G3310AA 6300 Series Security Pack Quick Start Guide

A guide to the 21 CFR Part 11 compliance add-on for the 6300 Series Ion Trap software

Use this reference to install and get started with the Agilent 6300 Series Security Pack software.

What are the 21 CFR Part 11 compliance features of the 6300 Series Security Pack software?

The 1997 Food and Drug Administration (FDA) ruling 21 CFR Part 11 defined criteria for FDA acceptance of electronic records and electronic signatures. The 6300 Series Security Pack software includes the following features to address these requirements:

- Limited system access and authority checks
- Audit trails
- Electronic signatures
- Results history

This *Quick Start Guide* introduces you to these capabilities. See the online help for more information on each of these features.

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Concepts

Key requirements of 21 CFR Part 11 include limited system access and authority checks. The 6300 Series Security Pack software helps laboratories to meet these requirements via a UserManagement Administration Tool, which enables a system administrator to set up users, passwords, and rights. In the case where there is only one Ion Trap LC/MS PC in the laboratory, it is most efficient to install the security pack software on that PC. Then the single PC acts as both client and server. In the case were there are multiple Ion Trap LC/MS PCs, it is best to install the software on a central server, as shown in Figure 1. The users, passwords and rights that are set up on the central server then apply to all the clients. Administrators invoke a UserManagement Configuration dialog box on the clients to establish the server as the control point for UserManagement. (See Figure 2.) Table 1 lists the software packages applicable to servers and clients.

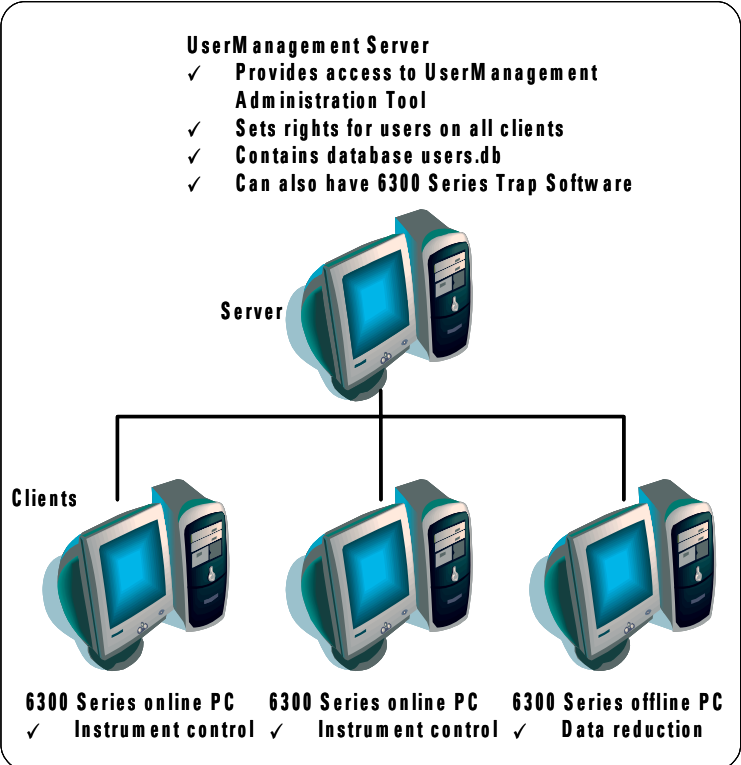**UserManagement Server**
- ✓ Provides access to UserManagement Administration Tool
- ✓ Sets rights for users on all clients
- ✓ Contains database users.db
- ✓ Can also have 6300 Series Trap Software

Server

Clients

6300 Series online PC
- ✓ Instrument control

6300 Series online PC
- ✓ Instrument control

6300 Series offline PC
- ✓ Data reduction

Figure 1   UserManagement software installed on central server

Name or IP address of server

Enter server port (generally keep default)

Location of User Management database on server (keep default)

UserManagement Server Configuration

To enable your local PC to communicate with the UserManagement Server, some information is needed.
You need to know the server name or IP address of your UserManagement Server and the port that is used for the server on that PC.

Server name or IP: localhost

Port: 12347

DB Location: C:\Program Files\Bruker Daltonik\UserManagement\Data\users.db

OK   Cancel

If UserManagement program is on local PC, keep default of localhost.

If UserManagement program is on remote PC, enter server name or IP

Figure 2   Client configuration of connection to UserManagement Server

Other requirements of 21 CFR Part 11 include audit trails and results history. These are accomplished at the client level once the compliance license number is installed in DataAnalysis on the Ion Trap LC/MS PC. Electronic signatures are implemented on the client PCs, but the rights to electronically sign are governed by the UserManagement Administration tool on the server.
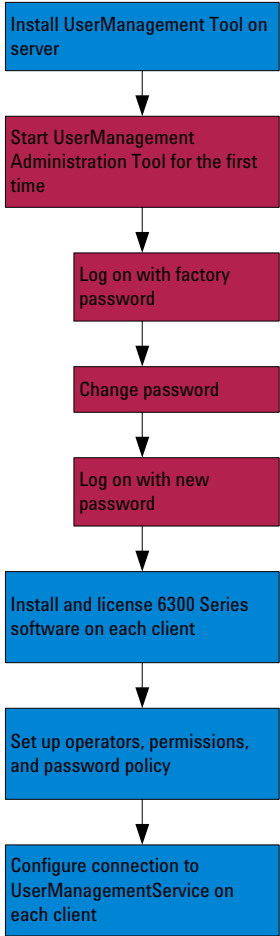
Table 1   Software to install on UserManagement Server and Ion Trap LC/MS clients

