** Options dialog box – E-mail page




# Setting Up Automatic Notifications

Automatic notifications are e-mail messages that are sent every time a specific event occurs. Automatic notifications are set up by a data system user with system administration privileges. They can be set up for an individual instrument, for location/groups, or for the entire Enterprise.

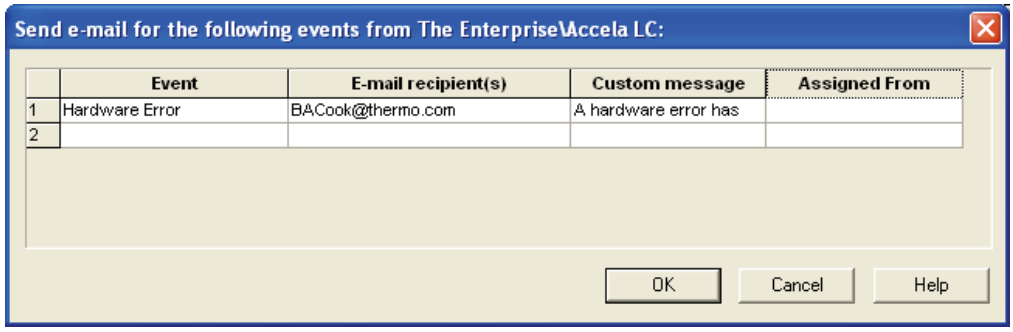
**Note** Automatic notifications for an instrument are inherited from the group and Enterprise of which it is a member. For example, if you create an automatic notification for hardware error for the Enterprise, that event automatically appears in the spreadsheet for every instrument in the Enterprise.

### ❖ To set up automatic notifications

1. Decide if the event is global to the Enterprise or specific to an instrument in the Enterprise:

   - If the event is global, from the Main Menu window, select the Enterprise icon and choose **File > Configure > E-mail** to open the dialog box called Send e-mail for the following events from The Enterprise.
   - If the event is specific to an instrument in the Enterprise, right-click an instrument icon in the Main Menu window. From the shortcut menu, choose **Configure > E-Mail** to open the Send e-mail for the following events from The Enterprise\Instrument dialog box. See Figure 17.

   **Figure 17.** Send e-mail for the following events from the Enterprise\Accela LC dialog box

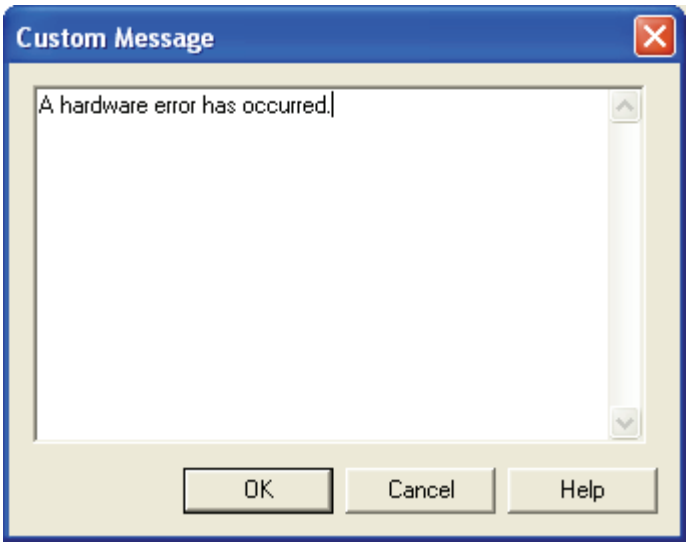



2. Fill in a row of the spreadsheet for each notification you want to occur.

   - Select the event from the Event list. If this event occurs during a run, the custom e-mail message is sent to the designated recipients.
   - Specify a recipient in the E-Mail Recipient(s) box.

     The recipients are listed in the "To" field of the message. This must be an SMTP compliant e-mail address of a valid user. You can add multiple addresses separated by a semi-colon.
   - Click the down arrow to enter an optional custom text message for this event. The Custom Message dialog box appears (see Figure 18). Type a custom text message to be sent with an event e-mail. Click **OK** to close the Custom Message dialog box.

**Figure 18.** Custom Message dialog box




- In the Assigned box, enter the origin of the event. Depending on the Enterprise configuration, the origin of the event can be the Enterprise or the name of a location/group. If you are using ChromQuest in the stand-alone mode, leave this box blank.

3. Click **OK** to accept the settings and close the dialog box.

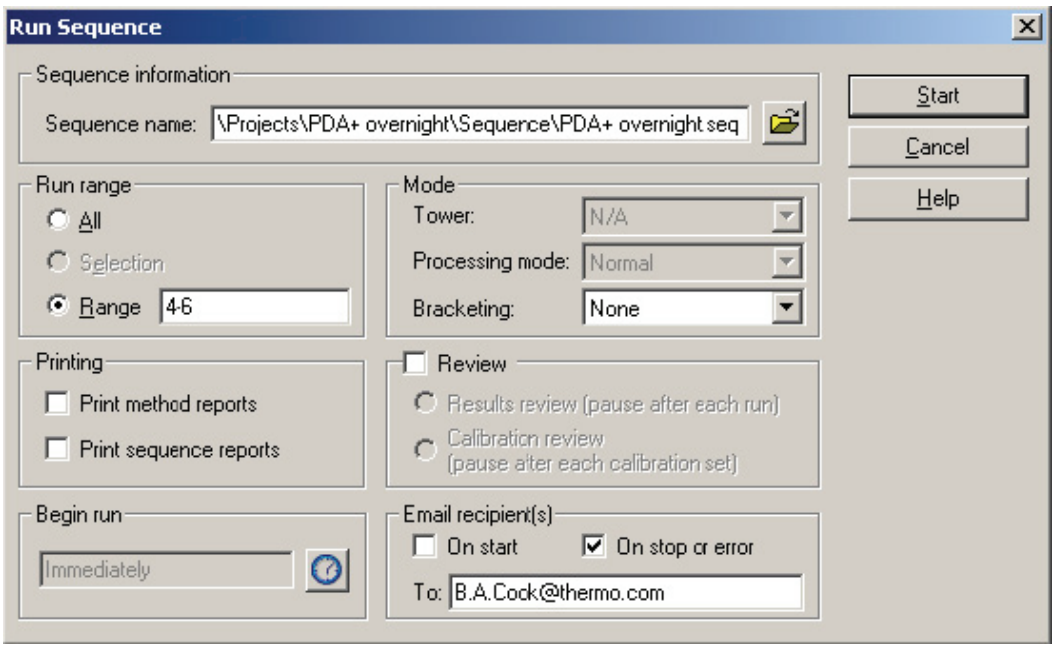
# Setting Up Specific Notifications

Specific notifications are one-time events that can be set up by any user of the ChromQuest data system. An example of this type of event is a notification that an individual sequence has completed.

A user activates a specific notification within the Instrument window by filling in the information for that event in the dialog box initiating that action.

In this Run Sequence dialog box, the entries specify that the user (with a user name of BACook) is to be notified by e-mail when the sequence stops or pauses due to an error.

**Figure 19.** Run Sequence dialog box



# Using the System Administration Wizards

This chapter describes how to use the system administration wizards to assign instrument and system administration privileges and to create projects.

**Contents**



## System Administration Wizard

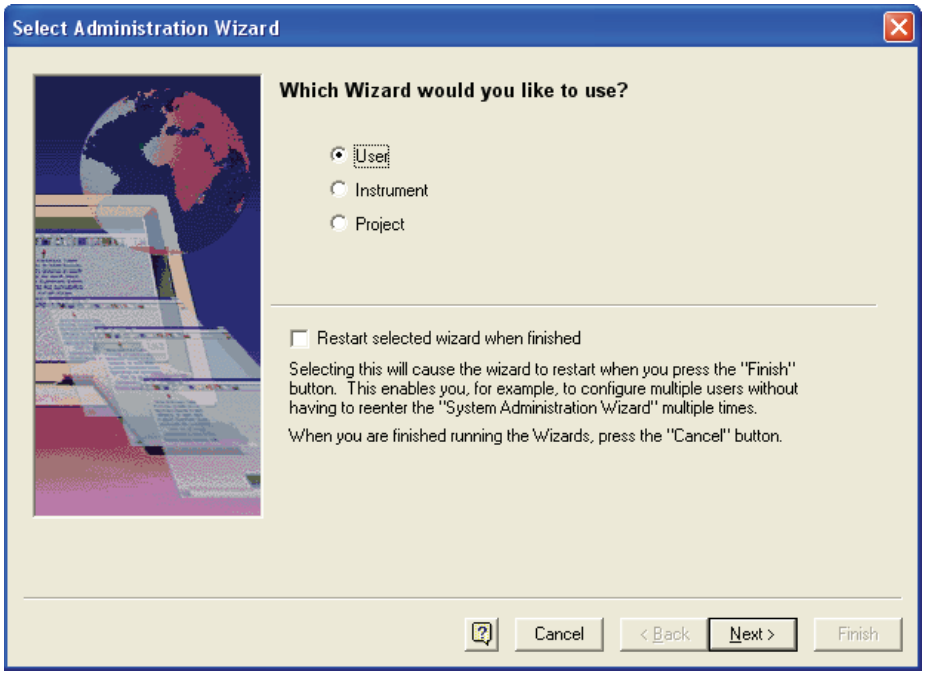
To require logins to specific projects, follow the instructions in "Enabling the System Administration Functions" on page 5 and "Enabling Instrument Login and Project Management" on page 10.

### ❖ To start the System Administration Wizard

1. Do one of the following:
   - Click the **System Administration Wizard** icon on the toolbar of the Main menu
   - Choose **Tools > System Administration Wizard**.

   The Select Administration Wizard page appears (see Figure 20).

**Figure 20.** Select Administration Wizard page




2. Select the **Restart selected wizard when finished** check box if you want to continue using the selected wizard after completing the current definition. For example, set up multiple new projects without restarting the Project Wizard.

# User Wizard

Use the User Wizard to modify system access for users and groups.

If you want to add or edit more than one user or group, select the **Restart selected wizard when finished** check box. When this check box is selected, the User Wizard restarts when you click **Finish**; you can then add or edit additional users or groups.

**Note** Users are defined through the Microsoft Windows 2000/XP domain controller administration. See your network administrator or Microsoft Windows 2000/XP documentation for details.

### ❖ To set up access for users and groups

1. In the Select Administration Wizard page of the System Administration Wizard, select the **User Wizard** option. Click **Next** to continue.

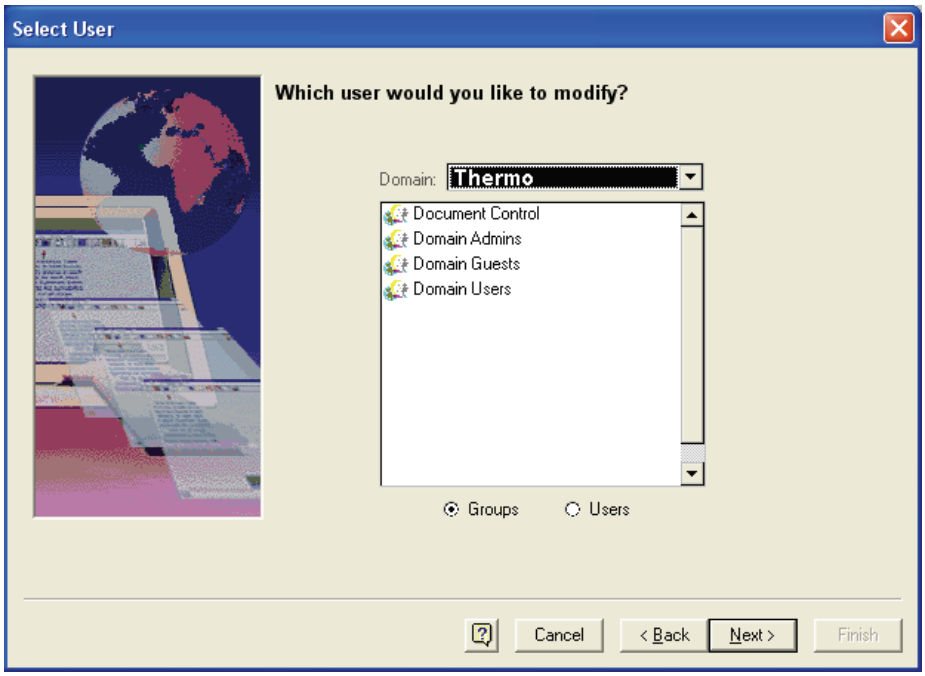
   The options on the Select User page depend on whether you enable logins from a domain controller or the data system. Logins are enabled by selecting the Enable Instrument Logins and Project Management check box on the **Tools > Options > Enterprise** page.

2. Do one of the following:
   - If the Enterprise is set up to enable logins from a domain controller, go to step 3
   - If the Enterprise is set up to enable logins from the data system computer, go to step 4
3. If user and group lists are accessed from a domain controller, do the following:
   a. Select a domain from the list of available domains (see Figure 21).

      A domain is a functional portion of the network that has been set up by the Windows 2000/XP Domain Controller. Once you have selected a domain, a list of defined groups within that domain appears.

   b. Select the **Groups** or **Users** option.
   c. Select a user or a group.
   d. Click **Next** to continue with setting administrative privileges for this user or group.

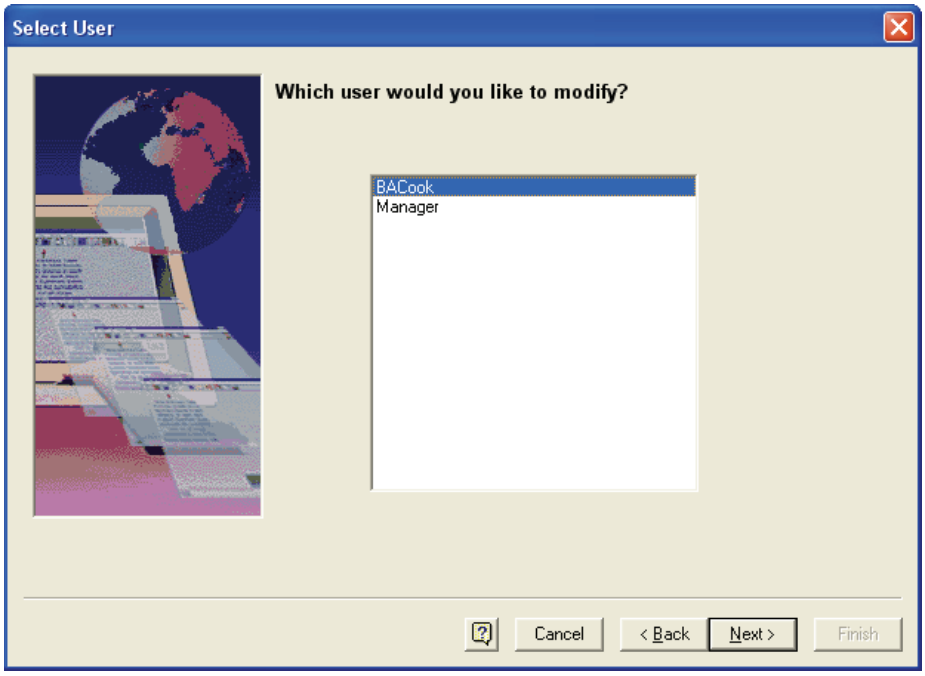
**Figure 21.** Select User page




**Note** If you plan to assign the same administration privileges, instrument privileges, and project privileges to all users in a group, it is faster to perform this function based on a **Group** selection, rather than assigning each user individually.

4. If the users list is accessed from the data system, select the user that you would like to modify (see Figure 22). Then click **Next**.

**Figure 22.** Select User page



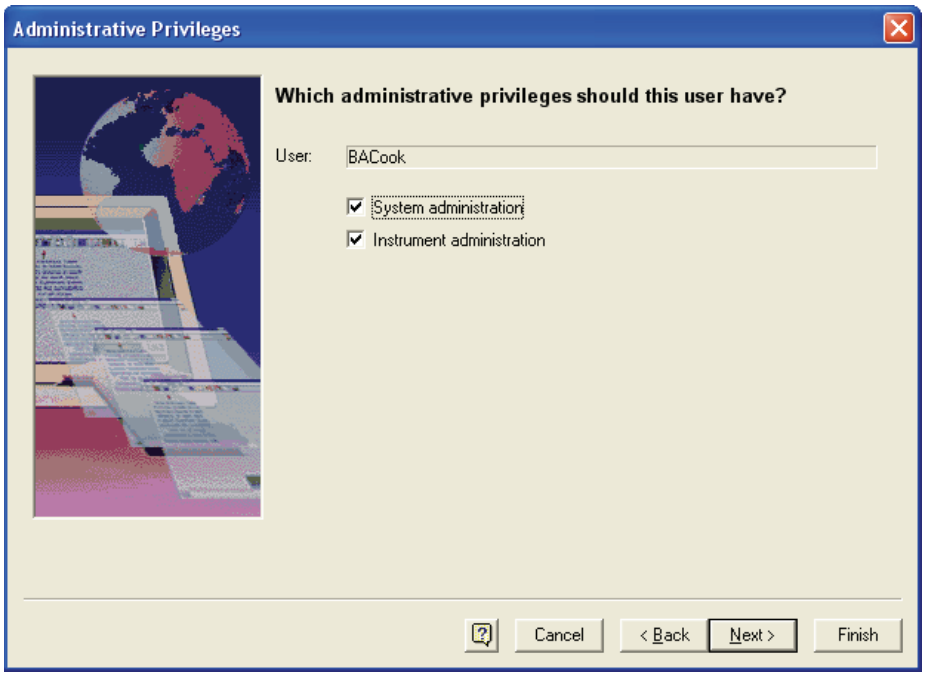

5. In the Administrative Privileges page (see Figure 23), do the following:

   a. Select the administrative privileges for this user:

      - To allow access to System Administration functions, select the **System administration** check box. These include access to the user wizard, instrument wizard, and project wizard.
      - To allow access to Instrument Administration functions, select the **Instrument administration** check box. When this box is selected, the user has access to adding, deleting, and configuring instruments.

   b. Click **Next**.

**Figure 23.** Administrative Privileges dialog box

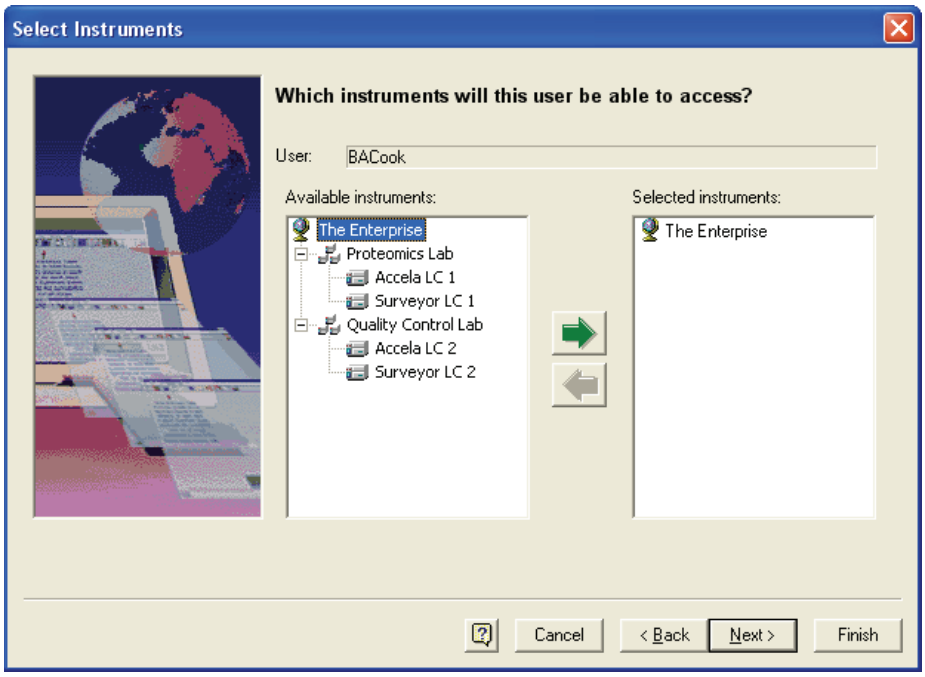



6. In the Select Instruments page (see Figure 24), select the instruments that users or groups can access, and then click **Next**.