	Server	Client
Purpose of PC	Central location for managing Ion Trap LC/MS users and rights	Offline or online Ion Trap LC/MS installation
Minimum software	UserManagement Administration Tool (G1330AA Security Pack Software)	Ion Trap software
Optional software	Ion Trap software	

Installation and Getting Started Roadmap

This diagram shows the steps for administrators and other users to get started with the 6300 Series Security Pack software. This guide and the online help explain these steps.
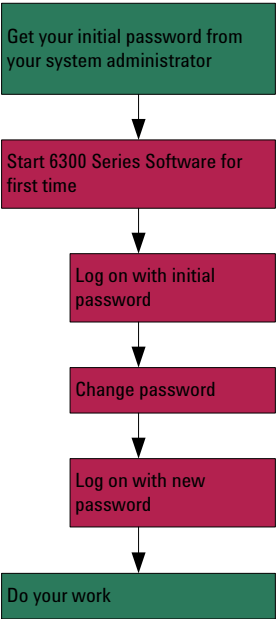
Administrators

All Users

Install UserManagement Tool on server

↓

Start UserManagement Administration Tool for the first time

↓

Log on with factory password

↓

Change password

↓

Log on with new password

↓

Install and license 6300 Series software on each client

↓

Set up operators, permissions, and password policy

↓

Configure connection to UserManagementService on each client

Get your initial password from your system administrator

↓

Start 6300 Series Software for first time

↓

Log on with initial password

↓

Change password

↓

Log on with new password

↓

Do your work

Figure 3   Getting started workflow diagram

Server Installation

The Security Pack for the Agilent 6300 Series Ion Trap LC/MS consists of two components: a server component and a client component. The server component can be installed on an Ion Trap Control PC or any other PC.

Step 1. Start the installation

1 Decide whether you want to install the server component on a centralized server PC for the entire laboratory, or on a local PC.

- If you have multiple Ion Trap LC/MS in the laboratory, install the software on a central server.
- If you have only a single Ion Trap LC/MS, install the software on the local instrument control PC.

← *6300 Series Ion Trap System LC/MS Installation Guide* →

2 If the server PC is or will also be an Ion Trap LC/MS Control PC or an offline data processing PC, start the installation according to the instructions in the *Agilent 6300 Series Ion Trap System Installation Guide* as if you are upgrading the PC.

Continue at the next Step only when instructed to by the *Installation Guide*.

If Ion Trap LC/MS Control PC already has a previous release of the Ion Trap LC/MS Software installed, make sure to you do "Step 2. Upgrade from Windows NT4 or to a compliant system" in the *Installation Guide* to restore the entire PC using the Emergency Recovery CD kit.

If you want to set up a data processing only PC in a compliant mode, use a dedicated PC, remove all previously installed Ion Trap LC/MS software, and separate data previously acquired in a non-compliant mode from data acquired in compliant mode on the Ion Trap LC/MS Control PC. You can purchase another Ion Trap LC/MS Control PC for this purpose, and benefit from the included Emergency Recovery CD kit.

Step 2. Install the UserManagement software

1 Insert the G1330AA 6300 Series Security Pack Software CD into the CD drive.

2 Display the files on the CD.

3 Double-click the folder **Install**.

4 Double-click **AgilentServerSetup.exe** to run the server setup program.

5 In the welcome screen, click **Next >**.

6 Carefully read the license agreement.

7 If you accept the terms, click **I accept the terms of the license agreement**.

8 Click **Next >** to continue.

9 Select a **Complete** as the **Setup Type**.

   Both the Server Component and Administration Tool are installed on the server PC.

10 Click **Next >** to continue.

11 Click **Install** to begin the installation.

12 If you are prompted to enter the license for the Trap UserManagement software, do so. You can find the license on the software certificate provided in the G1330AA Security Pack Software kit.

13 When you see the screen to **Enter Trap UserManagement Server Name and Port**, retain the defaults and click **OK**. The default port was specifically chosen because it is a free port on most PCs.

14 Click **Finish**.

Step 3. Start the UserManagement Administration Tool for the first time

1 Log onto the UserManagement Administration Tool:

    a From the **Start** menu on the UserManagement server, select **All Programs > 6300 Series Ion Trap LCMS > Administration > UserManagement Administration Tool**.

    b In the logon dialog box, for **Operator** enter **Administrator** and for **Password** enter **administrator**. Note that passwords are case-sensitive.

    c Click **Log On**.

2 When you see the message that instructs you to change your password, click **OK**.

3 Fill in the **Change Password** form as described on "To change your password" on page 22.

4 Log on again with your new password.

5 If you see the Create New Operator dialog box (see Figure 4 on page 9, click Cancel to go to the UserManagement Administration Tool main window (see Figure 5 on page 9).

6 Click **Close** to close the UserManagement Administration Tool, Click **Yes** when asked to confirm.

Step 4. Finish the Ion Trap Control LC/MS PC or offline data processing PC installation

←

6300 Series Ion Trap LCMS System Installation Guide

→

- If the UserManagement software is being installed on an Ion Trap LC/MS Control PC or an offline data processing PC, return to "Step 9. Install the Ion Trap Software" in the *Installation Guide* to complete the system installation.

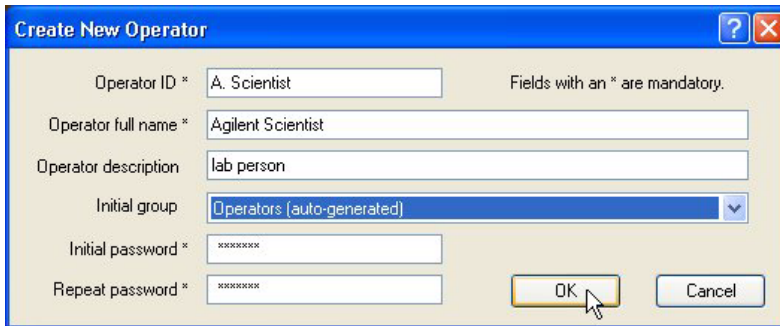Continue at the next Step when you are instructed to do so by the *Installation Guide*.

Step 5. Use the UserManagement Administration Tool to set up operators, rights and password policies

1 Log onto the UserManagement Administration Tool:

   a From the **Start** menu on the UserManagement server, select **All Programs > 6300 Series Ion Trap LCMS > Administration > UserManagement Administration Tool**.

   b In the logon dialog box, for **Operator** type Administrator and for **Password** type the password that you set in "Step 3. Start the UserManagement Administration Tool for the first time" on page 7. Note that passwords are case-sensitive.

   c Click **Log On**.

2 From the **Operators** tab, click **Create New Operator**.

3 Verify that you see the form shown in Figure 4.

4 Fill in the form to set up the first operator.

   • As a minimum, you need to complete the boxes that are marked with an asterisk.

   • For **Group**, select one of the preconfigured groups, or keep the default setting of **None**. You will have a chance to change the group later. The group assignment is what determines the operator's rights.

5 Click **OK**. You will see a message that states that the operator was created successfully.

6 When you see the **UserManagement Administration Tool** dialog box, use the information shown in Figure 5, along with the online help, to proceed with additional **UserManagement Administration Tool** tasks. These include:

   • Customize the password policy and timeout for your laboratory.

   • Modify **Rights, Group Assignments** and **Groups** as desired.

   • Add more **Operators** as desired.

7 When you are done, click **OK** to close the form.

←

6300 Series Ion Trap LCMS System Installation Guide

→

8 Return to "Step 13. Create a backup image of Programs and Archive partitions" in the *Installation Guide* to make a custom backup image of your system.

NOTE   If you have ChemStation installed, but do not see it in the **Application** list under the **Rights** tab, then close the UserManagement Administration Tool, launch ChemStation, and open the UserManagement Administration Tool again.
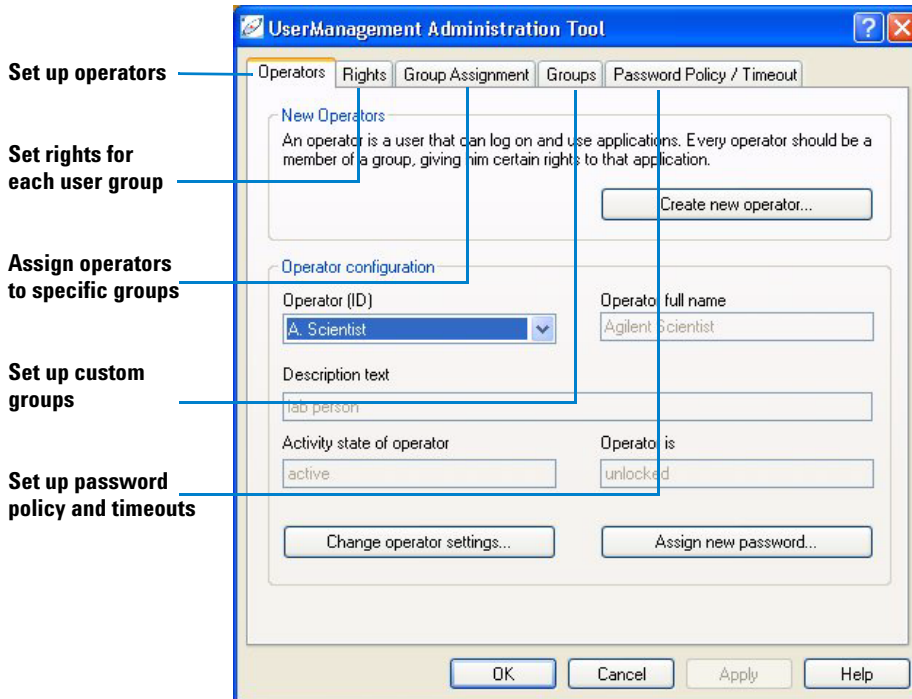
Figure 4   Setting up an operator

Set up operators

Set rights for each user group

Assign operators to specific groups

Set up custom groups

Set up password policy and timeouts

Figure 5   UserManagement Administration Tool

Client Installation

If the Client PC also functions as the UserManagement Server PC, and has been installed according to "Step 2. Install the UserManagement software" on page 6, then it is already properly configured, and you have nothing more to do.

If you have configured the UserManagement Server on a central PC, then follow the steps in this section for all the Client PCs. Client PCs can be Ion Trap LC/MS Control PCs or off-line (data-processing only) PCs.

Step 1. Install and license the Ion Trap LC/MS software on each client

1 If the 6300 Series Ion Trap LC/MS Software is already installed on your system, according to the instructions in the *Installation Guide*, then:

   a Click **Start > Programs > 6300 Series Ion Trap LCMS > Administration > License Manager**.

   b Enter the license key for the Ion Trap LC/MS Security Pack software.

   c Click **Add**.

   d Finish the license installation as instructed.

2 If the 6300 Series Ion Trap LC/MS 5.2 Software is *not* installed on your system:

   a Follow the instructions in the *Installation Guide* to start a regular installation or upgrade, not one for a compliant system.

   b When you are prompted to enter license numbers, make sure you enter the Ion Trap LC/MS Security Pack license number.

   c Finish the installation or upgrade as instructed.

NOTE   If the User database is located on a central UserManagement Server, but the Administrator wishes to administer the user database from a client PC as well, please install the entire UserManagement software with the Complete option on the client PC, just as for the central server (see "Step 2. Install the UserManagement software" on page 6).