   From the list displayed in the Available instruments box, select the instruments for this user (or group): either double-click the instrument, or click once to highlight the instrument and then click the green arrow. The list of instruments to be accessed by this user (or group) is displayed in the Selected instruments window. If no instruments appear in the Available instruments window, expand the enterprise by double-clicking locations until the desired instruments appear.

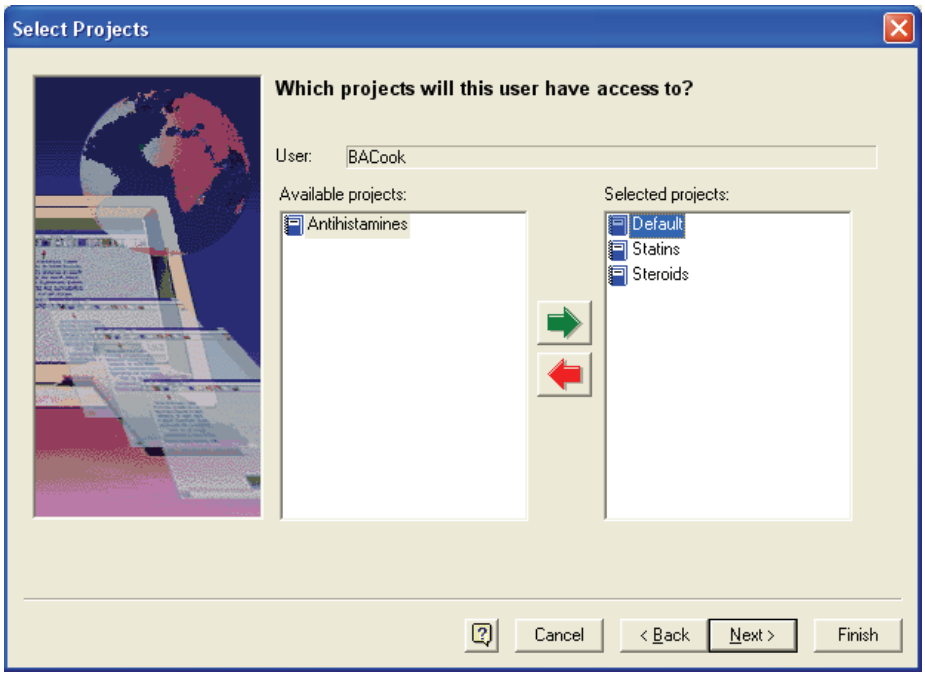
   You can also assign all instruments within a laboratory or location to a user/group by selecting the entire location from the Available instruments box. When a location (for example, QC Lab) appears in the Selected instruments box, this means that all instruments in that location are selected.

**Figure 24.** Select Instruments dialog box



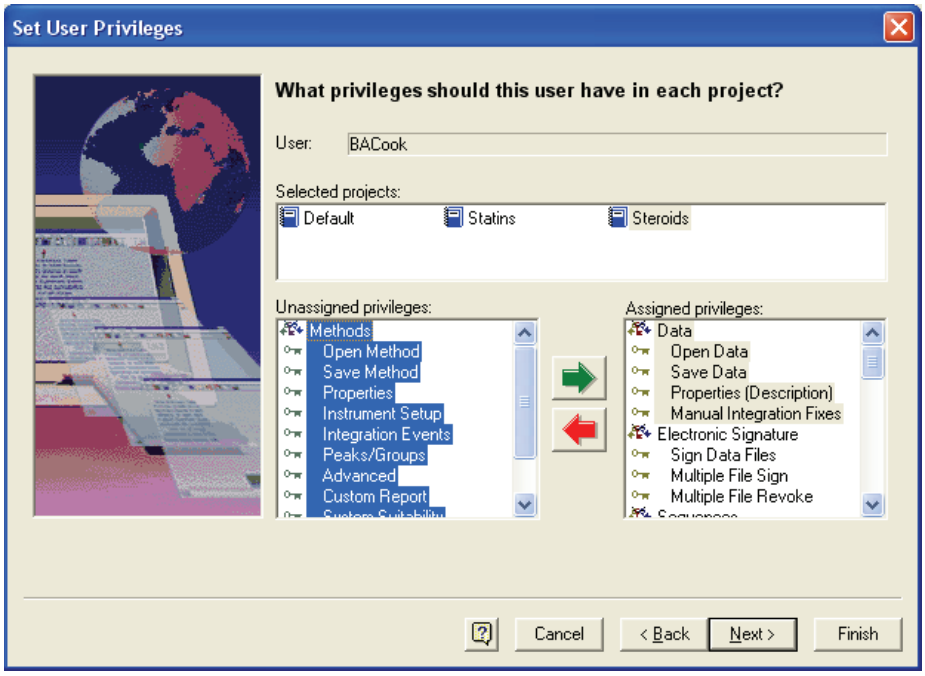

7. In the Select Projects page (see Figure 25), select the projects that the current user/group can access. From the Available projects box, either double-click a project, or click to highlight the project and then click the green arrow. The list of Selected projects are the projects the current user/group can access. When you have completed assigning projects, click **Next**.

**Figure 25.** Select Projects page



8. In the Set User Privileges page (see Figure 26), for each selected project, assign privileges by highlighting the privileges in the Unassigned privileges box, and then click the **green arrow** to move them to the Assigned privileges box. You can also double-click the privileges to quickly assign them. When you have completed assigning privileges for desired projects, click **Next**.

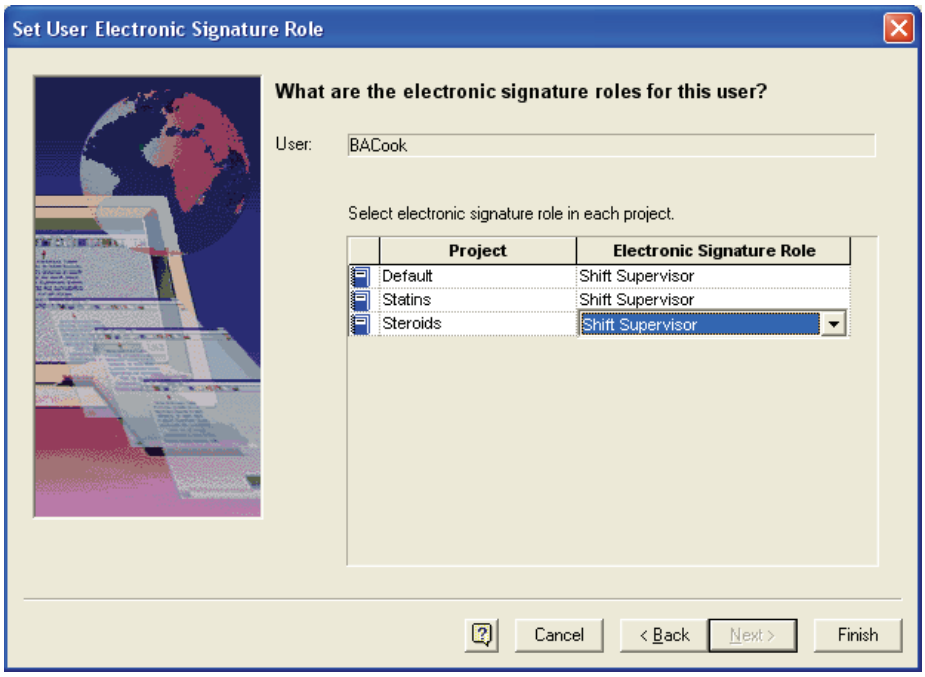
**Figure 26.** Set User Privileges page




**Note** The "Calibrate" privilege allows the user to run a calibration sample to update the method calibration. To create or modify the calibration parameters in a method, the user must have the "Save Method" privilege assigned.

9. In the Set User Electronic Signature Role page (see Figure 27), select the electronic signature roles for each project that the user has privileges to. When you are finished, click **Finish**.

**Figure 27.** Set User Electronic Signature Role page



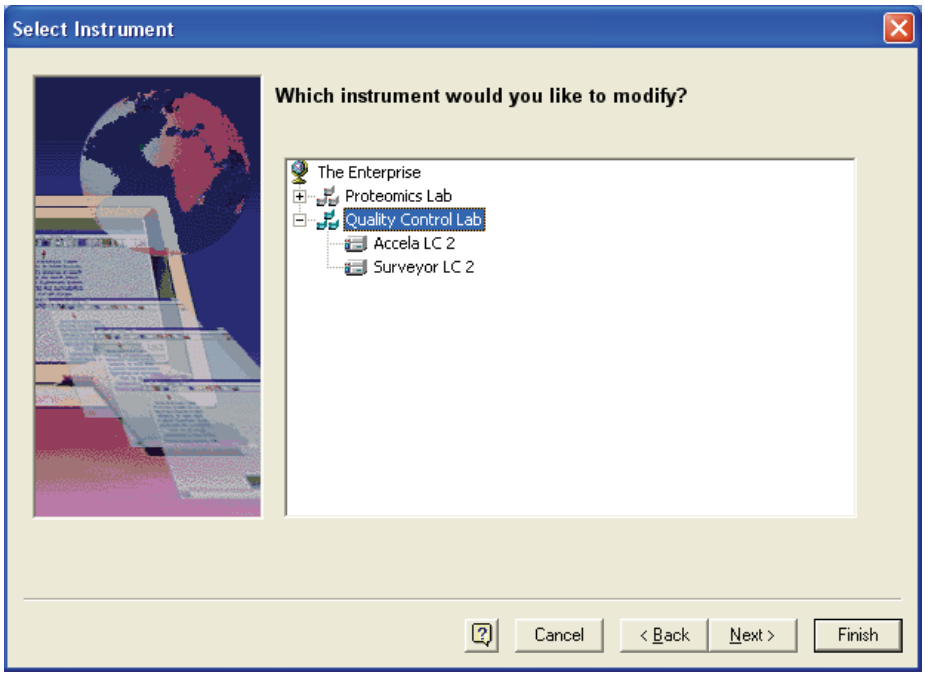

# Instrument Wizard

Use the Instrument Wizard to assign Users/Groups to an instrument or to all instruments in a given Enterprise location.

### ❖ To assign users and groups to an instrument

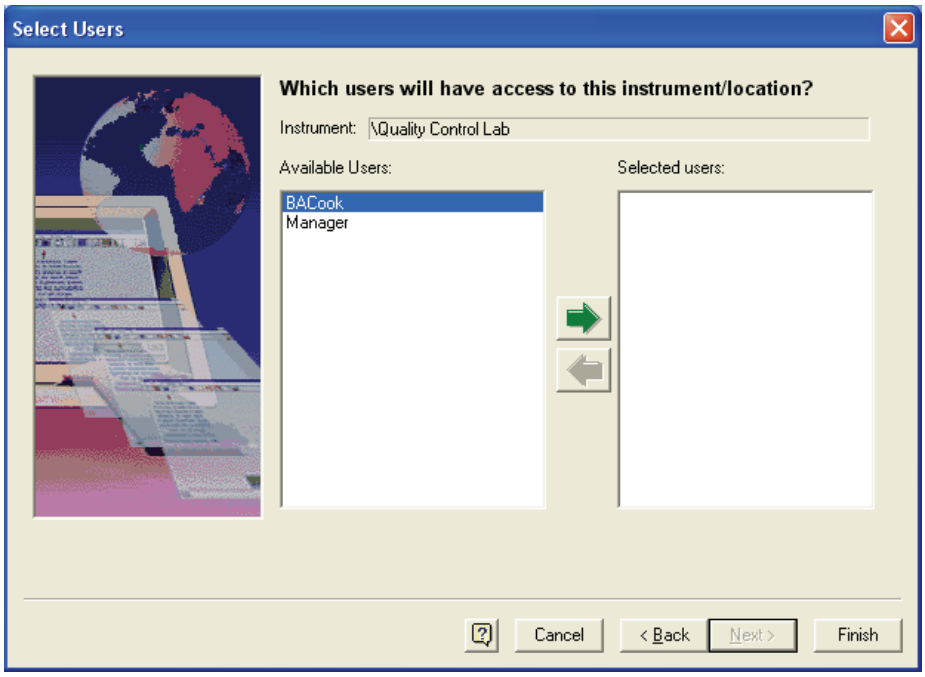
1. In the Select Wizard page of the System Administration Wizard, select the Instrument Wizard option.
2. In the Select Instrument page (see Figure 28) of the Instrument Wizard, select an individual instrument or a location containing multiple instruments. To view individual instruments within a location, double-click the location until the instrument names appear. After you select the location or instrument, click **Next**.

**Figure 28.** Select Instrument page




3. In the Select Users page (see Figure 29), for the instrument or location selected, choose the Groups/Users who will have access. First, select the Windows 2000/XP domain from the Domain list. Then select either the groups or users (radio button-controlled) from the list displayed. Double-click a user or group to add it to the list. Or, select multiple users or groups, and then click the **green arrow**. (Highlight one entry followed by SHIFT + click to highlight all selections in between, or use CTRL + click to highlight multiple non-contiguous entries.) Use the red arrow to remove entries from the selected list. When you have completed the list of users for this instrument/location, click **Finish**.

**Figure 29.** Select Users page




# Project Wizard

Use the Project Wizard to define, edit, or delete system projects, and assign users and groups to projects. A project consists of a set of directories for storage of Methods, Data, Sequences, and Templates, along with a project description. Using Projects facilitates data management by ensuring related data are stored in designated directories that are consistent for all users.

Use the Project Wizard to perform the following tasks:

- Creating a Project
- Assigning Users to a Project
- Changing a Project's Settings
- Removing Projects

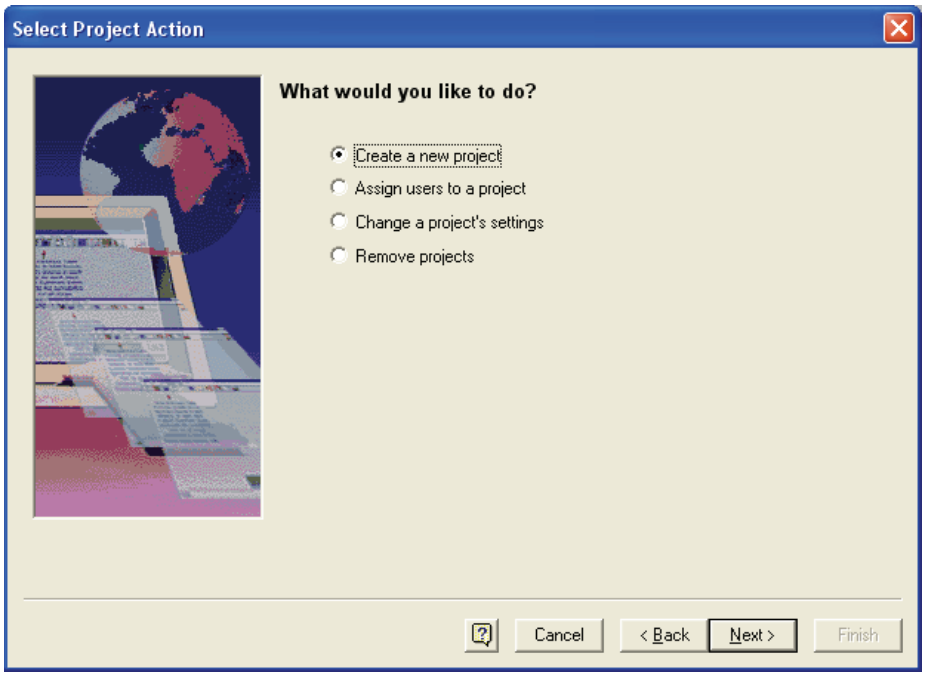
**IMPORTANT** When a project is removed using the wizard, access to the specified directories is removed. The actual data directories defined for the project are not deleted. Removal of data directories must be done by the Windows 2000/XP Administrator (if desired) after proper backup has been performed.

# Creating a Project

### ❖ To create a project

1. In the Select Project Action page (see Figure 30) of the Project Wizard, select the Create a New Project option, and then click **Next**.

   **Figure 30.** Select Project Action page




2. In the General Project Settings page (see Figure 31), do the following:

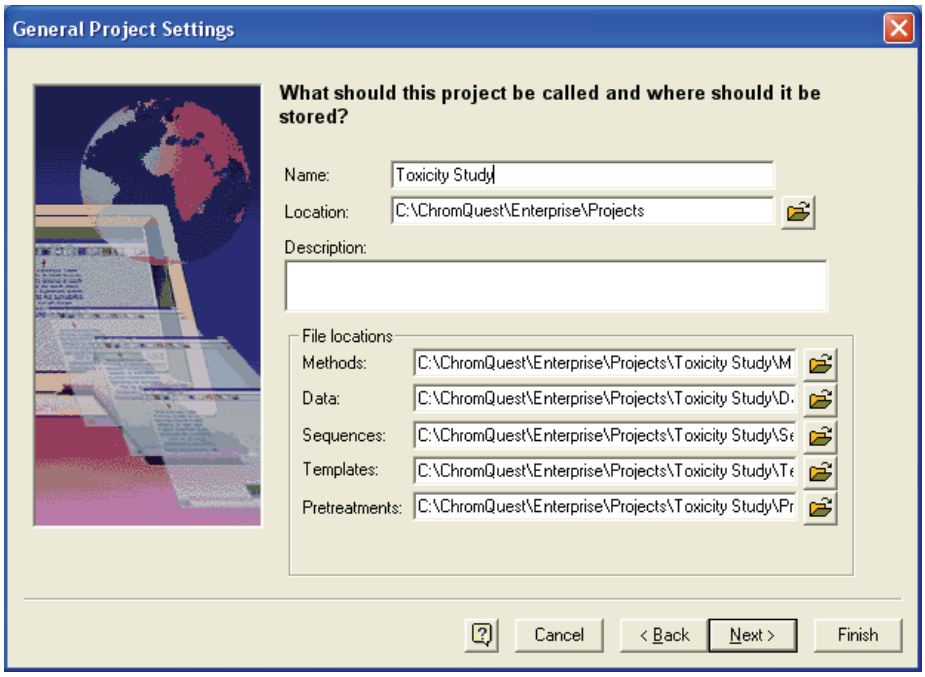
   a. Make the following entries and selections, and then click Next:

   - In the Name box, type a name for the project.
   - In the Location box, click  , and then browse to and select the location for the project definition. The location entered in this box sets up default directories for the project Method, Data, Sequences, and Templates directories.
   - In the Description box, type a text description of the project.

   File locations for your project are automatically created for you based on your entry for the Location field. If you wish to change any of these, you may type in the new location, or select it from available directories by clicking  .

   b. Click **Next**.

**Figure 31.** General Project Settings page




3. In the General Project Settings - Audit Settings page (see Figure 31), select the auditing options for the project as follows:

   a. In the list box, select one of the following:

      - All audit trails
      - Advanced report audit trail
      - Method audit trail
      - Pretreatment audit trail
      - Sequence audit trail

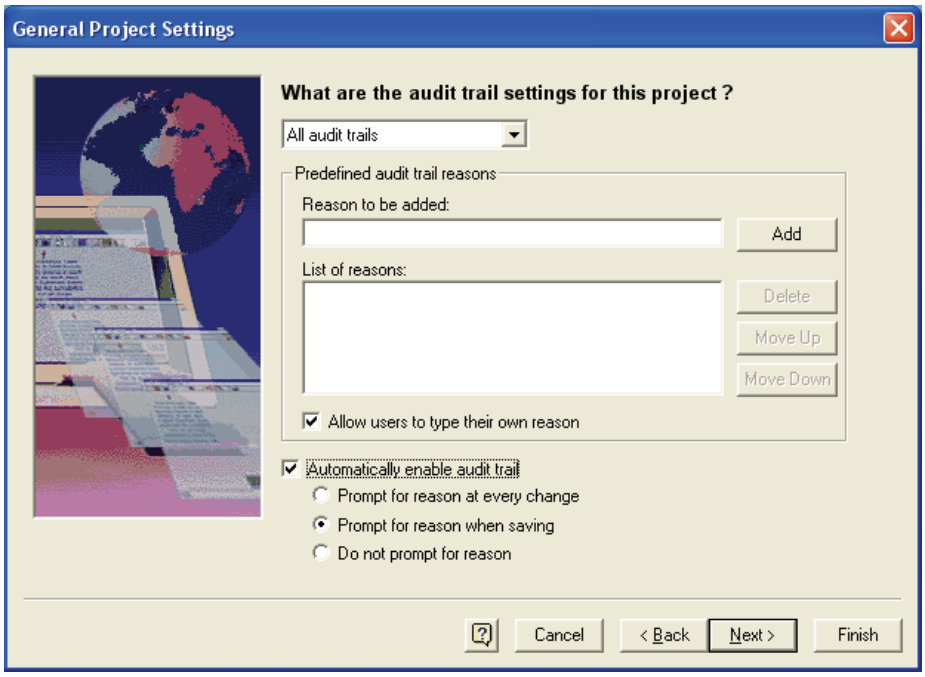
      To view the audit trails, in the Instrument window, choose **File > Data > Audit trail**, **File > Method > Audit trail**, **File > Sequence > Audit trail**, or **File > Advanced Report > Audit trail**.

   b. In the Predefined audit trail reasons area, add more reasons to the programs set of predefined reasons. To add reasons, type a reason in the Reasons to be added box, and then click **Add**. The reason appears in the List of reasons box. Use the Delete, Move Up, and Move Down buttons to modify the list of reasons.

   c. To allow users to type undefined reasons to the audit trail, select the Allow users to type their own reasons check box.