Step 2. Configure the UserManagement Server connection on each client

1 Click **Start** > **Programs > 6300 Series Ion Trap LCMS > Administration > UserManagement Configuration**.

2 In the UserManagement Server Configuration dialog box:

   a Enter the server name or IP address in the **Server Name or IP** text box.

   b Keep defaults for **Port** and **DB Location** unless the User database is located in a different path on the UserManagement Server.
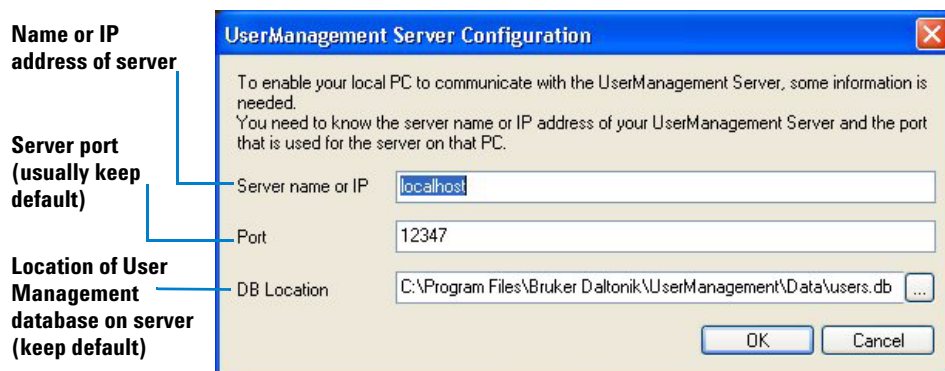
Name or IP address of server

Server port (usually keep default)

Location of User Management database on server (keep default)

Figure 6   Configuring the client connection to the UserManagement Server

To remove the 6300 Series Security Pack

1 Run **agilentserversetup.exe** on the software CD.

2 Select **Remove** from the setup panel.

CAUTION   Do not to use the **Windows Add/Remove Programs** function to remove the software. You might delete one or more Windows system files, which may interfere with Windows operation.

Quick Tutorial for System Administrators

This section assumes that installation is complete. If not, start with

To access the UserManagement Administration Tool

1 From the **Start** menu on the UserManagement server, select **All Programs > 6300 Series Ion Trap LCMS > Administration > UserManagement Administration Tool**.

2 In the logon dialog box, for **Operator** enter **Administrator** and for **Password** enter the password for Administrator. Note that passwords are case-sensitive.

3 Click **Log On**.

4 You will see the **UserManagement Administration Tool** dialog box, as shown in Figure 5. Use this to set up operators, rights, and passwords.

To sign or delete an electronic record

When you sign or delete an electronic record, you accept or delete the processed results. The original data file is not affected.

When you sign or delete an electronic record in DataAnalysis, you accept or delete a single set of processed results for a single data file. When you sign or delete an electronic record in QuantAnalysis, you accept or delete a single set of processed results, for all data files included in the quantitation set.

An electronic record may be signed more than once, by more than one person.

To use the Result History menu item in DataAnalysis

1 From **DataAnalysis**, load a data file if you have not already done so. This example uses the **SulfMS01.d** data file from the **Example Data** directory on the G1330AA Security Pack Software CD.
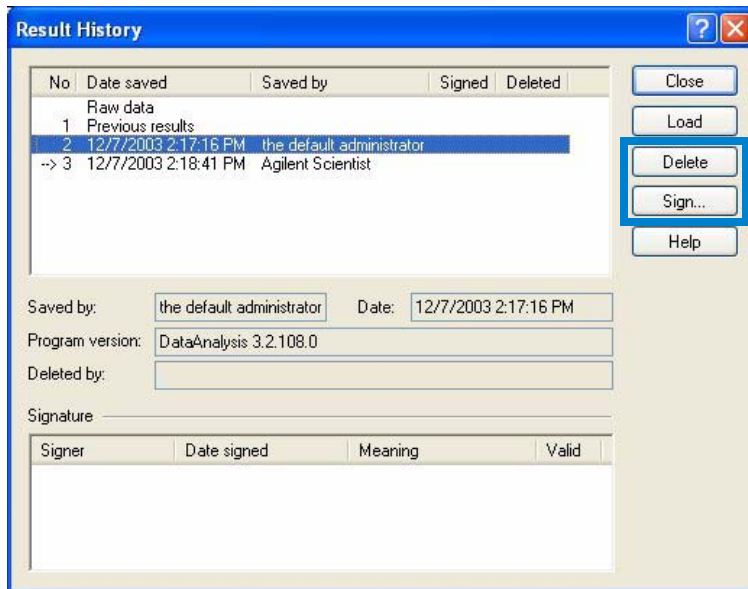
2 Select **File > Result History**.

Figure 7   Result History in DataAnalysis

3 To sign the record:

  a Click the item in the **Result History** that you wish to sign. (See Figure 7.)

  a Click **Sign...**.

  b Sign the electronic record.

    • Enter your operator name, password, and the meaning you intend to convey with your signature.

    • See Figure 8 as an example.

    • Remember that passwords are case-sensitive.

  c In the **Sign Electronic Record** dialog box, click **Sign**.

  d Check that your signature is reflected in the data record. You should see **yes** in the **Signed** column of the **Result History**.