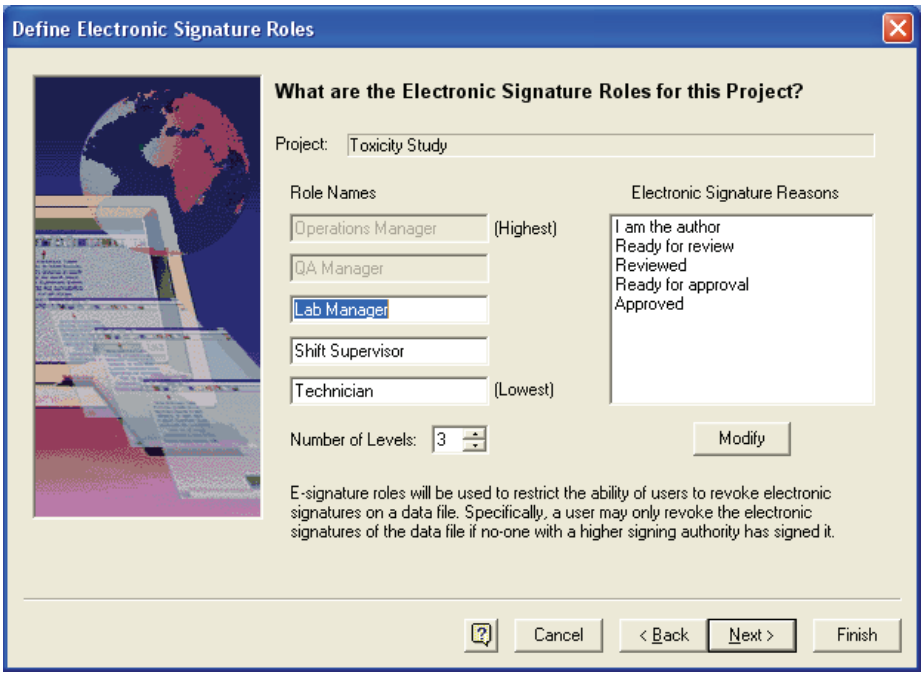
   d. Select the **Automatically enable audit trail** check box to enable auditing, and then select one of the auditing options.

**Figure 32.** General Project Settings page



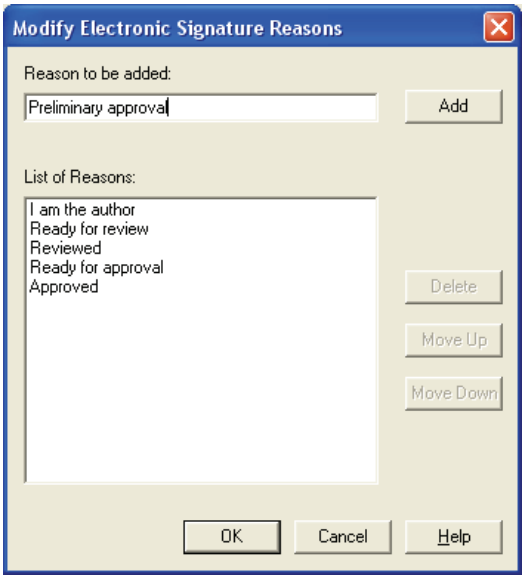

4. Click **Next**. The Define Electronic Signature Roles page appears (see Figure 33).
5. In the Define the electronic signature roles page, do the following:
   a. In the Number of Levels box, type or select the number of signature roles for this project. You add up to five signature roles to each project. You can change the names of the roles and you can change the reasons for the signatures.

**Figure 33.** Define Electronic Signature Roles page




b. To change the signature reasons, click **Modify** to open the Modify Electronic Signature Reasons dialog box (see Figure 34). Type a reason in the Reason to be added box and click **Add**. The new reason appears in the List of Reasons box. Use the Delete, Move Up, and Move Down buttons to modify the list. Click **OK** to close the Modify Electron Signatures Reasons dialog box.

**Figure 34.** Modify Electronic Signature Reasons dialog box



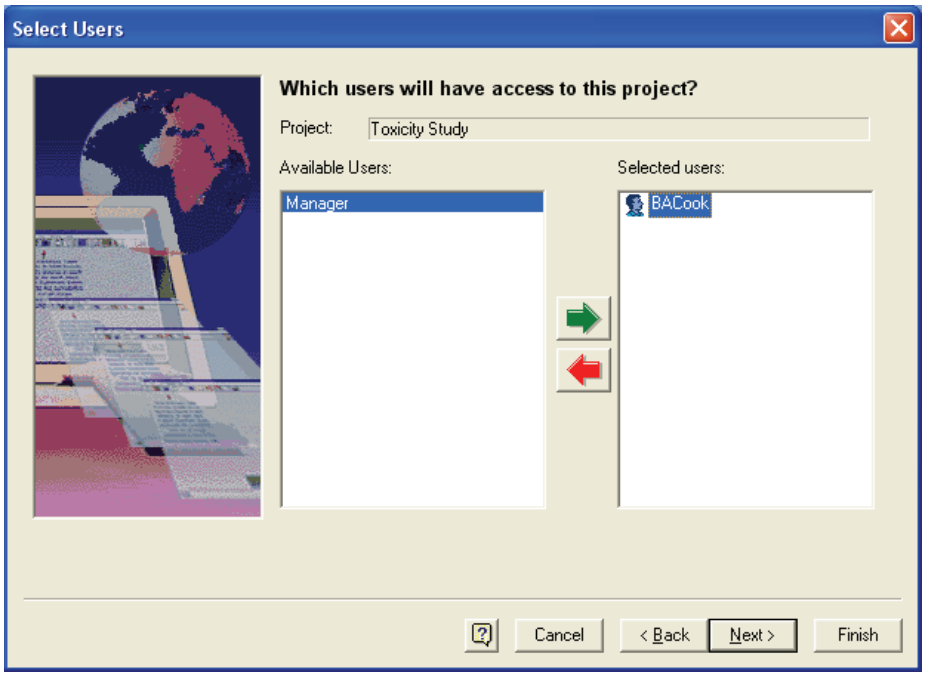

c. Click **Next**. The Select Users page appears.

6. In the Select Users page of the Project Wizard, do the following:

   a. Select the Windows 2000/XP domain from the list. Select either the groups or users (radio button-controlled) from the list displayed.

   b. Double-click a user or group to add it to the list. Or, select multiple users or groups, and then click the green arrow. (Highlight one entry, followed by SHIFT + click to highlight all selections in between, or use CTRL + click to highlight multiple non-contiguous entries.) Use the red arrow to remove entries from the selected list.

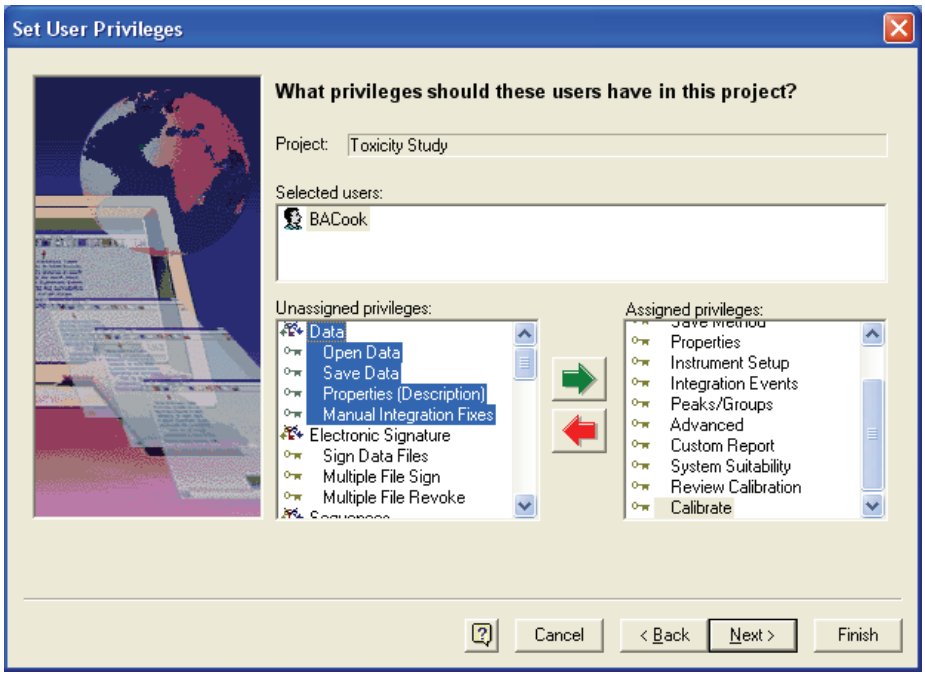
**Figure 35.** Select Users page




7. Click **Next** to continue. The Set Project User Privileges page appears. See Figure 36.

   Use the Set Project User Privileges page to assign software command access for the selected users/groups with access to this project. Once you have set the user privileges for a given project, the user/group has access only to the functional commands assigned for the defined project. You may grant full functional privileges (including method development and data acquisition control), or you may grant a subset of the software commands to a given user/group.

**Figure 36.** Set User Privileges page




8. In the Set Project User Privileges page, do the following:

   a. Assign privileges:

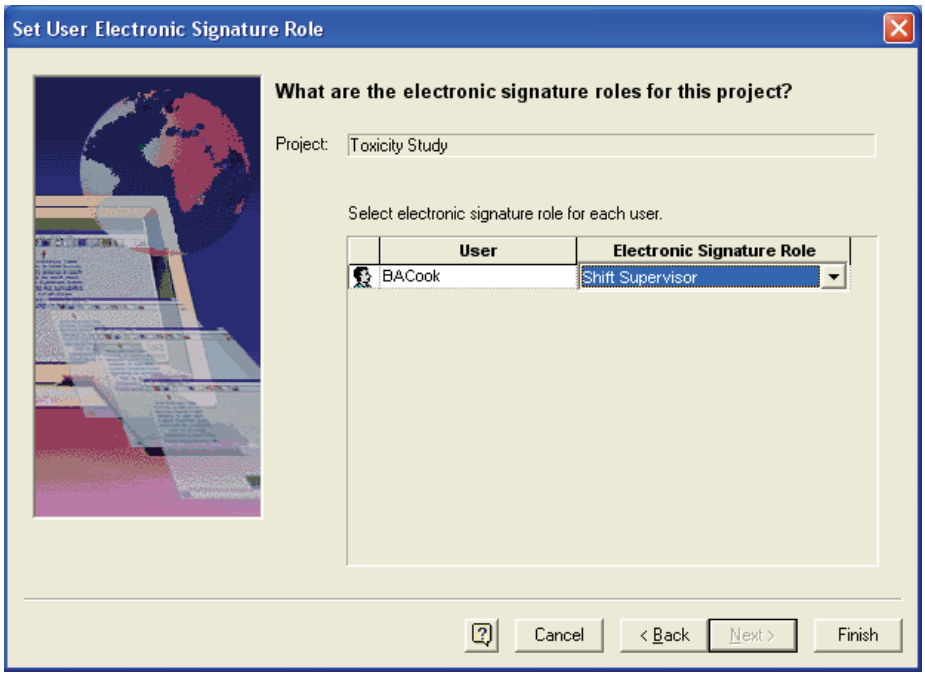
   - To assign individual privileges, highlighting them and click the **green arrow**.
   - To assign complete groups of related privileges (such as Data commands), double-click the main privilege type (Methods, Data, Sequences). This automatically selects all available commands for that functional area.

   **Note** The "Calibrate" privilege enables the user to run a calibration sample to update the method calibration. In order to create or modify the calibration parameters in a method, the user must have the "Save Method" privilege assigned.

   b. Click **Next** to continue to the next page of the Project Wizard.

9. In the Set Electronic Signature Role page (see Figure 37), assign the electronic signature roles for the user.

**Figure 37.** Set User Electronic Signature Role page




10. When you have completed selection of project privileges, click **Finish** to complete the project definition.

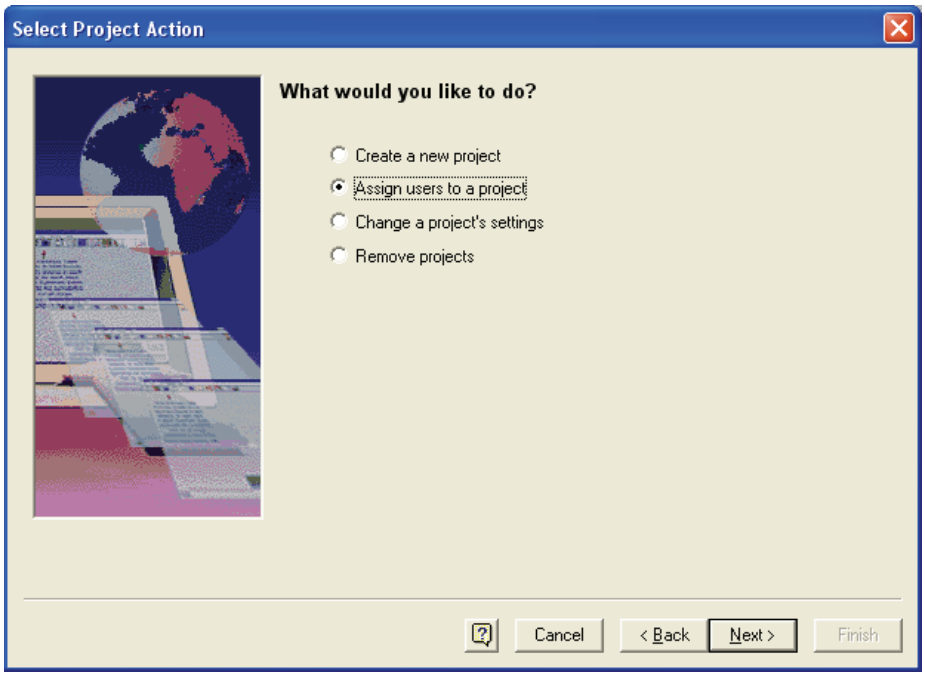
## Assigning New Users/Groups to a Project

Once you have one or more projects defined for your system, you can add or change the assigned users/groups using this option.

### ❖ To assign new users or groups to a project

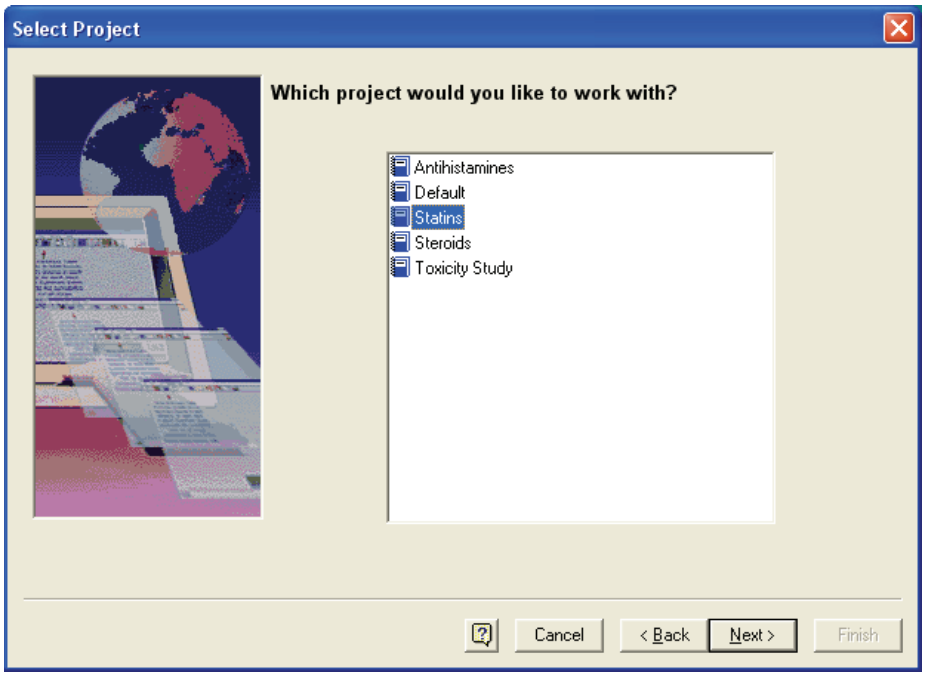
1. Select the **Assign Users to a Project** option (see Figure 38), and then click **Next** to continue.

**Figure 38.** Select Project Action page



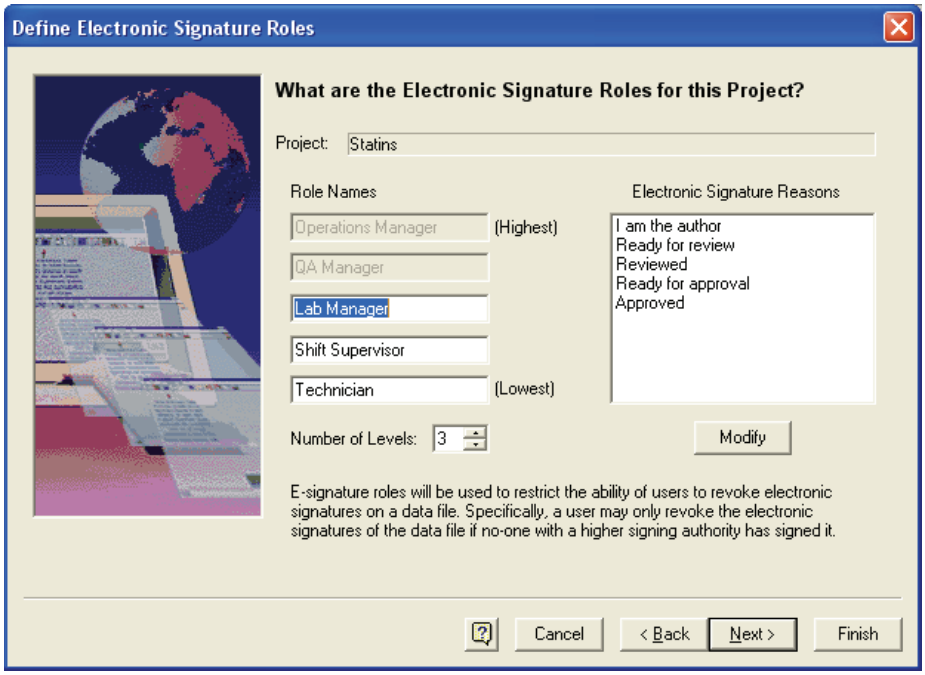

2. In the Select Project page (see Figure 39), select the project to work with, and then click **Next**.

**Figure 39.** Select Project page



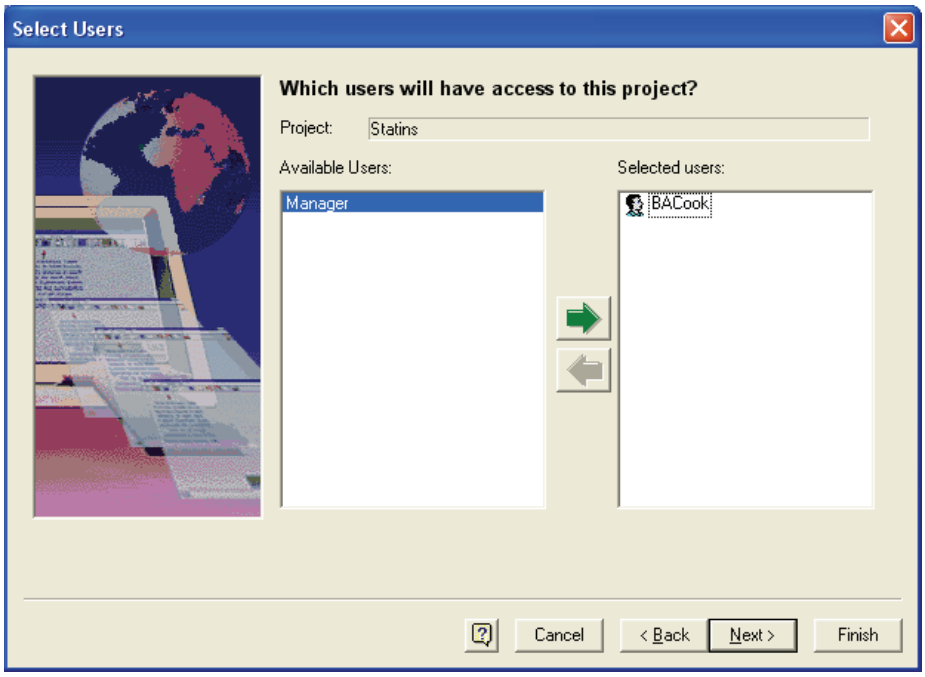
3. In the Define Electronic Signature Roles page (see Figure 40), define the electronic signature roles for this project. Then click **Next**.

**Figure 40.** Define Electronic Signature Roles page




4. In the Select Users page (see Figure 41), for the selected project, choose a Windows 2000/XP domain from the list. Select the users/groups you want to have access to this project from the available users/groups displayed. When a user/group is selected, it appears in the Selected Users list on the right. Select a user/group by double-clicking it with the mouse, or perform a multiple selection using SHIFT + click (to select contiguous users/groups) or CTRL + click (to select multiple, non-contiguous users/groups). Then click the **green arrow**.

**Figure 41.** Select Users page




5. When you have completed your selection, click **Next** to continue or **Finish** if you are done.

6. In the Set User Privileges page (see Figure 42), do the following:

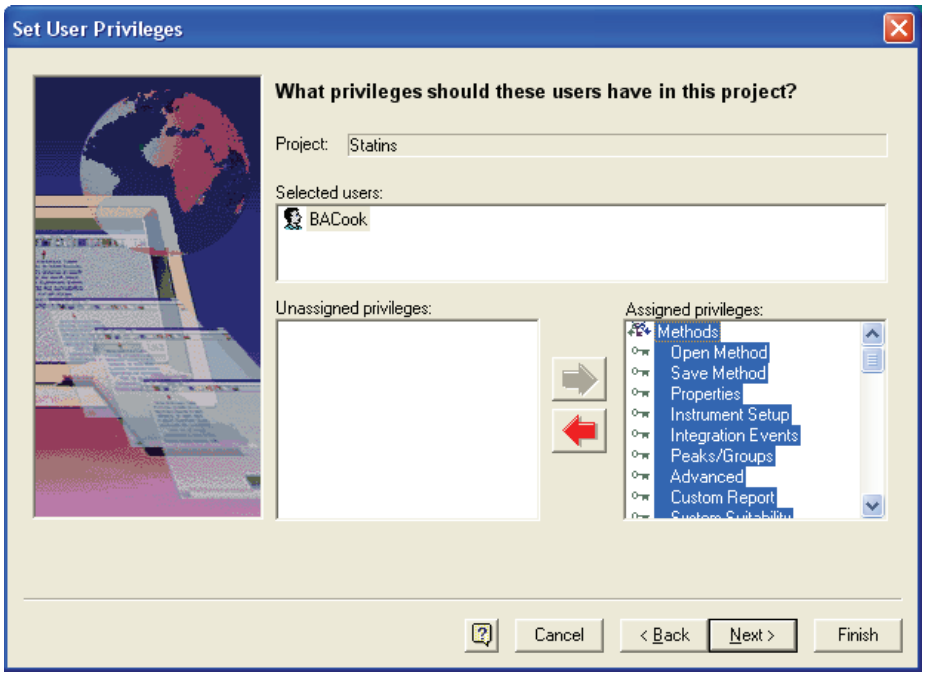
   a. Assign software command access for the selected users/groups with access to this project. Once you have set the user privileges for a given project, the user/group has access only to the functional commands assigned for the defined project. You cam grant full functional privileges (including method development and data acquisition control), or you can grant a subset of the software commands to a given user/group.

      To assign a privilege, highlight it with the mouse, and then click the **green arrow**. To assign a complete group of related privileges (such as Data commands), double-click the main privilege type (Methods, Data, Sequences). This automatically selects all available commands for that functional area.

      **Note** The "Calibrate" privilege enables the user to run a calibration sample to update the method calibration. In order to create or modify the calibration parameters in a method, the user must have the "Save Method" privilege assigned.

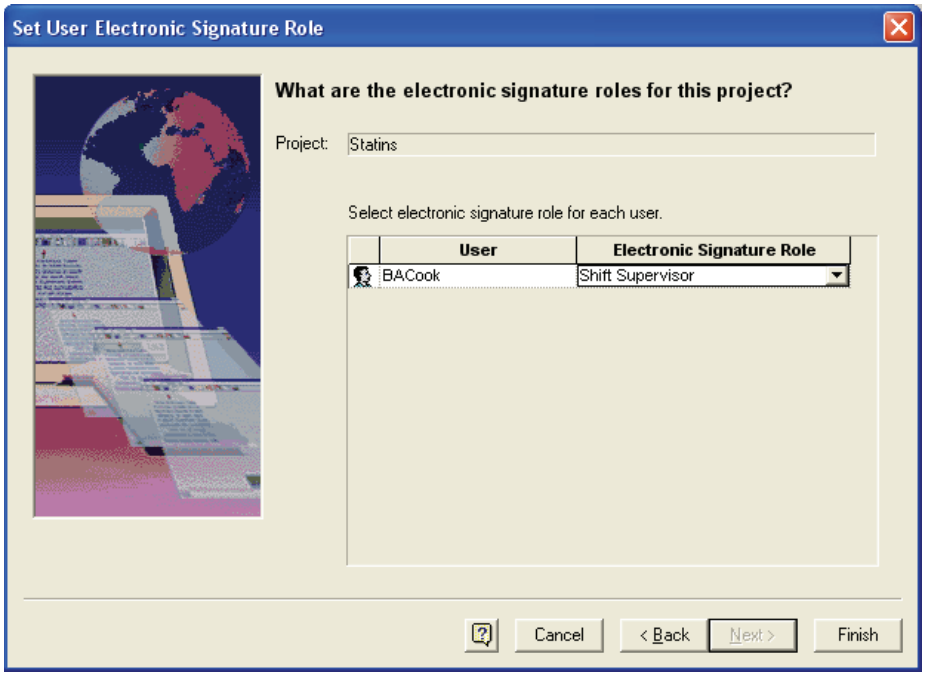
   b. Click **Next**.

**Figure 42.** Set User Privileges page




7. In the Set User Electronic Signature Role page (see Figure 43), assign the electronic signature roles for the user or group.

**Figure 43.** Set User Electronic Signature Role page




8. When you have finished, click **Finish**.

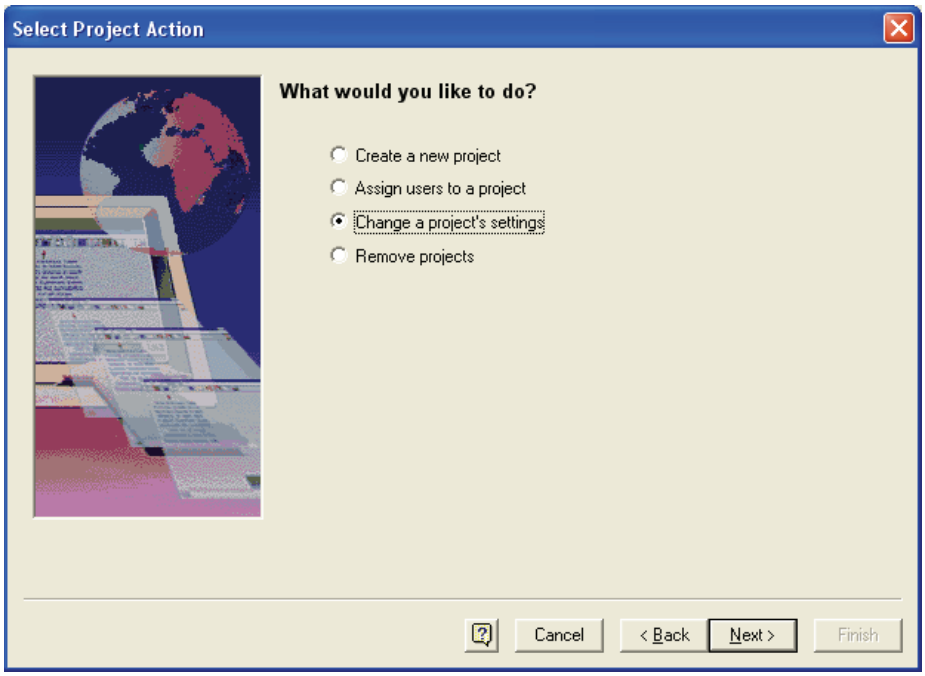
## Change a Project's Settings

Use this option to change the definition of an existing project in your Enterprise. You can change the project description, user/groups assignment, and privilege assignments. You cannot change a project's location after it has been created, however.

### ❖ To change a project's settings

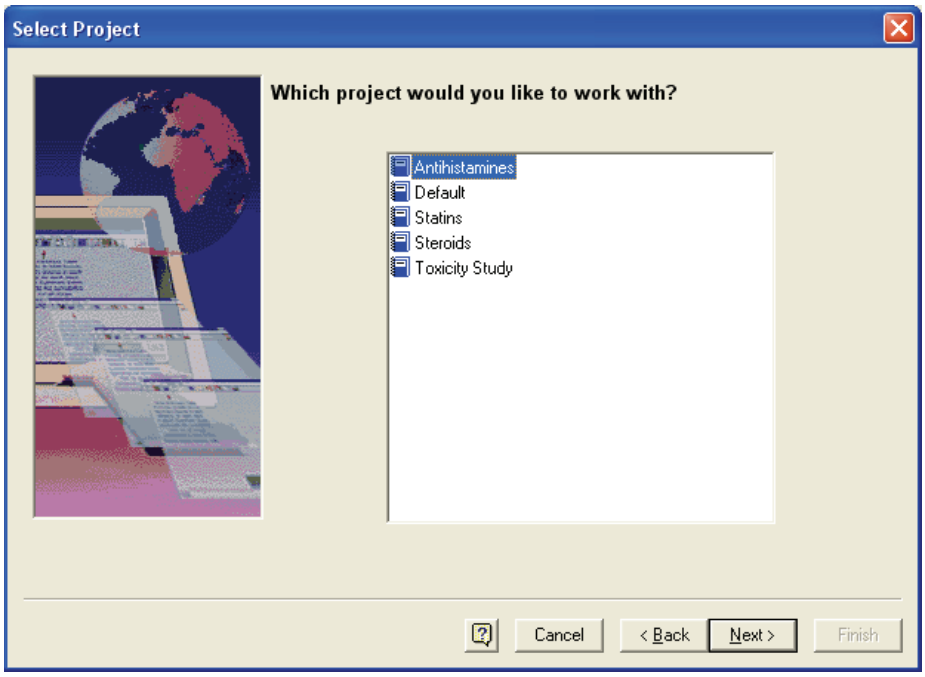
1. Select the **Change a project's settings** option (see Figure 44). Then click **Next** to continue.

   **Figure 44.** Select Project Action page

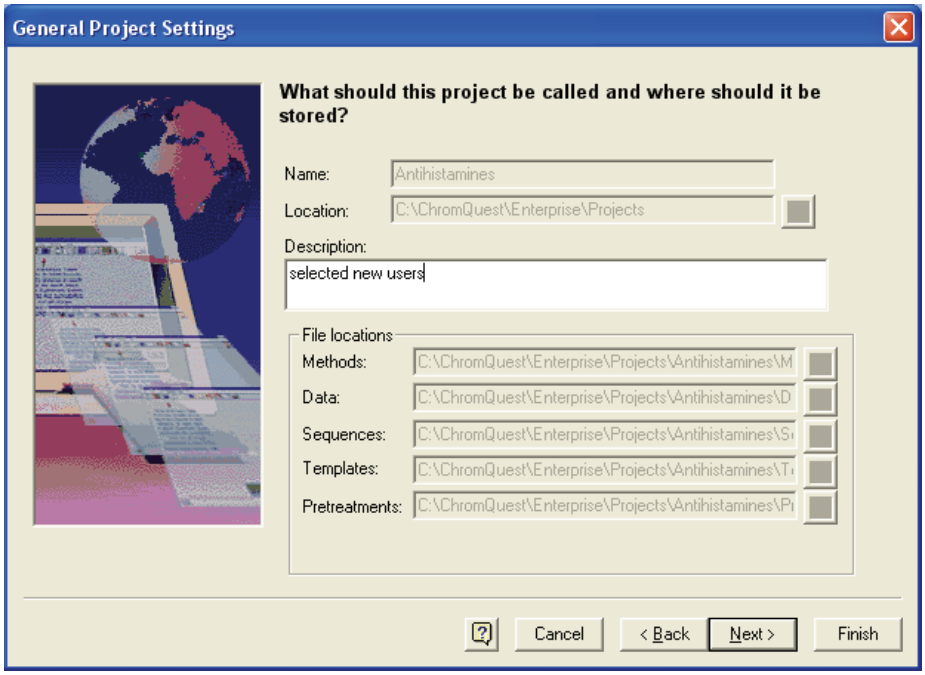
2. In the Select Project page (see Figure 45), select the project to work with, and then click **Next**.

**Figure 45.** Select Project page



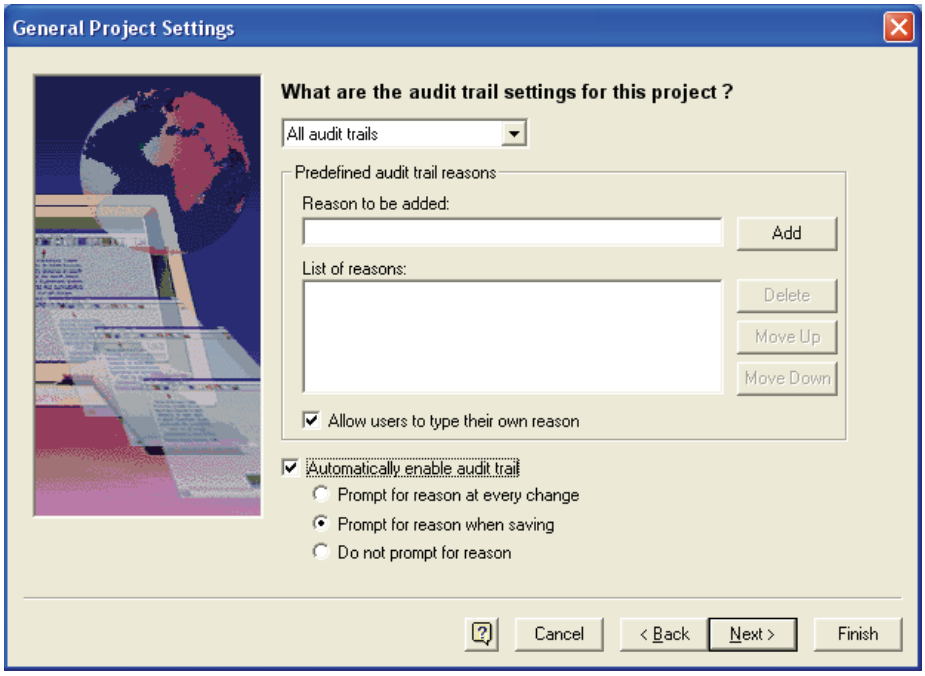

3. In the General Project Settings page (see Figure 46), review the current project settings and change the project description if desired. When you have completed the project setting changes, click **Next** to continue, or **Finish** if done.

**Figure 46.** General Project Settings page



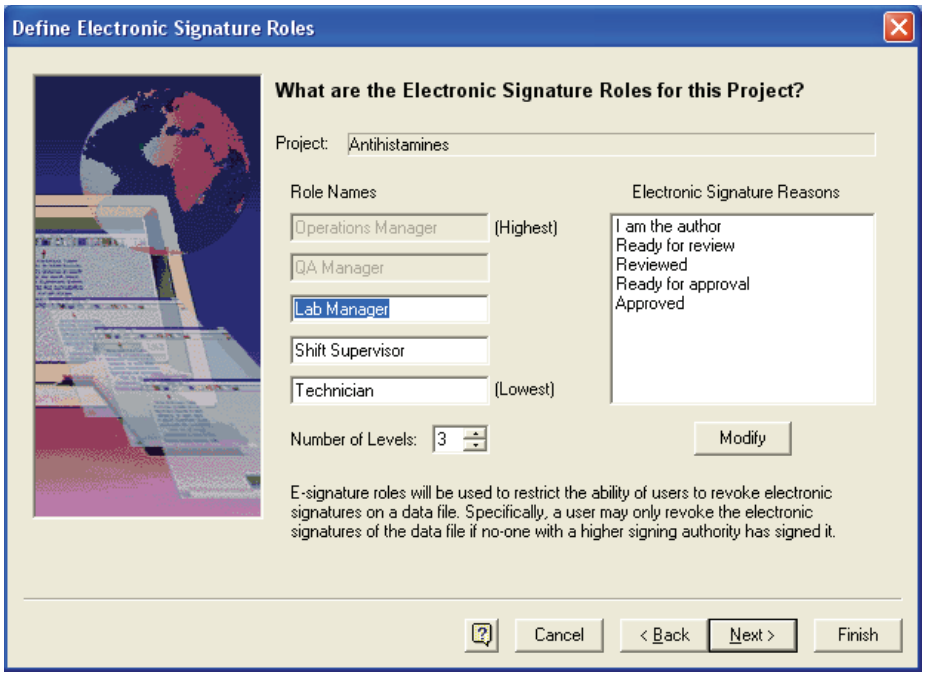
4. In the General Project Settings – Audit trail page (Figure 47), modify the audit settings, and then click **Next** or **Finish**.

**Figure 47.** General Project Settings – Audit trail page




5. In the Define the Electronic Signature Roles page (Figure 48), define the electronic signature roles for this project. Click **Next** to continue or **Finish** if done.

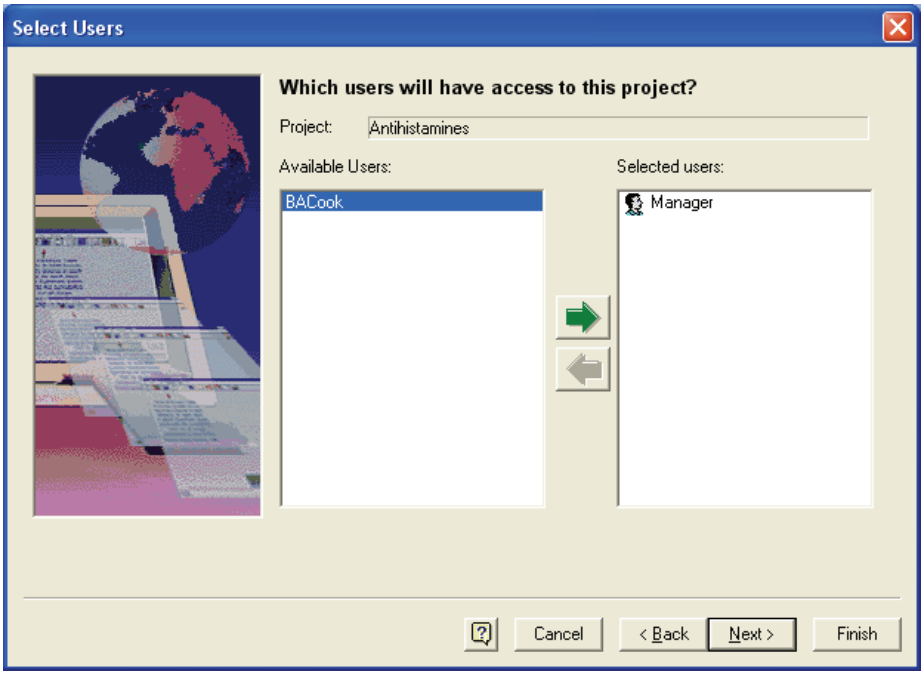
**Figure 48.** Define the Electronic Signature Roles page



6. In the Select Users page, do the following:

   a. Change the users/groups who have access to the project. First, select the Windows 2000/XP domain from the list. Then select either the groups or users from the list displayed. Double-click a user or group to add it to the list. Or, select multiple users or groups, and then click the **green arrow**. (Highlight one entry, followed by SHIFT + click to highlight all selections in between, or use CTRL + click to highlight multiple non-contiguous entries.) Use the red arrow to remove entries from the selected list.