4 To delete the record:

    a Click the item in the **Result History** that you wish to delete. (See Figure 7.)

    b Click **Delete**.

    c When you see the message that requests you to confirm deletion, click **Yes**.

    d Check that your deletion is reflected in the data record. You should see **yes** in the **Deleted** column of the **Result History**.
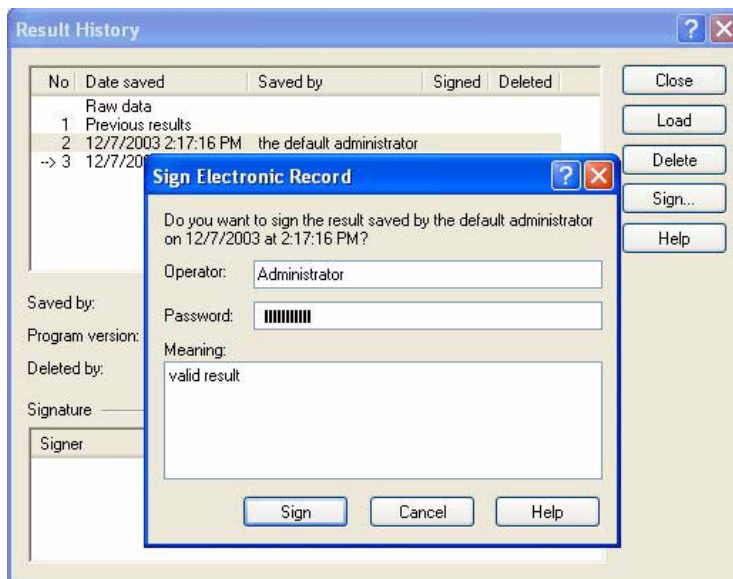

Figure 8   Signing an electronic record in the **Result History**

To use the Sign Electronic Record menu item in DataAnalysis

1 From **DataAnalysis**, load a data file if you have not already done so. This example uses the **SulfMS01.d** data file from the **Example Data** directory on the G1330AA Security Pack Software CD.

2 If you wish to load a specific result within a data file:

    a Select **File > Open**.

    b Click the file name.

    c At the bottom of the **File Open** dialog box, click the **Result** arrow and select the specific result you wish to open. See Figure 9. Unlike the **Result History**, deleted results do not appear in this list.

    d Click **Open**.
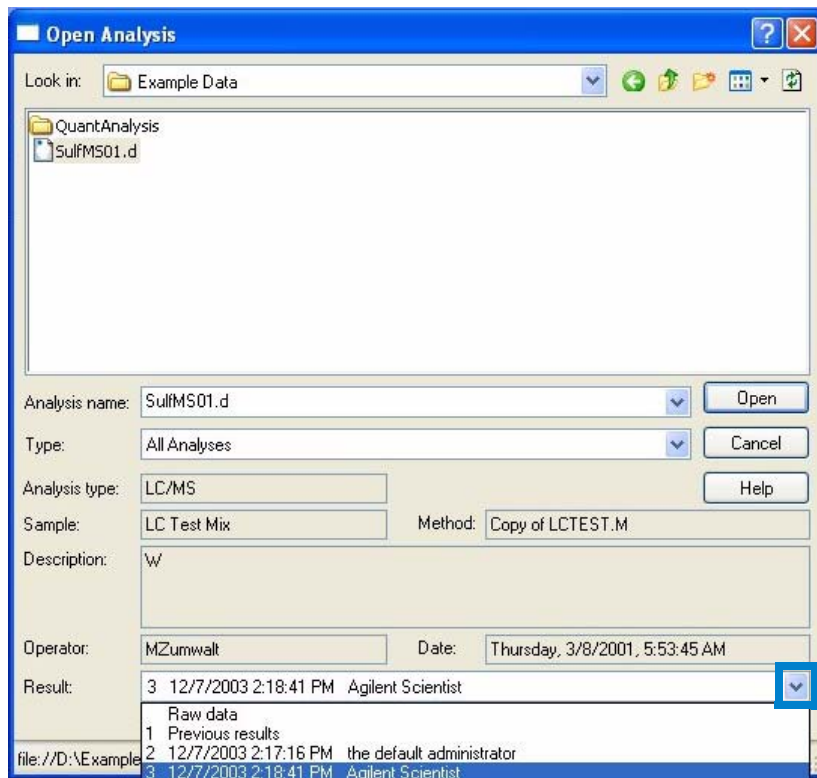
Figure 9   Opening a specific result associated with a data file

3 Select **File > Sign Electronic Record**.

4 Check to see whether the electronic record indicated at the top of the dialog box (as shown in Figure 10) is the one you wish to sign. The record indicated will be one of the following:

- The last record saved, i.e., the result of the most recent action on the data
- The last result opened with **File > Open**
- The last record selected and loaded in the **Result History**

Figure 10   Signing an electronic record

5 To sign the electronic record, enter your operator name and password. Remember that passwords are case-sensitive.

6 Enter a **Meaning** to describe what you intend to convey with your signature.

7 Click **Sign**.

To use the History... button in QuantAnalysis

1 In **QuantAnalysis**, load a quantitation batch file if you have not already done so. This example uses the **Seqtable.btc** batch file from the **Example Data\QuantAnalysis** directory on the G1330AA Security Pack Software CD.