   **Figure 49.** Select Users page



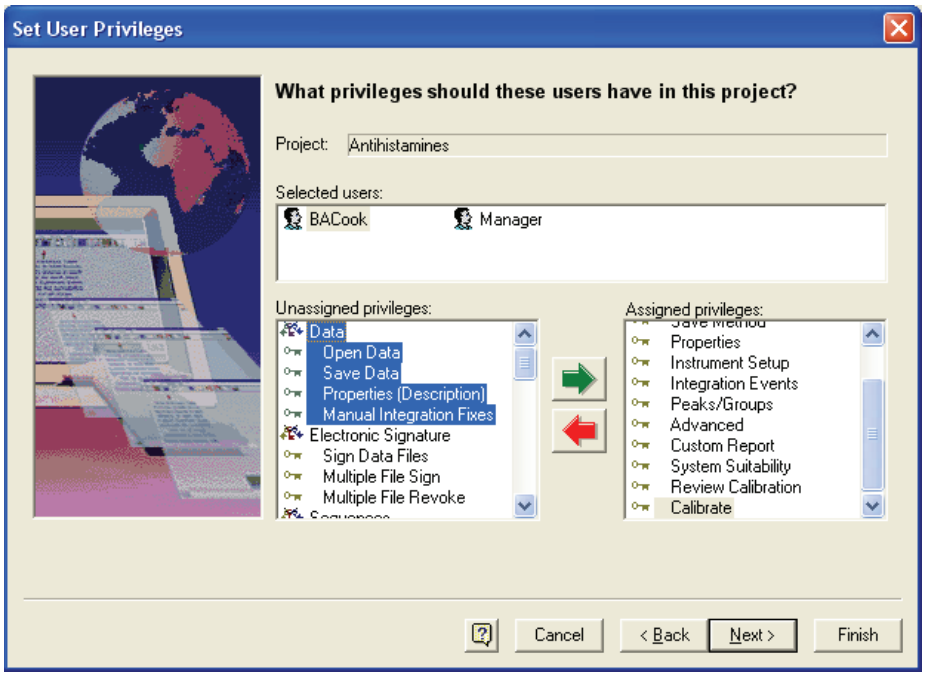

   b. Click **Next** to continue or **Finish** if done.

7. In the Set User Privileges page (see Figure 50), do the following:

   a. Change the assigned software command access for the selected users/groups with access to this project. Once you have set the user privileges for a given project, the user/group has access only to the functional commands assigned for the defined project. You can grant full functional privileges (including method development and data acquisition control), or you can grant a subset of the software commands to a given user/group.

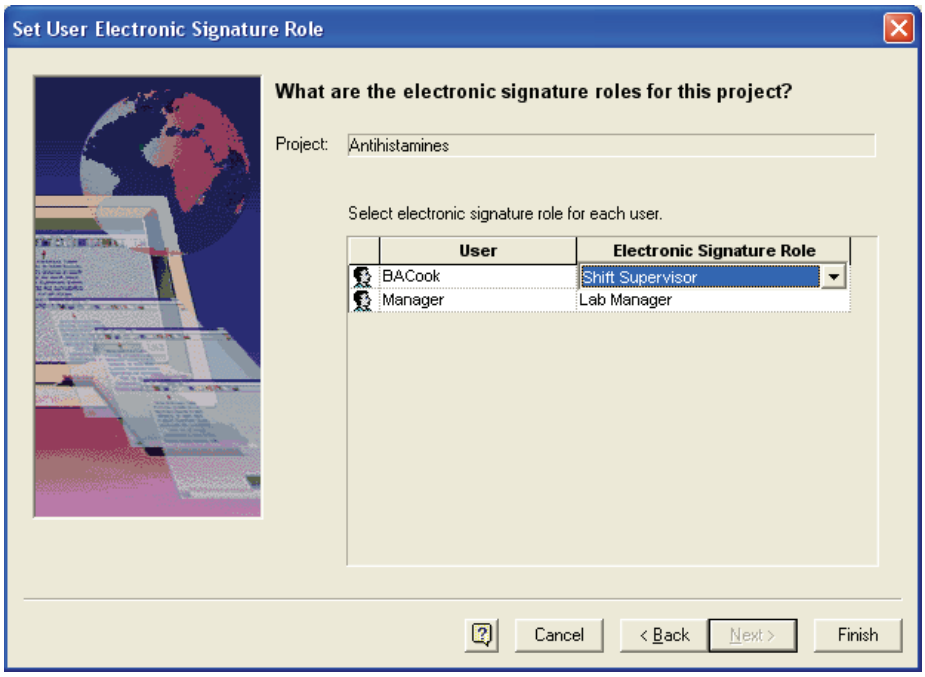
   b. Click **Next** to continue or **Finish** if done.

**Figure 50.** Set User Privileges page




8. In the Set User Electronic Signature Role page, assign the electronic signature roles for the user or group.

**Figure 51.** Set User Electronic Signature Role page




9. When you have completed selection of project privileges, click **Finish** to complete the project definition changes.

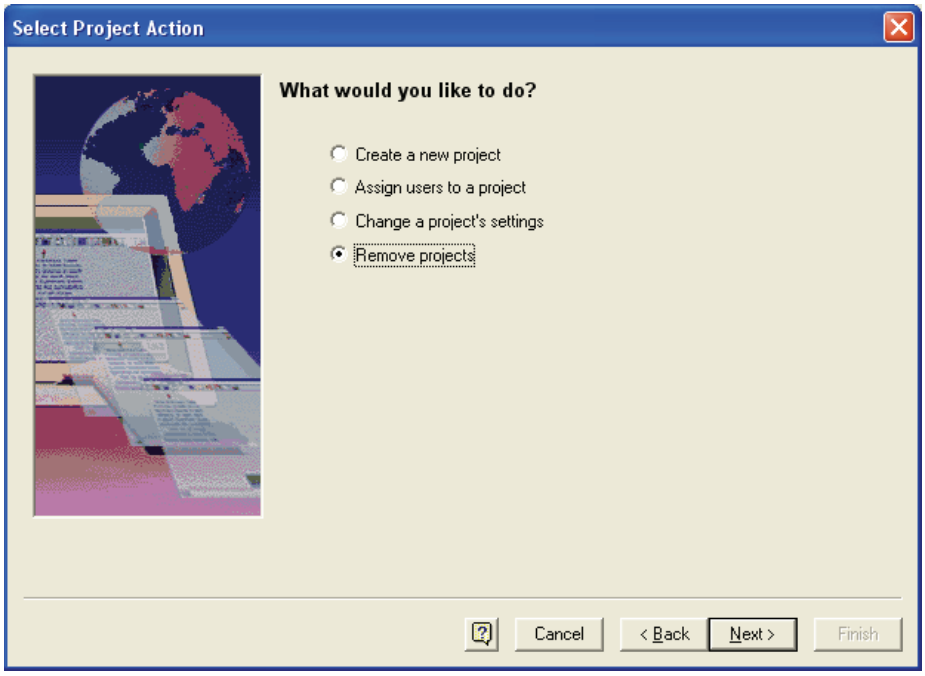
# Remove a Project

Use this option to remove a project from active use. The directories remain on the Windows 2000/XP; however, access to the project from within are no longer possible.

### ❖ To remove a project

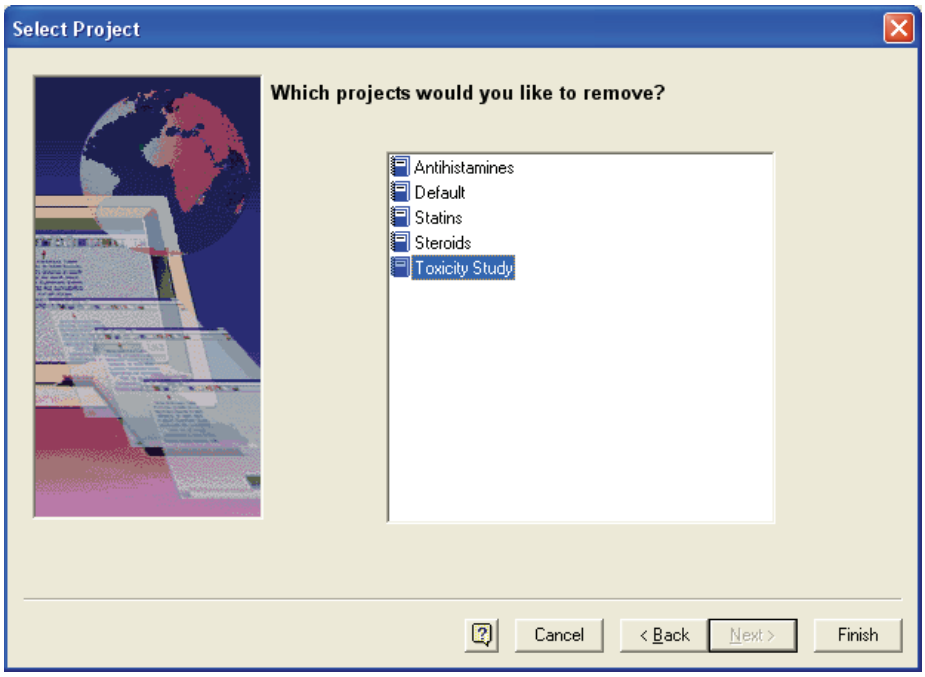
1. Select the **Remove projects** option. Then click **Next**.

   **Figure 52.** Select Project Action page




2. In the Select Project page (see Figure 53), select the project to be removed. Then click **Finish**.

**Figure 53.** Select Project page




The following dialog box appears (see Figure 54).

**Figure 54.** Warning message


3. Click **OK** to remove the project from the list of available projects.

# Configuring Instruments

This chapter contains general information about configuring the instruments in the Enterprise. For specific information about configuring the SpectraSYSTEM LC and Surveyor Plus LC modules, refer to the sections at the back of the *ChromQuest 5.0 User Guide*.

**Contents**



## Configuring the Enterprise, Instruments, and Detectors

Configuration of the Enterprise is the process of defining the system and its hardware. There are main areas for configuration:

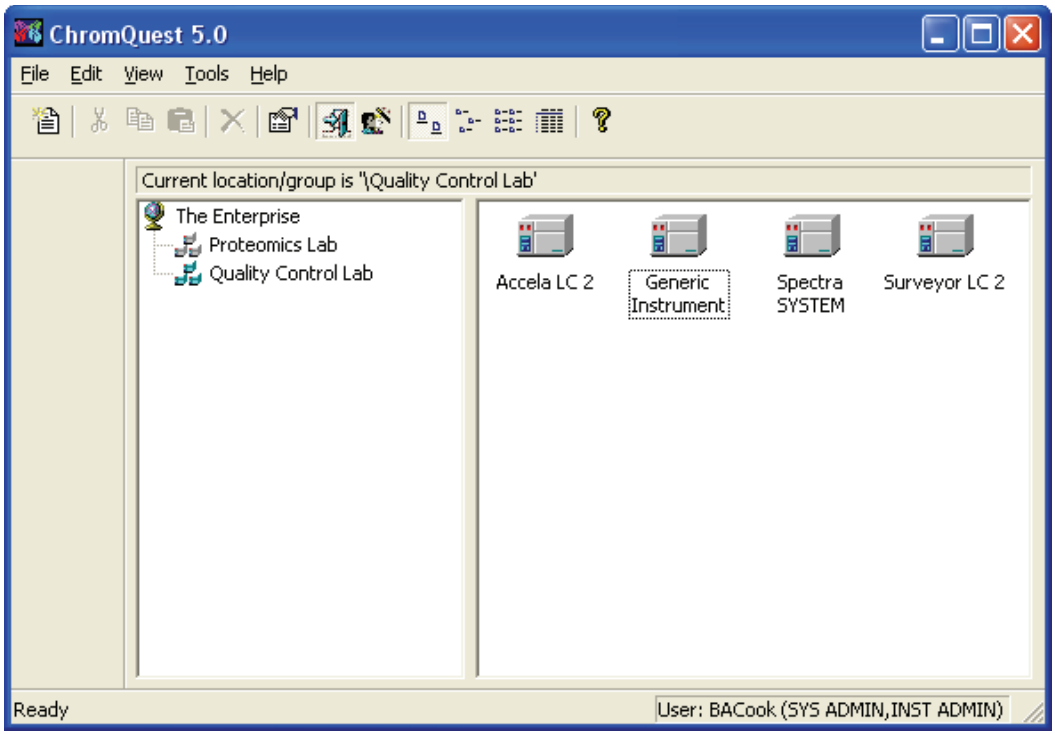
- **Interface Configuration**. This is where you set up the configurable options for the SS420x analog to digital interface board.
- **Instrument Configuration**. Each instrument controlled from the ChromQuest data system has cofigurable options. In ChromQuest, these options are specified from the Main Menu window. In ChromQuest SI, the instrument configuration application is opened by choosing **Start > All Programs > Chromatography > ChromQuest SI Config**.

# Main Menu

The Main Menu window is the first window that appears when you start the ChromQuest data system. From this window, you can view the entire Enterprise, including any locations and instruments that have been configured on the system.

**Note** ChromQuest SI does not have a Main Menu window.

**Figure 55.** ChromQuest Main Menu window




By default, the left pane of the Main Menu window displays the defined system enterprise locations. The Enterprise is displayed as a hierarchy, where each location is displayed as a "folder" containing locations or instruments configured within it.

Click a location in the left pane to display its contents on the right. Click the plus signs (+) to display more locations. To change the size of either pane, drag the bar that separates the two sides. To quickly open a location and display its contents, double-click the location in the left pane.

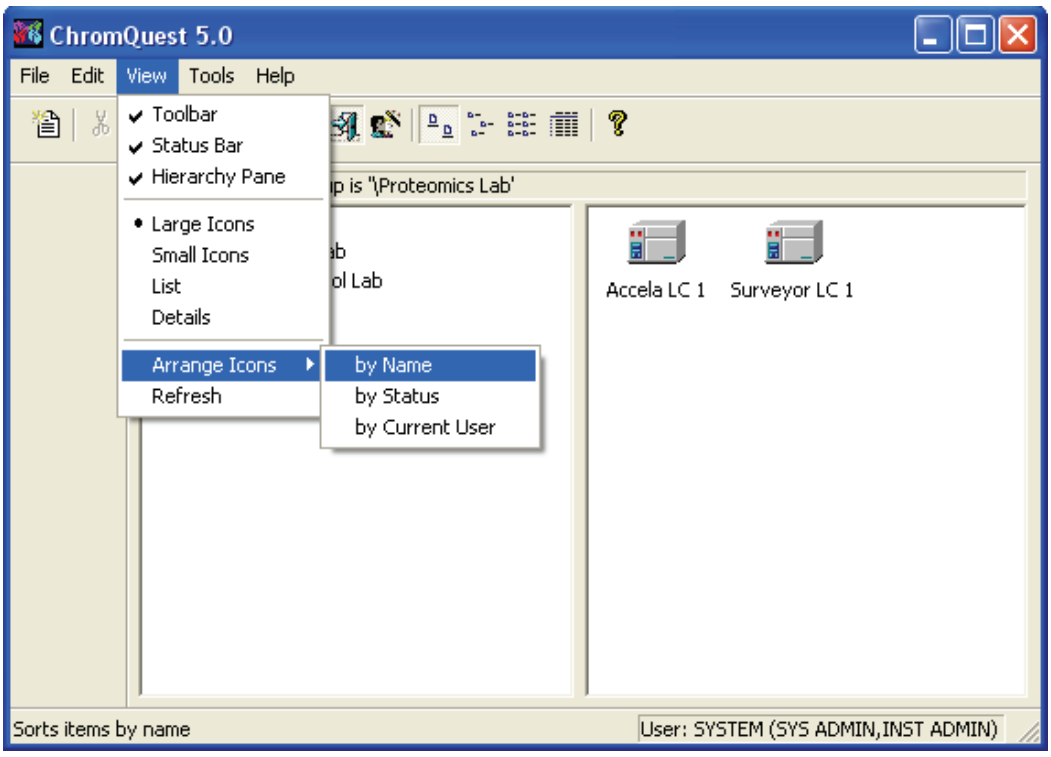
## Instrument Access

To access an instrument for method development, sequence generation, and data acquisition; double-click the icon of the instrument you wish to access.

## Changing the View

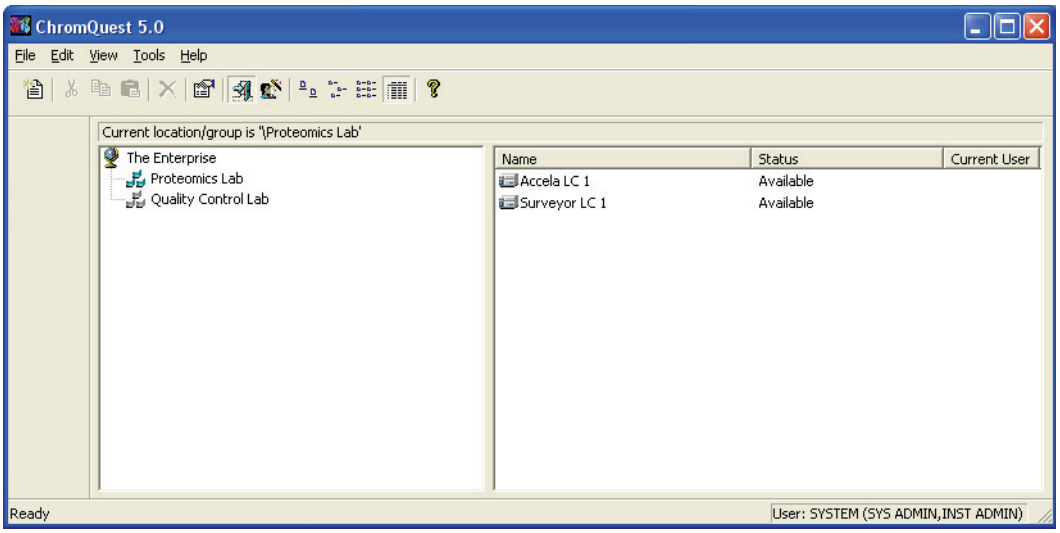
By default, instruments configured on the system are displayed as icons (see Figure 56). You can change how the Main menu appears using the commands located in the View menu. Using these commands, you can turn the toolbar and status bar on and off, change the size of the icons, or arrange the icons. Options for changing the icon sizes or viewing details are also available as buttons on the toolbar.

**Figure 56.** Chromquest – View menu




You can view status details of instruments configured on the system in the Main Menu window (see Figure 57). To view status, choose the **View > Details** command from the menu bar, or click the **Details** icon. Instruments for the current location are displayed with status information.

**Figure 57.** ChromQuest Main Menu window with details



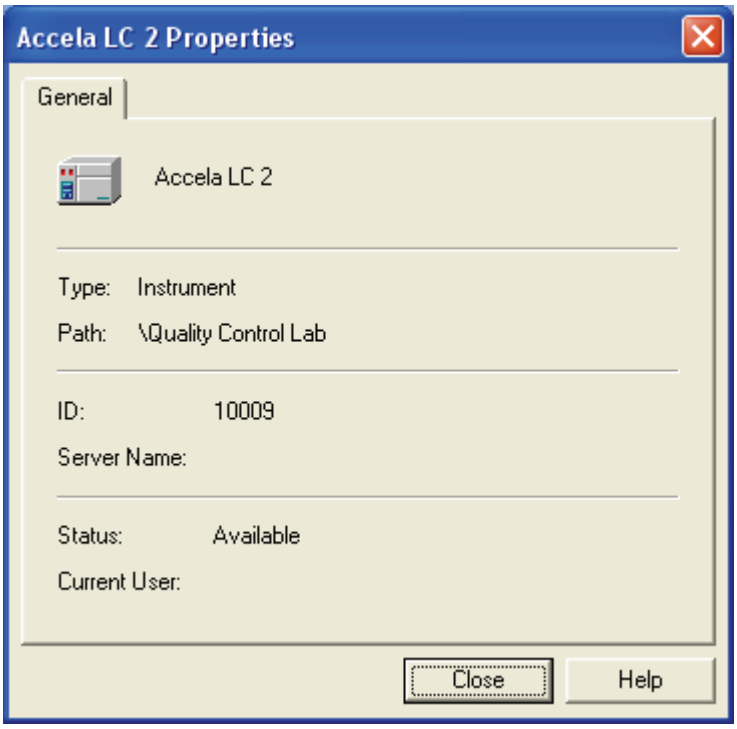

When you view a location in "details" mode, the right pane of the window displays the instrument name, current instrument status (available, idle, running), and the current user of that instrument. The status is updated periodically, as defined by the Status Update Interval set in **Tools > Options > Workstation**.

You can also view the Main menu without the entire enterprise displayed. To remove the Enterprise or Hierarchy pane, choose **View > Hierarchy Pane**. If this selection is not checked, the Enterprise is not displayed.

## Item Properties

You can view details of an instrument by right-clicking the instrument icon, choosing **Properties** from the shortcut menu. An information dialog box appears with current instrument information. See Figure 58.

**Figure 58.** Instrument Properties dialog box



# Enterprise Configuration

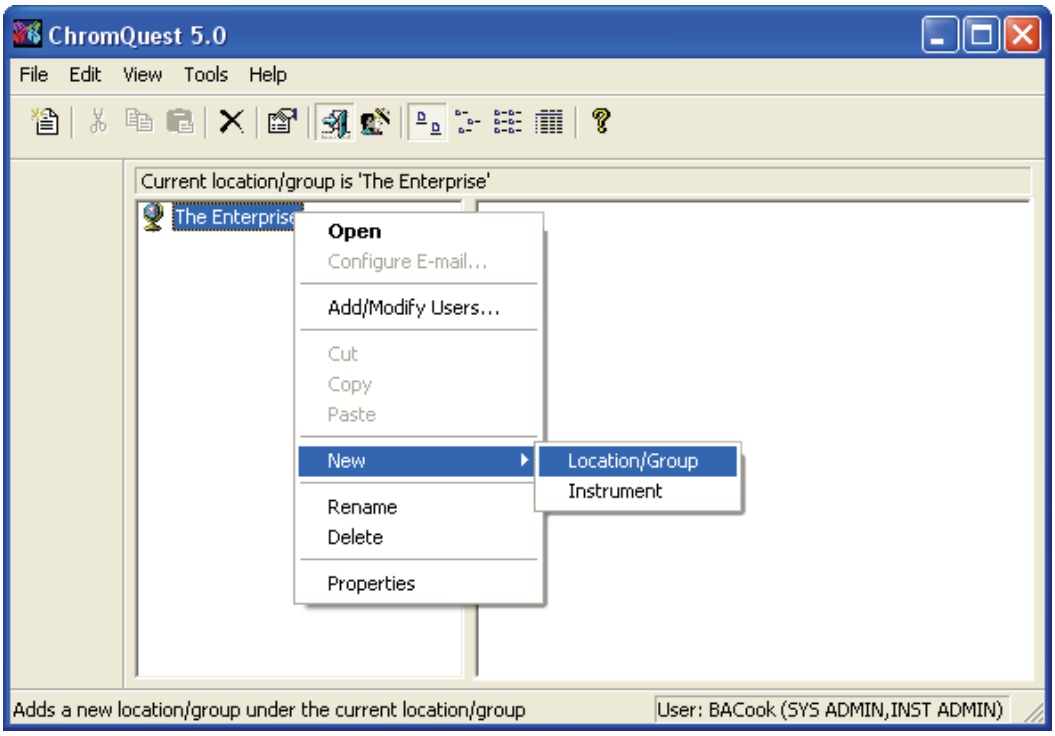
When is first started, the Main Menu window has no Enterprise defined. The system administrator must define the Enterprise before instruments can be configured and used.

You can rename the Enterprise by right-clicking the enterprise name and choosing **Rename** from the shortcut menu. Type the new Enterprise name.

## Adding an Enterprise Location

To add a location to your Enterprise, right-click the Enterprise pane, and choose **New > Location Group**.

**Figure 59.** Adding a location or group

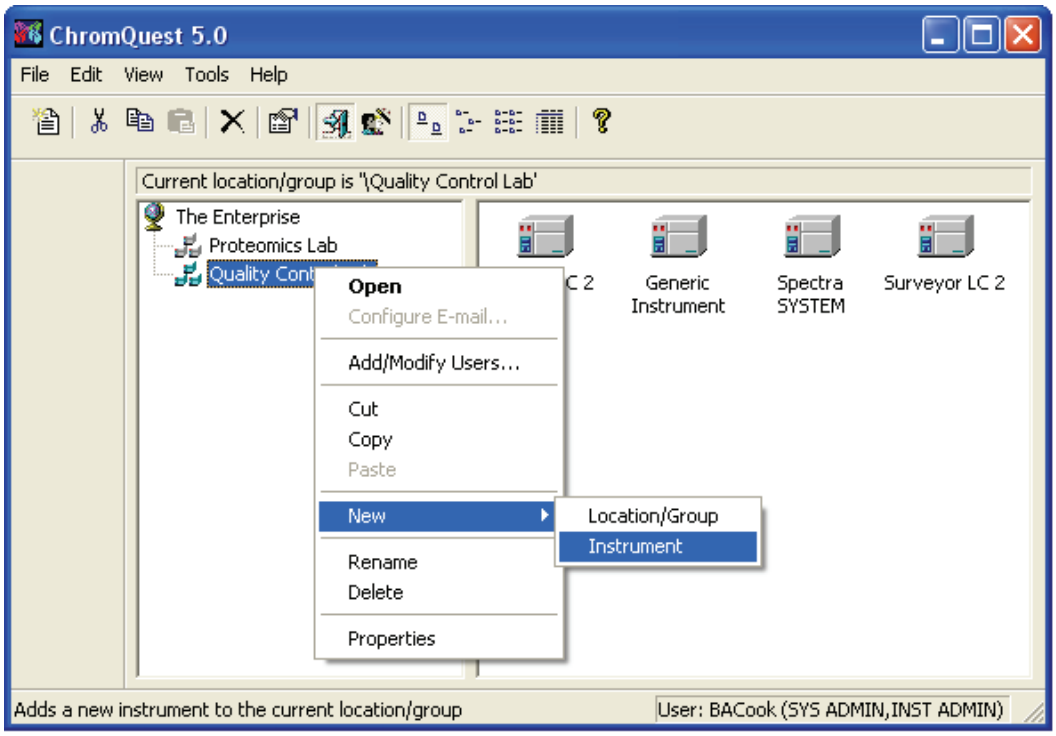



A new entry appears below the Enterprise. You can give the new location or group a name. Continue adding locations or groups to the Enterprise until the Enterprise configuration matches that of your company or group.

## Adding an Instrument to the Enterprise

Before you can configure an instrument, you must add it to the Enterprise definition. To add an instrument, select the location where the instrument is found. Right-click and choose **New > Instrument** from the shortcut menu (see Figure 60). An icon for the new instrument appears in the right pane, and you can give it a name.

**Figure 60.** Adding an instrument




Continue to add locations and instruments until the system Enterprise matches your company/laboratory configuration. Then configure each of the instruments as described in "Configuring Instruments and Detectors" on page 66. You must also configure any A/D interfaces you will use on your system as described in "Interface Configuration" on page 64. Your completed Enterprise can be as simple as one lab with multiple instruments, or a complex list of buildings, laboratories, and instruments.

# Interface Configuration

If you are using an SS420x analog to digital converter for data acquisition, you must set up the interface configuration.

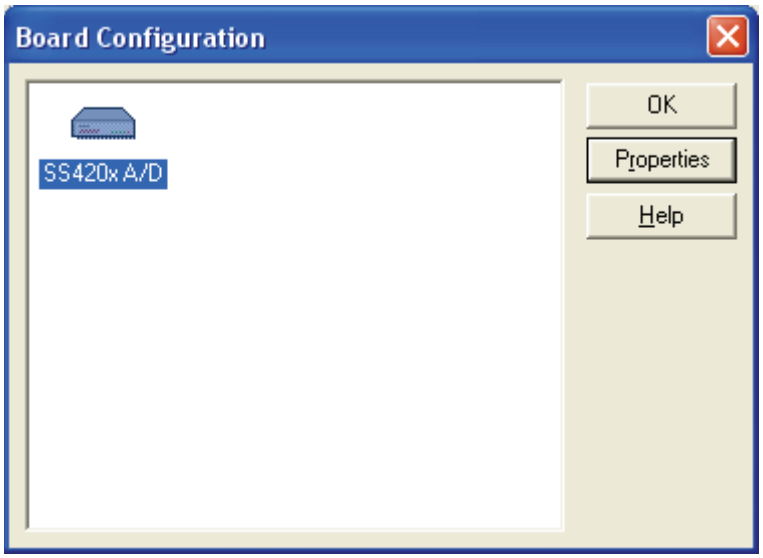
**Note** It is only necessary to perform interface configuration where the interface board is actually installed.

### ❖ To configure the data acquisition hardware

1. Depending on the data system, do one of the following:
   - For ChromQuest, from the Main Menu window, choose **Tools > Interface Configuration**.
   - For ChromQuest, from the Windows desktop, choose **Start > All Programs > Chromatography > ChromQuest SI Config**. The ChromQuest SI Configuration dialog box appears. Click **Interface Configuration**.

   The Board Configuration dialog box appears. See Figure 61.

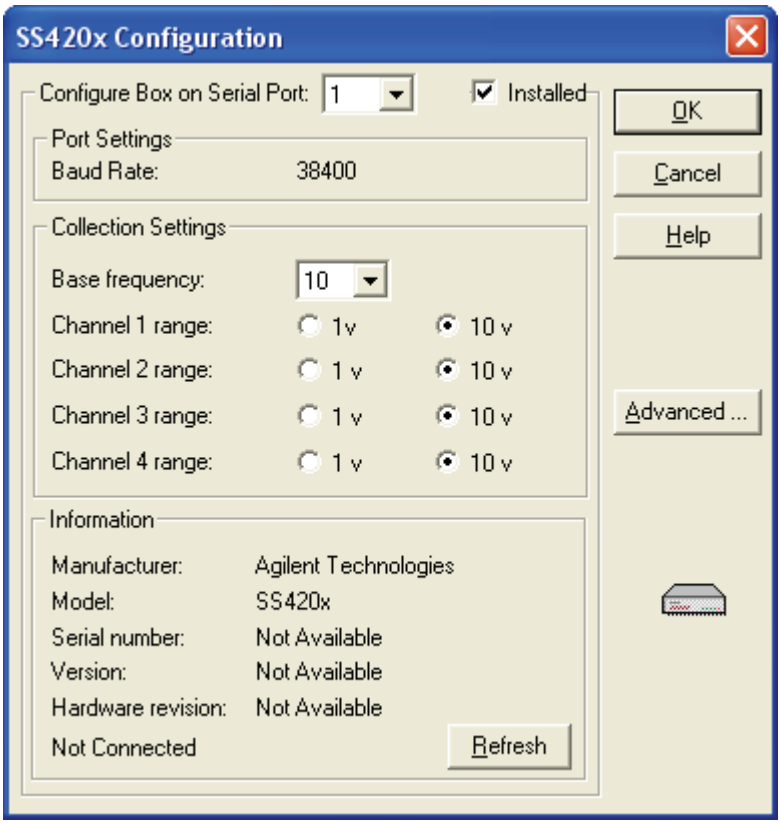
   **Figure 61.** Board Configuration dialog box




2. To configure the SS420x A/D converter:
   a. Click the SS420x A/D icon to select it, and then click Properties.

      The SS420x Configuration dialog box appears. See Figure 62.

**Figure 62.** SS420x Configuration dialog box




b. In the Configure Box on Serial Port list, select the serial port on the data system computer that the SS420x A/D converter is connected to.

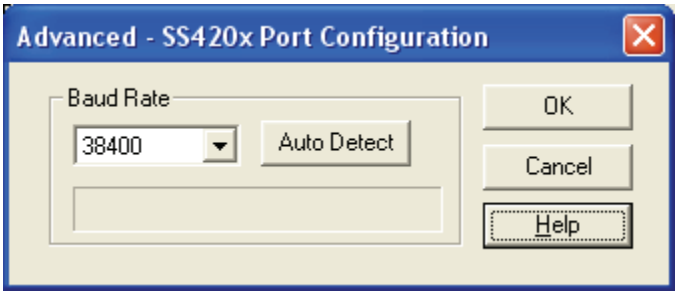
c. Select the **Installed** check box.

d. Select the appropriate base frequency and channel ranges.

e. Click **Advanced**.

The Advanced SS420x Port Configuration dialog box appears.

**Figure 63.** Advanced - SS420x Port Configuration dialog box




f. Click **Auto Detect**.

g. Click **OK** to close the Advanced SS420x Port Configuration dialog box.

h. Click **OK** to close the SS420x Configuration dialog box.

3. Click **OK** to close the Board Configuration dialog box.

   In ChromQuest, the Main Menu window appears. In ChromQuest SI, the ChromQuest SI Configuration dialog box appears.

4. For ChromQuest SI, click **Close** to close the ChromQuest SI Configuration dialog box and return to the Windows desktop.

# Configuring Instruments and Detectors

If you are controlling instruments from the ChromQuest data system and the system administrator has enabled user logins, you must have instrument administration privileges to configure instruments. The ChromQuest SI data system does not provide the login security feature.

This section contains the following topics:



## Configuring Instruments in ChromQuest and ChromQuest SI

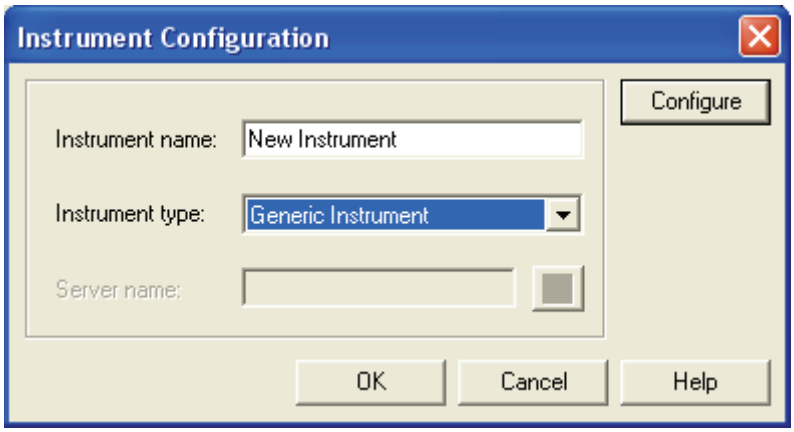
❖ **To configure instruments**

1. Do one of the following:
   - For ChromQuest, go to step 2.
   - For ChromQuest SI, choose **Start > All Programs > Chromatography > ChromQuest SI Config**. The ChromQuest SI Instrument Configuration dialog box appears. Click **Instrument Configuration**. Go to step 5.
2. In ChromQuest, choose **Start > All Programs > Chromatography > ChromQuest**.

   The Main Menu window appears.
3. Right-click the icon for the instrument you want to configure.
4. From the shortcut men, choose **Configure > Instrument**. For instructions on extracting an instrument configuration from a stored data file.

   The Instrument Configuration dialog box appears.

**Figure 64.** Instrument Configuration dialog box

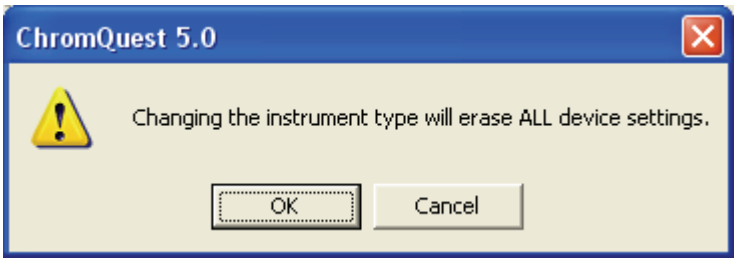



**Note** If you are using an HP5890 with or without an HP7673 autosampler, and want to use instrument and/or autosampler control features, you must select the **HP5890 + HP7673** type for the instrument. Details on how to configure HP instruments and how to control them are located in a separate control manual that comes with the instrument control option software.

5. Do one of the following:

   - To configure a new instrument, select the instrument type from the Instrument Type list. For the client/server mode, select the server. When you select an instrument type, the following dialog box appears (see Figure 65). Click **OK** to select the instrument type and close the warning dialog box.

     **Figure 65.** Warning that appears when you select an instrument type

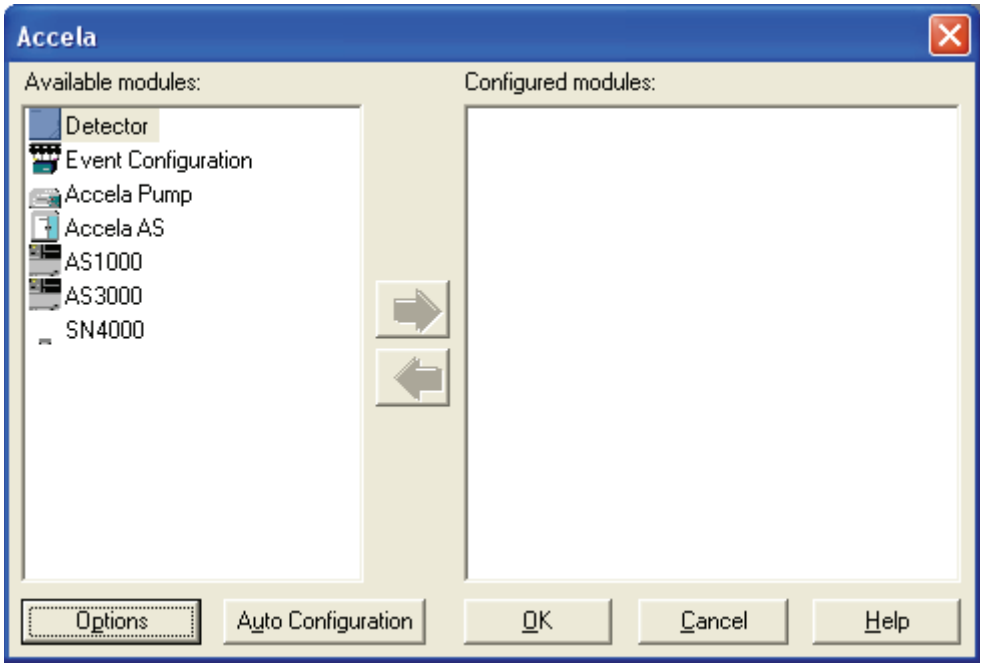
     
     

   - To modify the configuration of an existing instrument, do **not** select the instrument type, as doing so erases the current instrument configuration.

6. In the Instrument Configuration dialog box, click **Configure**.

   A dialog box containing the available modules for the selected instrument type appears. Figure 66 shows the dialog box for an Accela instrument.

**Figure 66.** Accela dialog box.




7. In the Available modules list, double-click the icons for the modules of your instrument. For a detector, double-click the Detector icon.

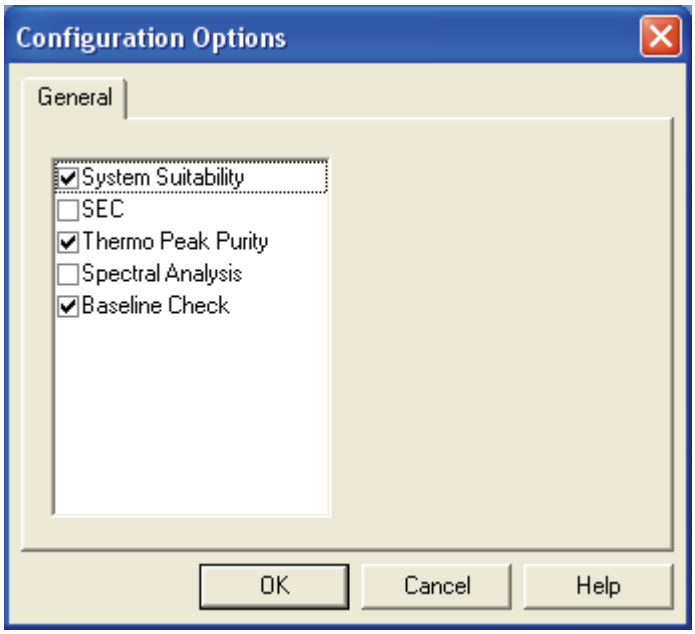
   The modules appear in the Configured modules list.