2 From the **Work Table View**, click the **History...** button, as shown in Figure 11.

3 To sign the record, see step 3 on page 13.
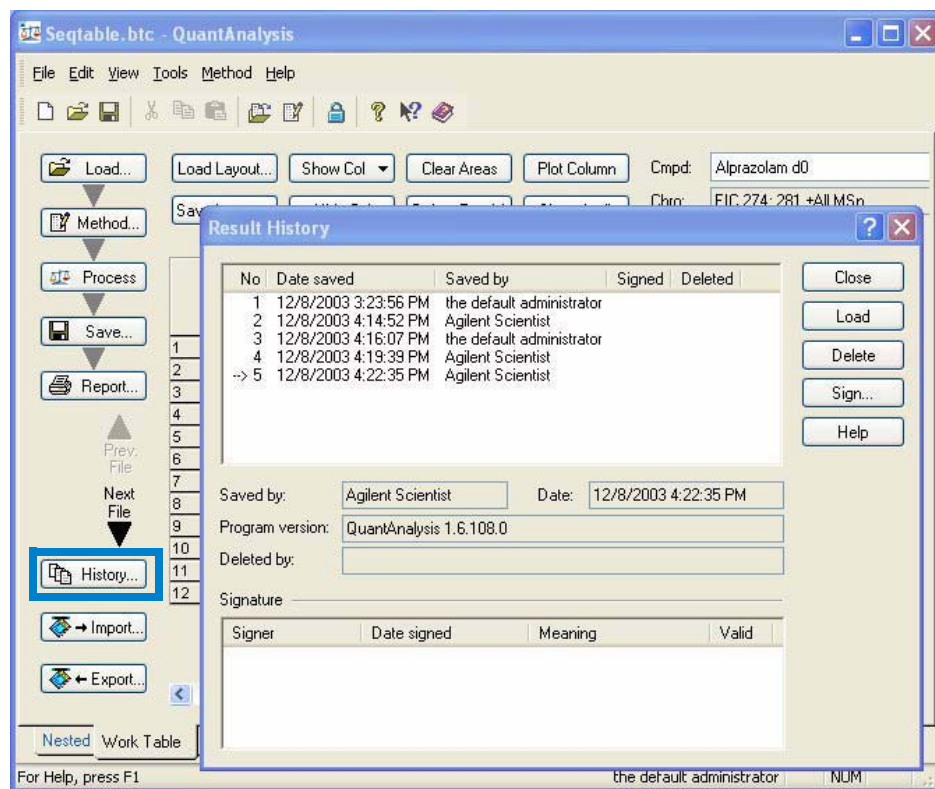
4 To delete the record, see step 4 on page 14.

Figure 11   Result History in QuantAnalysis

To recover from administrator's incorrect password entry

If as Administrator you type your password wrong too many times (as set by **Maximum wrong logons** in the **Password Policy**), the software will lock you out. To regain access to the software:

1 Stop the **BDalUserManagement Service**. To do this, see Figure 12 and follow these instructions:

    a Right-click **My Computer** and select **Manage**.

    b Click **Services and Applications** to expand it.

    c Click **Services** to expand it.

    d Right-click **BDal UserManagement Service** and select **Stop**.

2 Do one of the following:

    • If you do not remember your password, delete the user database (**X:\Program Files\Bruker Daltonik\UserManagement\Data\users.db**), where **X** is the drive where you installed the Ion Trap LC/MS software. Then do steps 3 - 5 below.

    • If you do remember your password, but just accidentally miss-typed it, do step 3 only.

3 Restart **BDalUserManagement Service**. (See Figure 12.)

    a Right-click **My Computer** and select **Manage**.

    b Click **Services and Applications** to expand it.

    c Click **Services** to expand it.

    d Right-click **BDal UserManagement Service** and select **Start**.

    e Close **Computer Management**.

4 Start the UserManagement Administration Tool, as described in "Step 3. Start the UserManagement Administration Tool for the first time" on page 7.

5 Start over to set up users, passwords, etc., as described in "Step 5. Use the UserManagement Administration Tool to set up operators, rights and password policies" on page 8.
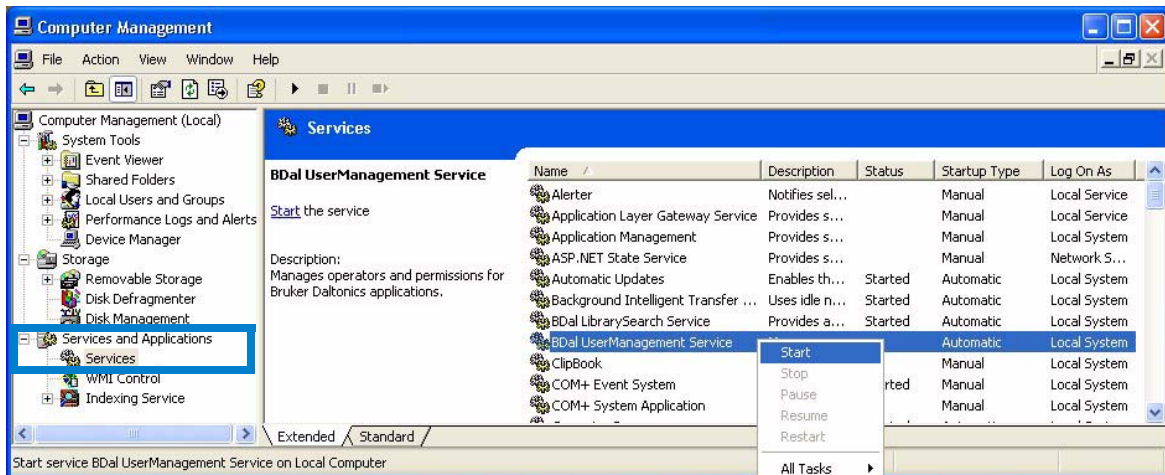
Figure 12   To start or stop the UserManagement Service

To unlock an operator who has entered his password incorrectly

If an operator types his password wrong too many times (as set by **Maximum wrong logons** in the **Password Policy**), the program will lock him out.

If the operator is the system administrator, see "To recover from administrator's incorrect password entry" on page 18. If the operator is another user, then follow these steps to allow him to regain access to the program:

1 Start the **UserManagement Administration Tool**, as described in "To access the UserManagement Administration Tool" on page 12.

2 In the **Operators** tab, select the **Operator ID** of the person who has been locked out.

3 Click **Change Operator Settings...**.

4 Clear the **Operator is locked** check box.

5 Click **OK**.

To uninstall the UserManagement program

1 Remove the 6300 Series Security Pack license:

Note that you must have Administrator privileges to remove the license.

a Click **Start > Programs > 6300 Series Ion Trap LCMS> Administration > License Manager**.

b Select **6300 Series Security Pack *x.x***, where *x.x* represents the version number, then click **Delete.**

c Click **Yes** when you are asked, **Do you really want to delete the selected license key?**

d Enter your password when prompted.

e Click **Close**.

CAUTION   You must uninstall the compliance license first before uninstalling the UserManagement Server program. Otherwise the system can get into an unusable status, and you will not be able to launch the Ion Trap LC/MS software.

2 Click **Start** > **Settings > Control Panel** (Windows 2000) or click **Control Panel** (Windows XP).

3 Double-click **Add/Remove Programs** (Windows 2000) or **Add or Remove Programs** (Windows XP).

4 Click **6300 Series Security Pack**.

5 Click the **Remove** button.

Quick Tutorial for Operators

To log on

1 Do one of the following:

- Start one of the Ion Trap LC/MS programs.
- If the program has already been started by another operator, select **Help > Operator...**.

2 Check that you see a logon dialog box similar to the one shown in Figure 13.

3 Enter your user name and password.

- Remember that the password is case-sensitive.
- See your system administrator if you do not know your password.

4 Click **Log On**.

5 Note that the first time you log on, you will be prompted to change your password. Fill in the form as shown in Figure 14.
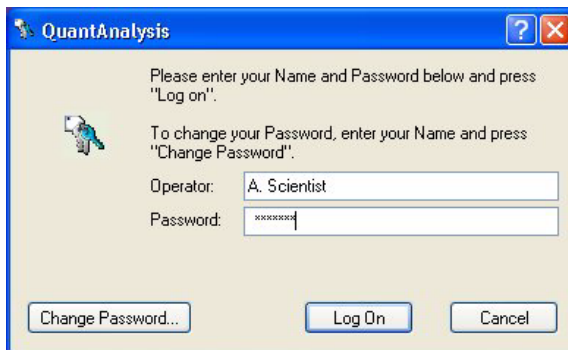
Figure 13   Logging on

To change your password

1 In the logon dialog box (Figure 13 or similar), click **Change Password...**.

2 Fill out the information shown in Figure 14.

3 Click **OK**.

Figure 14   Changing passwords

To view audit trail information for QuantAnalysis

Click the **Show Audit** button in the QuantAnalysis window. See Figure 15. The example shows the **Seqtable.btc** batch file from the **Example Data\QuantAnalysis** directory on the G1330AA Security Pack Software CD.
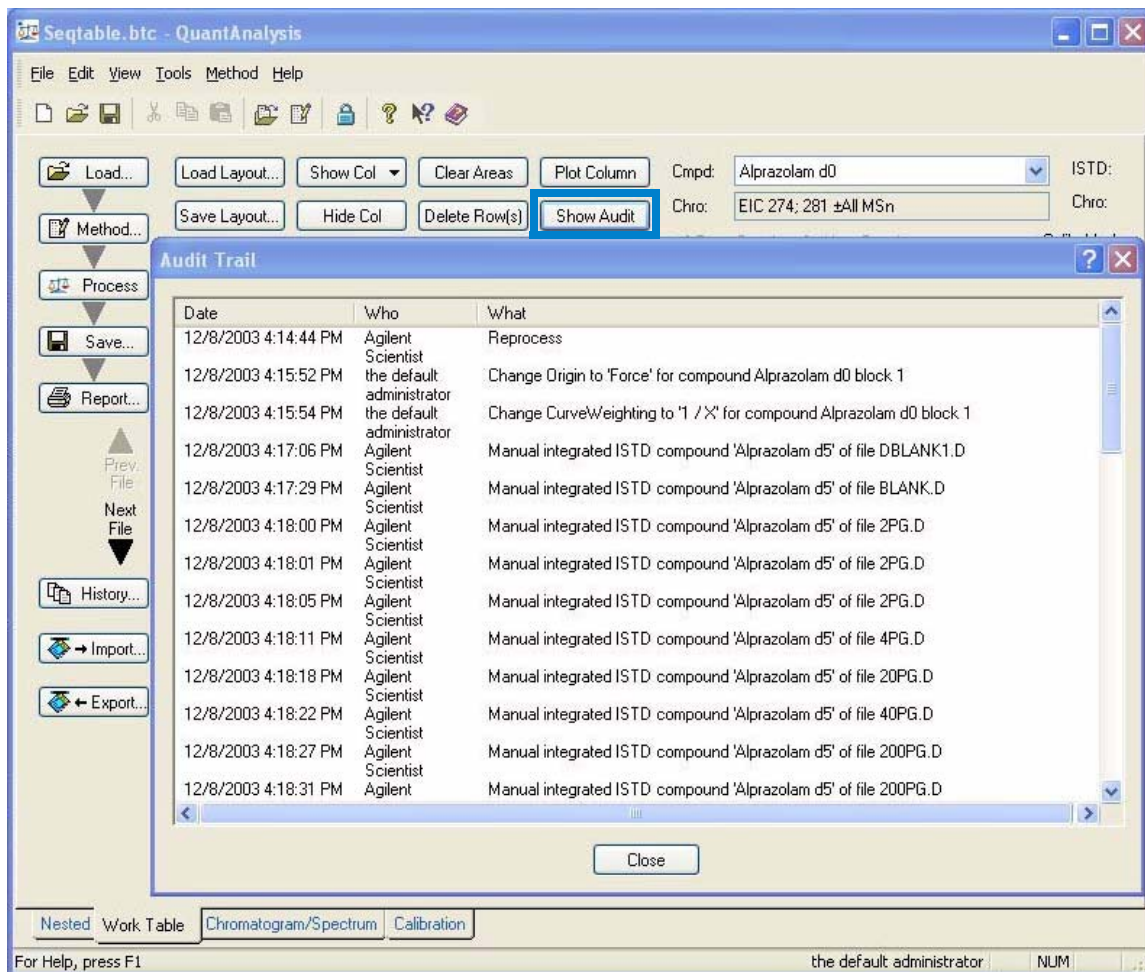
Figure 15   Audit trail in QuantAnalysis

To view other audit trail information

1 From DataAnalysis, select **File > Open** and open a data file. This example uses the **SulfMS01.d** data file from the **Example Data** directory on the G1330AA Security Pack Software CD.