8. Complete the configuration of each module in the Configured modules list.

9. Click **Options** to check the available options for the instrument.

   The Configuration Options dialog box appears. See Figure 67. If the instrument configuration contains a PDA detector or a UV3000 scanning wavelength detector, ChromQuest selects the Spectral Analysis check box when you close the instrument dialog box.

**Figure 67.** Configuration Options dialog box




10. and then click **OK** to close the Configuration Options dialog box.
11. Click **OK** to close the Instrument (Accela, Thermo Surveyor LC, Thermo SpectraSystem, and so on) dialog box.
12. For ChromQuest SI, click **Close** in the ChromQuest SI Configuration dialog box to accept the configuration and return to the Windows desktop.

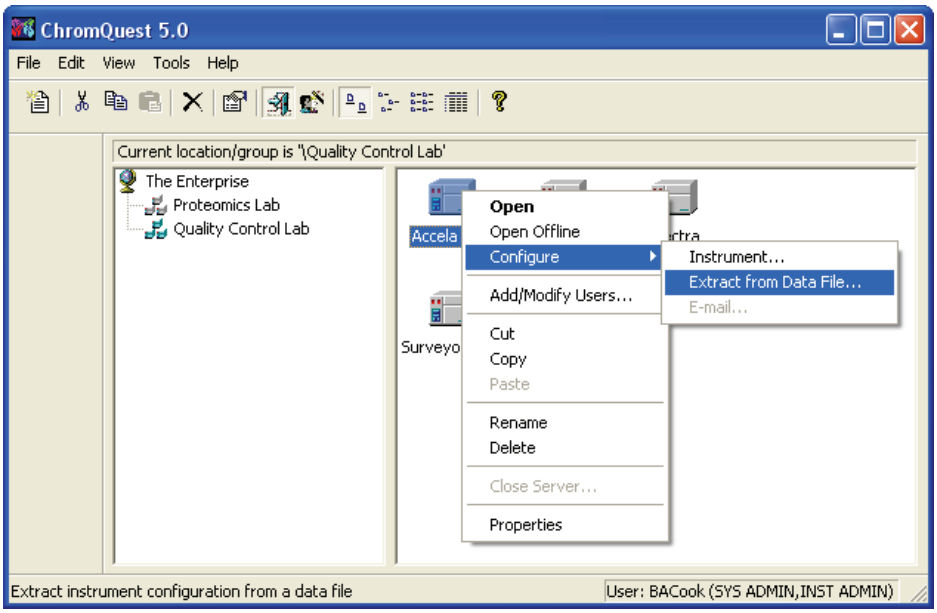
## Extracting an Instrument Configuration from a Data File

Use the Extract From Data File command to extract an instrument configuration from a stored data file.

### ❖ To extract an instrument configuration from a stored data file

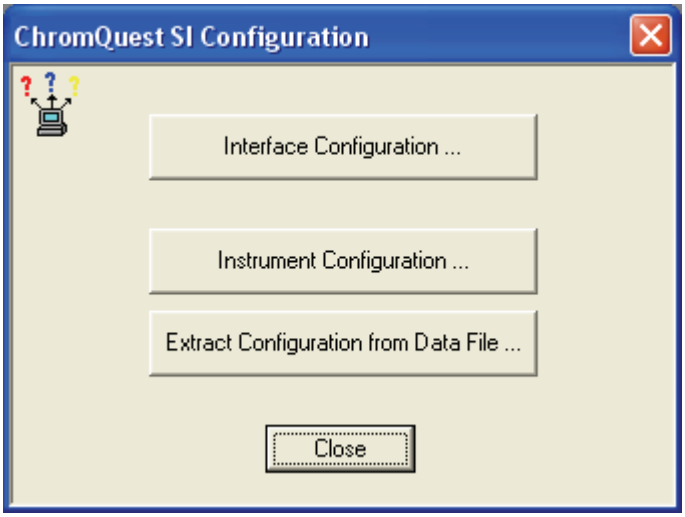
1. Depending on the data system, do one of the following:
   - For ChromQuest, from the Main Menu window, right-click the icon for the instrument you want to configure, and choose **Configure > Extract From Data File**. See Figure 68.

**Figure 68.** ChromQuest Main Menu window



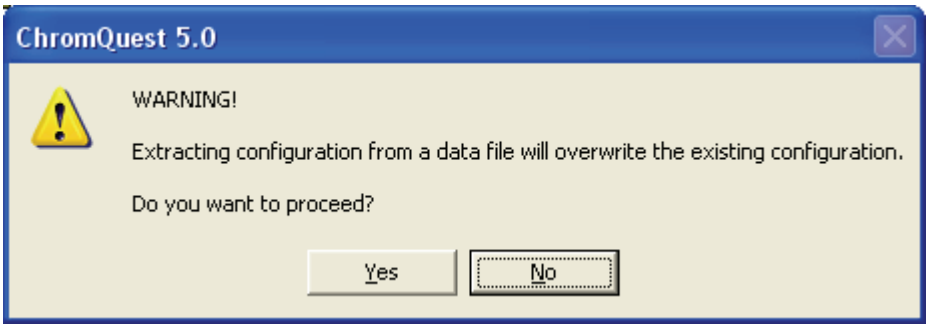

- For ChromQuest SI, choose **Start > All Programs > Chromatography > ChromQuest SI Config**. The ChromQuest SI Configuration dialog box appears (see Figure 69). Click **Extract Configuration from Data File**.

**Figure 69.** ChromQuest SI Configuration dialog box



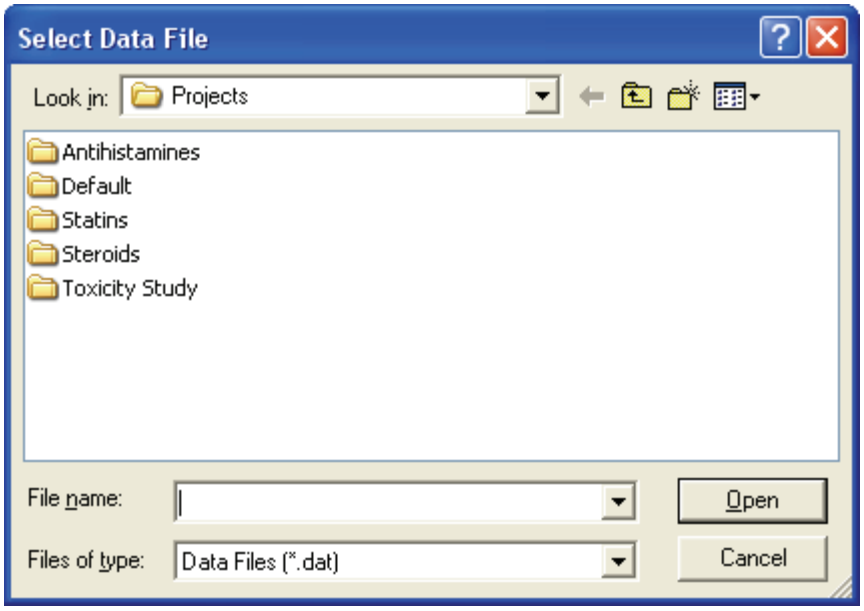

When you choose Extract from Data File, the following warning message appears. See Figure 70.

**Figure 70.** Warning dialog box



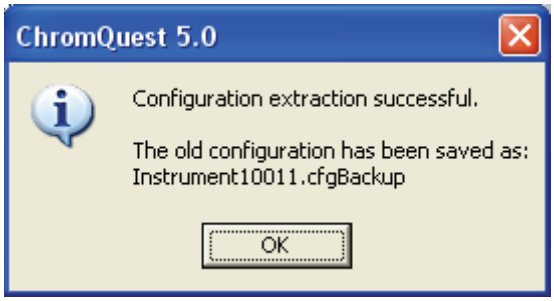

2. Click **Yes** to open the Select Data File dialog box. See Figure 71.

**Figure 71.** Select Data File dialog box




3. Select a stored data file and click Open.
4. The dialog box shown in Figure 72 appears.

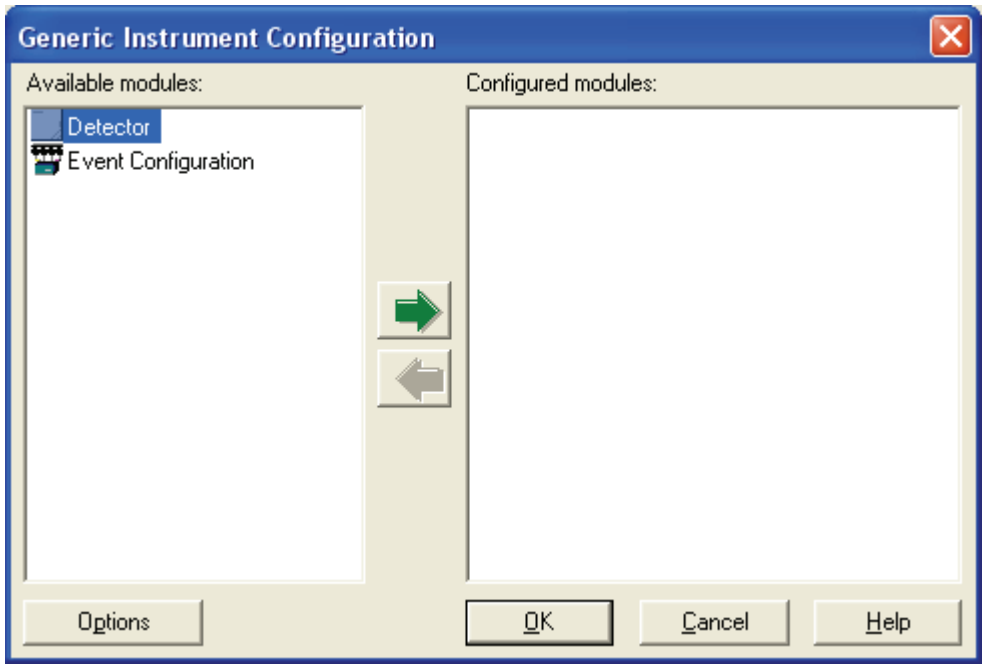
**Figure 72.** Configuration extraction successful dialog box



## Configuring a Generic System

Use the Generic System Configuration dialog box (see Figure 73) to add and define detectors and external events for your instrument.

**Figure 73.** Generic System Configuration dialog box




### ❖ To create a generic instrument

1. Depending on the data system, do one of the following:
   - For ChromQuest, open the Main Menu window. Right-click the **Enterprise** or **Location** and choose **New > Instrument**. Right-click the new instrument and choose **Configure > Instrument**.
   - For ChromQuest SI, choose **Start > All Programs > Chromatography > ChromQuest SI Config**. Double-click **Instrument Configuration**.

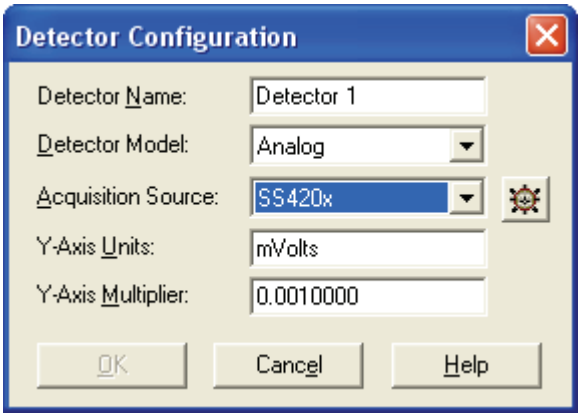
     The Instrument Configuration dialog box appears.
2. In the Instrument Type list, select **Generic Instrument**. Then click **Configure**. The Generic Instrument Configuration dialog box appears.

   The Available Modules box contains one or more icons.
3. To add a detector to the configuration:
   a. In the Available Modules box, click the **Detector** icon, and then click the green arrow button.

      The Analog icon appears in the Configured Modules box.
   b. Double-click the Analog icon.

The Detector Configuration dialog box appears. See Figure 74.

**Figure 74.** Detector Configuration dialog box



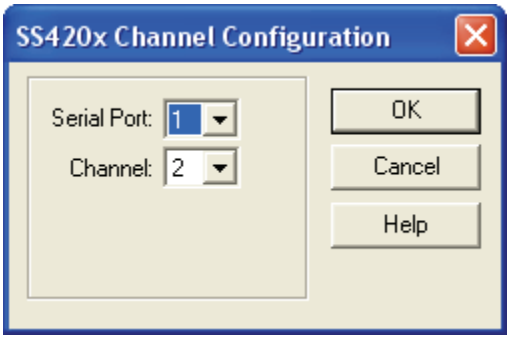

c. Type a name in the Detector Name box.

d. Select an acquisition source from the Acquisition Source list.

e. Click  .

A dialog box for the selected acquisition source appears. Figure 75 shows the dialog box for the SS420x analog to digital board.

**Figure 75.** SS420x Channel Configuration dialog box




f. Make the appropriate entries and selections in the dialog box for the selected acquisition source, and then click **OK**.

g. Click **OK** to close the Detector Configuration dialog box and return to the Generic Instrument Configuration dialog box.

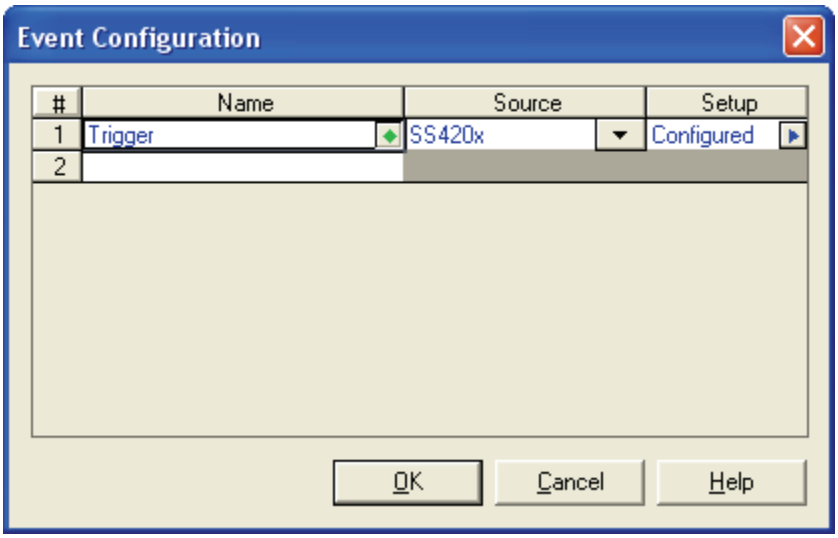
4. To set up an event for the SS420x analog to digital converter:

a. In the Available Modules list, double-click the **Event Configuration** icon.

b. In the Configured Modules list, double-click the **Event Configuration** icon.

The Event Configuration dialog box appears. See Figure 76.

**Figure 76.** Event Configuration dialog box

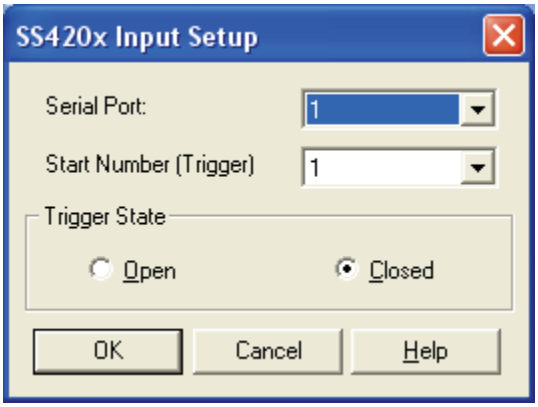



c. From the Name list, select **Trigger** or **Ready**.

d. In the Setup column, click the blue arrow.

The SS420x Input Setup dialog box appears. See Figure 77.

**Figure 77.** SS420x Input Setup dialog box




e. In the SS420x Input Setup dialog box, make the appropriate selections and entries. Then click **OK**.

f. Click **OK** to close the Event Configuration dialog box.

5. Click **OK** to close the Generic Instrument Configuration dialog box.

6. For ChromQuest SI, click **Close** in the ChromQuest SI Configuration dialog box to accept the configuration and exit the configuration application program.

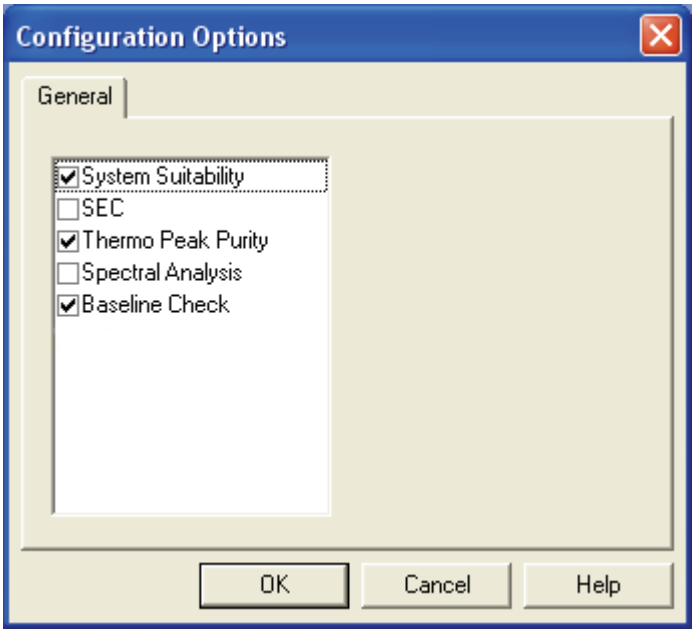
# Viewing Instrument Options

❖ **To view the available options**

In the configuration dialog box for the selected instrument type, click **Options**.

The Configuration Options dialog box appears.

**Figure 78.** Options dialog box




If the instrument contains a PDA detector or a UV3000 scanning wavelength detector, ChromQuest selects the Spectral Analysis check box when you close the configuration dialog box for the instrument.

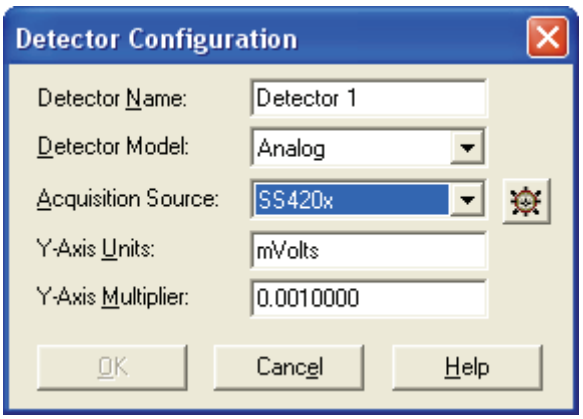
# Configuring Detectors

❖ **To complete the configuration of a detector**

1. Double-click the **Analog** icon in the Configured modules list.

   The Detector Configuration dialog box appears.

   **Figure 79.** Detector Configuration dialog box




2. In the Detector Name box, type a descriptive name for the detector.
3. In the Detector Model list, select the detector type.
4. In the Acquisition Source list, select the type of A/D board or device you are using from the list.
5. Click the  .

   The configuration dialog box for the selected detector appears. See the following topics:

   - "Configuring PE Nelson 760 Acquisition Source" on page 77
   - "Configuring PE Nelson 941 Acquisition Source" on page 78
   - "Configuring PE Nelson 960 Acquisition Source" on page 79
   - "Configuring a Generic System" on page 72

6. Make the appropriate entries and selections, and then click **OK** to close the dialog box.
7. In the Y-Axis Units box, type in the units to be displayed on the Y-Axis of your chromatogram. For example, microvolts or AU, depending on the detector units of measurement. acquires your analog signal and stores it in microvolts. If you want to display the signal in different units, you must use the correct multiplier. Consult the table below for commonly used Y-axis labels and corresponding multipliers.

8. In the Y-Axis Multiplier box, type the multiplier you want to use.

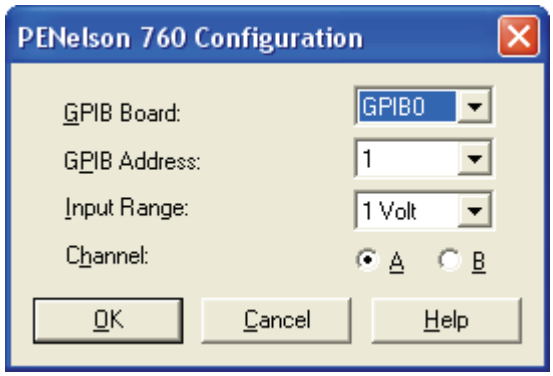
| Y-Axis Label | Y-Axis Multiplier |
|---|---|
| Volts | 0.000001 |
| Millivolts | 0.001 |
| Microvolts | 1 |
| Other | Enter a number that, when multiplied by microvolts, gives you the desired units. |

9. Click OK to close the Detector Configuration dialog box.

## Configuring PE Nelson 760 Acquisition Source

If you are using a PE Nelson 760 series interface to acquire your data, the following dialog box appears.

**Figure 80.** PE Nelson 760 Configuration dialog box



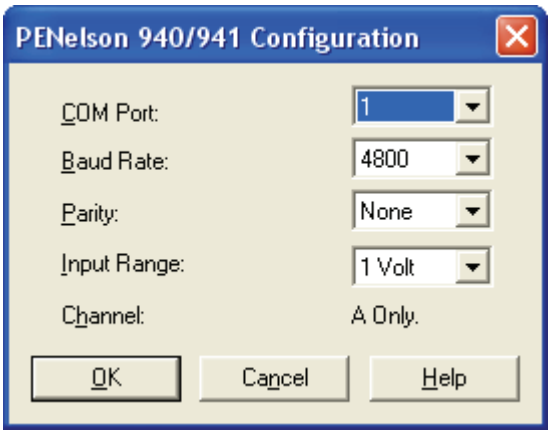

### ❖ To configure the PE Nelson 760 acquisition source

1. Select the GPIB Board number from the list. For most systems, select GPIB0.
2. Select the GPIB Device Address for the PE Nelson interface connected to this instrument. This address should match the address set on the PE Nelson interface.
3. Select a range for the detector from the Input Range list.
4. Select the Channel for this detector: A or B. The detector should be connected to this channel on the PE Nelson interface.
5. When you are done, click **OK** to return to the Detector Configuration dialog box.

## Configuring PE Nelson 941 Acquisition Source

If you are using a PE Nelson 940 or 941 interface to acquire your data, the following dialog box appears.

**Figure 81.** PE Nelson 940/ 941 Configuration dialog box



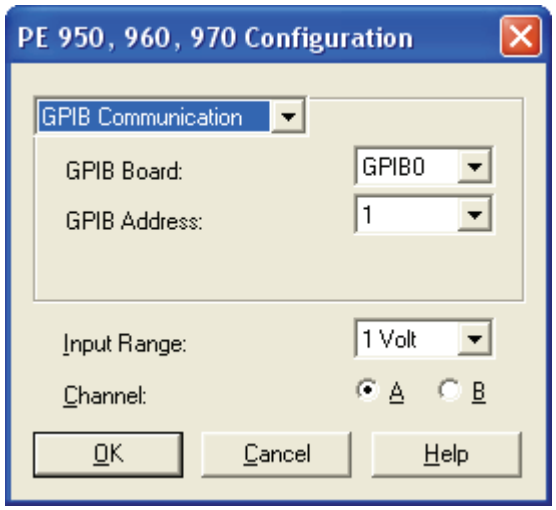

### ❖ To configure the PE Nelson 940 or 941 acquisition source

1. Select the Com Port from the list.
2. Select the Baud Rate the PE Nelson interface uses to communicate. This should match the baud rate set on the PE Nelson interface.
3. Select the Parity used from the list.
4. Select the Input Range for this detector.
5. Select the Channel that matches the channel where the detector is connected: **A** or **B**.
6. When you are done, click **OK** to return to the Detector Configuration dialog box.

## Configuring PE Nelson 960 Acquisition Source

If you are using a PE Nelson 950, 960, or 970 interface to acquire your data and the interface is set to communicate by way of GPIB, the following box appears.

**Figure 82.** PE Nelson 960 Configuration dialog box with GPIB communication



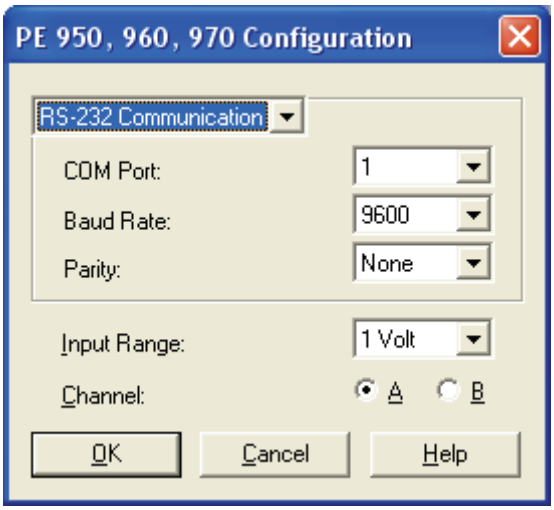

### ❖ To set up the configuration for a PE Nelson box using a GPIB board

1. In the GPIB Board list, select the number. For most systems, select GPIB0.
2. In the GPIB Device Address list, select the number that corresponds to the address set on the PE Nelson interface.
3. In the Input Range list, select an input range for the detector.
4. Select the Channel for this detector: **A** or **B**. The detector must be connected to this channel on the PE Nelson interface.
5. When you are done, click **OK** to return to the Detector Configuration dialog box.

### ❖ To set up the configuration for a PE Nelson box using RS232 communication

1. Select **RS232 Communication** from the list, and complete the following dialog box.

   **Figure 83.** PE Nelson950, 960, 970 Configuration dialog box for RS232 communication




2. Select the Com Port from the Com Port list.
3. Select the Baud Rate the PE Nelson interface uses to communicate. This must match the baud rate set on the PE Nelson interface.
4. Select the Parity used from the Parity list.
5. Select the Input Range for this detector.
6. Select the Channel that matches the channel where the detector is connected.
7. When you are done, click **OK** to return to the Detector Configuration dialog box.

## Configuring Valves and External Events

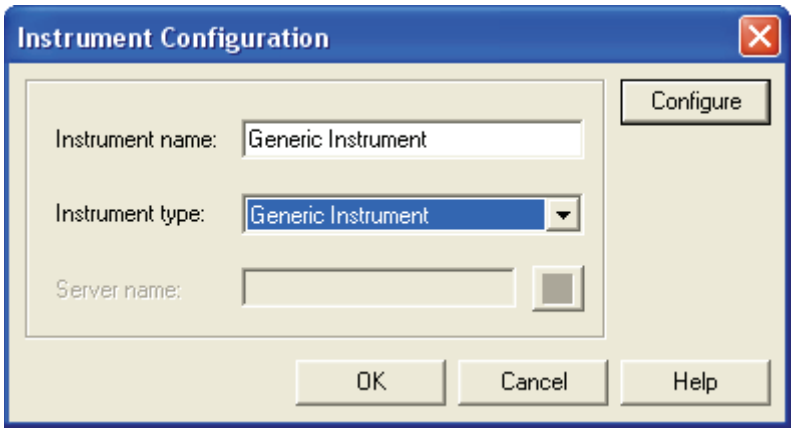
In order to configure a valve, trigger, or other external event, you must first make sure the event is properly connected to the system. Configuring an external event involves specifying which input lines are being used, so you must have this information available before you start the configuration.

In ChromQuest, valve and external event configuration is done from the Instrument Configuration dialog box.

### ❖ To configure an external event in ChromQuest

1. Open the Instrument Configuration dialog box.
2. In the Instrument type list, select **Generic Instrument**. See Figure 84.

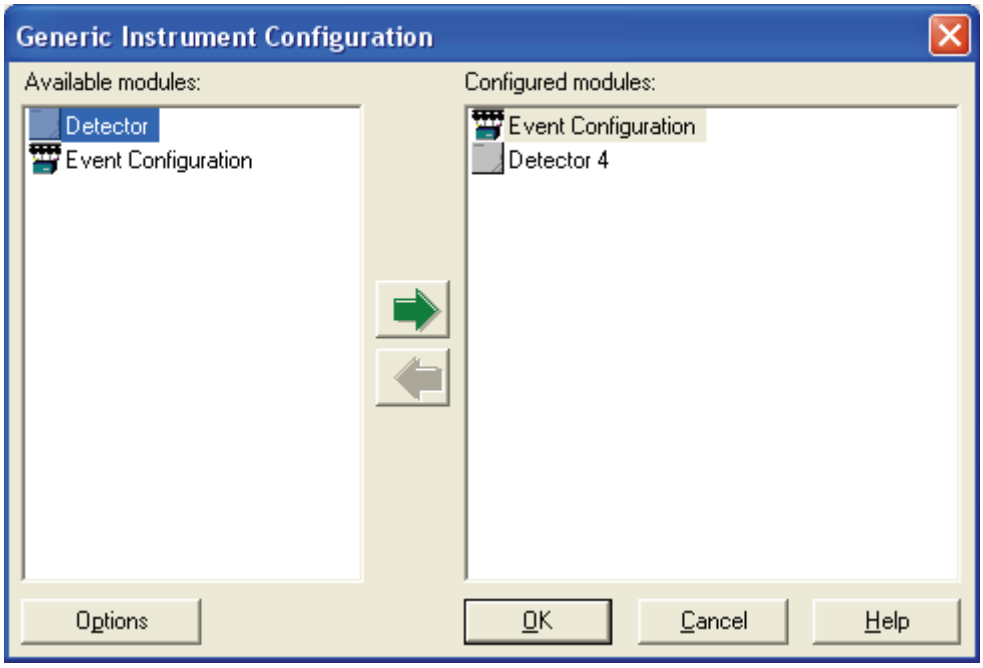
**Figure 84.** Instrument Configuration dialog box




3. Click **Configure**.
4. In the System Configuration window, double-click the **Events Configuration** icon.

   The Event Configuration icon appears in the Configured modules list. See

   **Figure 85.** Generic System Configuration dialog box



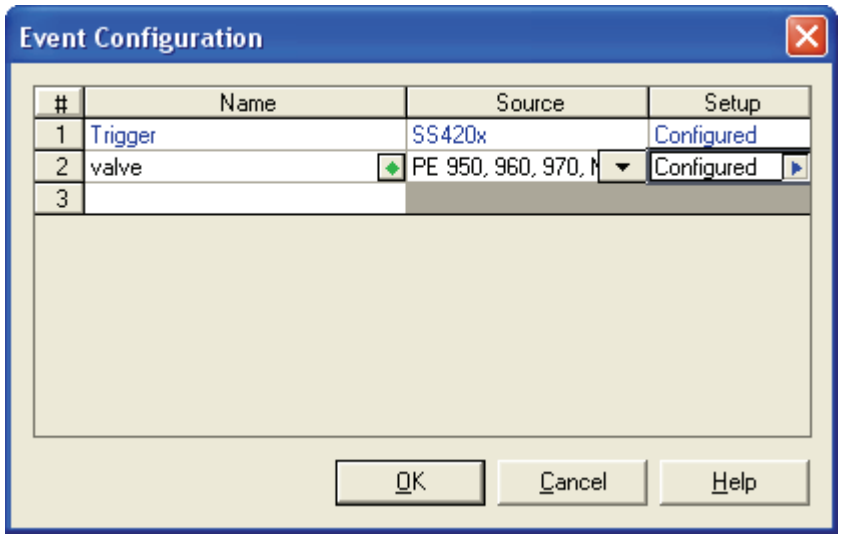

5. Double-click the **Event Configuration** icon in the Configured modules box.

   A spreadsheet appears where you can select the external events to configure.

## Event Configuration

When you double-click the Event Configuration icon, the following spreadsheet appears where you configure the events:

**Figure 86.** Event Configuration dialog box




### ❖ To configure events

1. In the Name list, do one of the following:
   - To configure an event, click  and select either **Trigger** or **Ready**.
   - To configure a valve or other external event, select the Name box and then type the name of the event or valve.
2. In the Source list, select the source of the event (the hardware from which the event comes). The PE Nelson selections are available for events that you have named. They are not available for the Trigger or Ready events.
3. In the Setup list, click  .

   A dialog box appears where you set up the appropriate information for the operation of this event.

Continue the external event configuration until all events for this instrument are configured. Programming of the external events into your method is done in the Instrument Setup section of the method, and is described in the Method Development section.

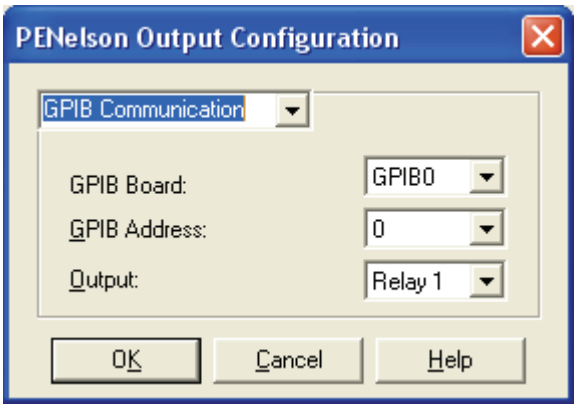
**Note**

1. The external events tab in Instrument Setup is not available unless you have configured your instrument with one or more external events.
2. It is possible to assign the same event to more than one instrument. Be careful to assign events so that conflicts between instruments do not occur.

## PE Nelson 760 Output Setup

When you configure a valve or other external device, the Setup field opens the Output Setup dialog box. Select the GPIB Board Number, GPIB Interface Address, and Output line to which the event is tied.

**Figure 87.** PE Nelson 760 Output Configuration dialog box

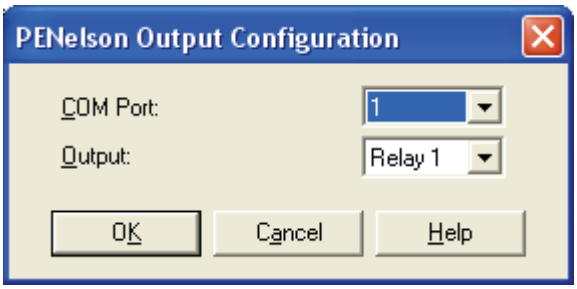



When completed, click **OK** to exit the dialog box.

## PE Nelson 941 Output Configuration

When you configure a valve or other external device, the Setup field opens the Output Configuration dialog box.

**Figure 88.** PE Nelson 941 Output Configuration dialog box




Select the COM Port where the interface is configured from the COM Port list.

Select the Output from the Output list.

When completed, click **OK** to exit the dialog box. Once the events are configured, you can program them from the Instrument Setup section of the methods.

## PE Nelson 960 Output Configuration

When you configure a valve or other external device, the Setup field opens the Output Configuration dialog box.

If the interface uses GPIB to communicate, select this option from the list.

**Figure 89.** PE Nelson 960 Output Configuration dialog box


Select the GPIB Board to which the interface is connected.

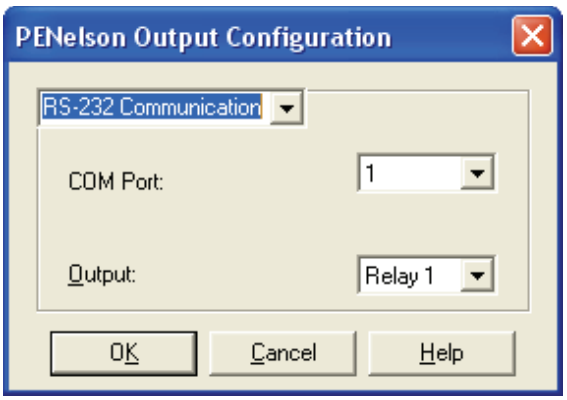
Select the GPIB Address that matches the address set on the interface.

Select the Output to configure.

Click **OK** to exit the dialog box.

If the 960 Interface communicates via RS232, select this option from the list, and the following dialog box appears.

**Figure 90.** PE Nelson 960 Output Configuration dialog box




Select the COM Port where the interface is configured.

Select the Output.

Click **OK** to exit the dialog box. Once the events are configured, you can program them from the Instrument Setup section of the methods.

# Verification of Analog Connections

Before attempting to inject samples on your chromatograph, ensure that the analog connections and triggers you have made are correct by looking at the actual detector signals.

## Using Preview to Verify Analog Connections

❖ **To do a quick preview of the signal without performing a run using the Preview function**

1. From the Main menu, click the icon that represents the instrument you wish to check, and log on to start the instrument application.

2. Locate the **Preview** button on the toolbar and click it or choose **Control > Preview Run**. The real time detector output from your instrument appears. If you inject a simple sample (that is, a solvent) you should see a peak elute, oriented in the correct direction. If you see no peaks, check to see if your connections and assignment of analog line numbers, and configuration are correct. If the peaks are in the wrong direction, reverse your detector signal lines and repeat.

3. When you are finished, click the **Stop Run** button. Note that in the **Preview** mode, the data is not integrated or analyzed.

   Once you have verified your analog signals and remote input lines are properly connected, you can start acquiring actual data. If you are using for the first time, take a few minutes to perform the Tutorial. This Tutorial takes you step-by-step through the basics of using the system, and can increase the pace of learning.

## Starting an Instrument

You can develop methods and sequences, create custom reports, and acquire data in the Instrument window.

❖ **To access the Instrument window in ChromQuest**

In the Main Menu window, double-click the instrument icon that represents your LC system. You might be required to log on before you can access the instrument window functions.

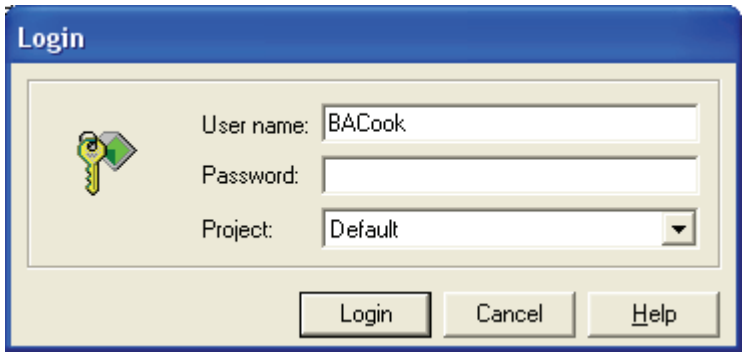
❖ **To access the Instrument window in ChromQuest SI**

From the Windows desktop, choose **Start > All Programs > Chromatography > ChromQuest SI**.

## Instrument Login

Whenever the instrument login and project management are enabled, you are required to login whenever you attempt to start an instrument application.

**Figure 91.** Login – User name dialog box




Enter the information as prompted, and then click **Login**.

- User name

  Enter the user name that has been assigned to you on the network.

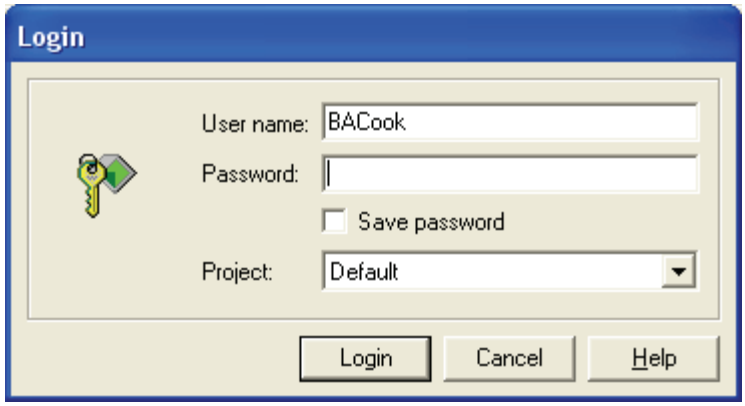
- Password

  Enter your assigned network password.

- Save Password

  If the Save password option is enabled by your system administrator, a Save password check box appears.

**Figure 92.** Login – Password dialog box




If you select this box, the password you type at login is saved when you click **Login**. Once the password has been saved, whenever you log on to the instrument, the saved password is used.

**Note** The password is saved when you click **Login**, whether or not the login is successful.

- Domain

  Select the domain you have privileges on from the list, or type in the correct domain. (The Domain list is not shown here, unless you are using a domain controller.)

- Project

  Select a project to log on to. This project becomes the default project path for methods, data, and sequences in the instrument. You can, however, create and save files in other locations, or change the selected project later, even though you have logged on to a designated project.

Once you have logged on to an instrument and selected a project, that project's paths for methods, data, sequences, and templates are used unless you designate a new project. To change the selected project, use **File > Select Project** from the menu bar.

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