2 Select **File > Audit Trail** to view the audit trail for that data file.

3 Check that you see the **AuditTrailViewer**, as shown in Figure 16.

4 Highlight an entry in the table to view details for that entry (also shown in Figure 16).

5 To view audit trail information for any other analysis or method:

  a Click the **Electronic Record** button at the top of the dialog box.

  b Navigate to the analysis or method and select it.

  c Confirm that you see the audit trail.

6 To view the UserManagement Audit Trail, click the **User Management** button.

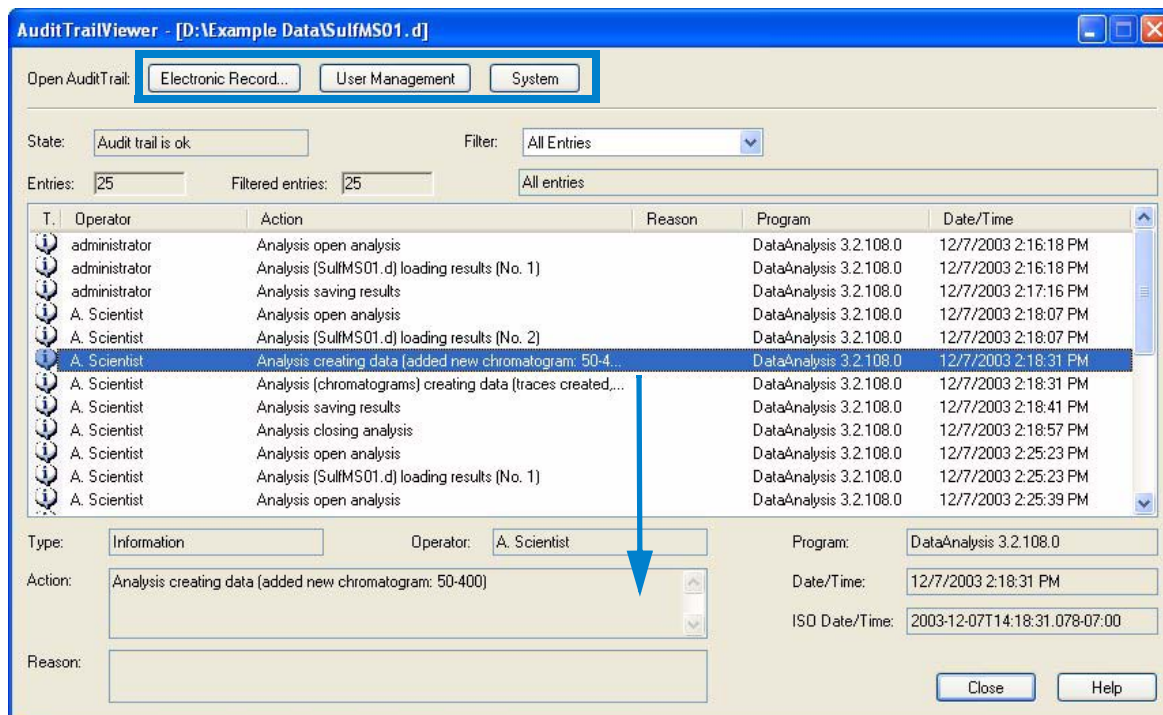**7** To view the System Audit Trail (on-line systems only), click the **System** button.

Figure 16 AuditTrailViewer opened in DataAnalysis

You can also open the **AuditTrailViewer** from the **Start** menu. Click **Start > All Programs > 6300 Series Ion Trap LCMS > Administration > AuditTrailViewer**.

Description of audit trail information

The following table shows the types and locations of audit trail information for the 6300 Series Ion Trap LC/MS system. (This does not include the QuantAnalysis audit trail discussed on .) The first four audit trails are implemented within the Ion Trap LC/MS software, and are accessed as described above. The the last four are implemented within the ChemStation program.

6300 Series and ChemStation audit trail files

Log	Contents	Location
Data log	Operations on the data file, data processing steps	<Data Folder>\AuditTrail.log
Method log	Changes to the method file	<Method Folder>\AuditTrail.log
User Management log	Valid and failed user logons	C:\BDALSystemData\UserAuditTrail\#\AuditTrail.log, where # is a folder named with a long alphanumeric string
System log	Logons, software versions, method loads, license number changes	C:\BDALSystemData\SystemAuditTrail\#\AuditTrail.log, where # is a folder named with a long alphanumeric string
Instrument log	Application-level logging	C:\HPCHEM\1\TEMP\Instr<Instrument #>.log
Sequence log	Sequence-level logging	D:\DATA\<Sequence Folder>\<something>.log
Run log	Run-level logging	D:\DATA\<Data Folder>\Run.log
Module log	State of modules over time	C:\HPCHEM\1\TEMP\<set of files>

To lock and unlock programs

1 From any Ion Trap LC/MS program, click **Help > Lock All Applications**.
2 To unlock, enter your password.
 • Administrators can unlock programs that have been locked by others.

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In this Book

The *Quick Start Guide* introduces you to the 6300 Series Security Pack features that are used for 21 CFR Part 11 compliance.

G3310-90002

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