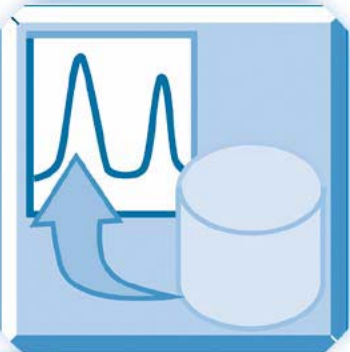


Agilent ChemStation OpenLAB Option



Concepts Guide



Agilent Technologies

Notices

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In This Guide ...

This guide contains installation and reference information for ChemStation OpenLAB Option G2189BA, the ECM interface between Agilent ChemStation and an Agilent Enterprise Content Manager (ECM) client/server system.

1 Introduction

This chapter introduces ECM, the implementation of OpenLAB Option in ChemStation, and the requirements of 21 CFR Part 11.

2 Installation

This chapter describes the installation and configuration of ChemStation OpenLAB Option.

3 Basic Concepts of ChemStation OpenLAB Option

This chapter describes how to log in to ECM in ChemStation, and explains the ECM-related user interface items and toolbars, as well as the main preference settings.

4 Working With ChemStation OpenLAB Option

This chapter describes the basic workflows with ChemStation OpenLAB Option. There are four data-related workflows and two workflows for methods and sequence templates.

5 Administration Regarding 21 CFR Part 11 Compliance

This chapter explains the purpose of 21 CFR Part 11 and its implementation in ChemStation with ChemStation OpenLAB Option.

6 Custom Fields

This chapter explains the purpose and usage of custom fields in ChemStation.

7 Treatment of ChemStation Legacy Data and Data Migrated from ChemStore

This chapter provides information on migrating legacy ChemStation sequence data to sequence container format, in order to be able to upload these data sets to ECM.

8 Interface to OpenLab Intelligence Reporter

This chapter provides information on the integration of OpenLAB Intelligence Reporter in Agilent ChemStation.

9 Attribute Extraction Services for ChemStation Data

This chapter provides an overview of the available ECM Attribute Extraction Services (AES) for ChemStation data. The AES extract metadata information from the ChemStation data files. These metadata make the ChemStation data searchable. For detailed information, refer to the ECM documentation.

10 Using Print Services in ChemStation

This chapter gives a brief overview of how to install and configure the Print Services. This enables you to automatically upload ChemStation reports to ECM in a PDF format.

11 Troubleshooting

The chapter gives some elementary troubleshooting hints.

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This chapter introduces ECM, the implementation of OpenLAB Option in ChemStation, and the requirements of 21 CFR Part 11.



What is ECM?

The Agilent Enterprise Content Manager (ECM) is a web-based electronic library that allows you to safely archive and catalog any electronic file. ECM allows you to store and index analytical raw data, reports, and all other types of documents. The stored files can be shared with other users.

You can store any electronic file type, such as Microsoft Office documents, Adobe PDF documents, images, and molecular drawings, as well as raw data and reports generated by ChemStation.

ECM allows you to easily collect, organize, search, and review all of your data. It automatically extracts searchable metadata from files, and provides powerful search capabilities. In addition, ECM provides embedded viewers for many file types.

The ECM interface is opened via Microsoft Internet Explorer, also referred to as the ECM Web Client.

Add-On Solution for ChemStation: OpenLAB Option

Starting with revision B.02.01 SR1, Agilent ChemStation provides an interface to the Agilent Enterprise Content Manager (ECM), which enables you to store analytical data and reports in a secure location. From ChemStation, you can log in to ECM and store methods, sequence templates, data files, and reports in ECM. Data storage can be either automatic (that is, at the end of a single run or sequence) or manual. ChemStation data stored in ECM can later be downloaded to ChemStation for review or reprocessing at any time.

Furthermore, ChemStation OpenLAB Option offers features that enable users to comply with 21 CFR Part 11 and similar regulations for electronic records and electronic signatures:

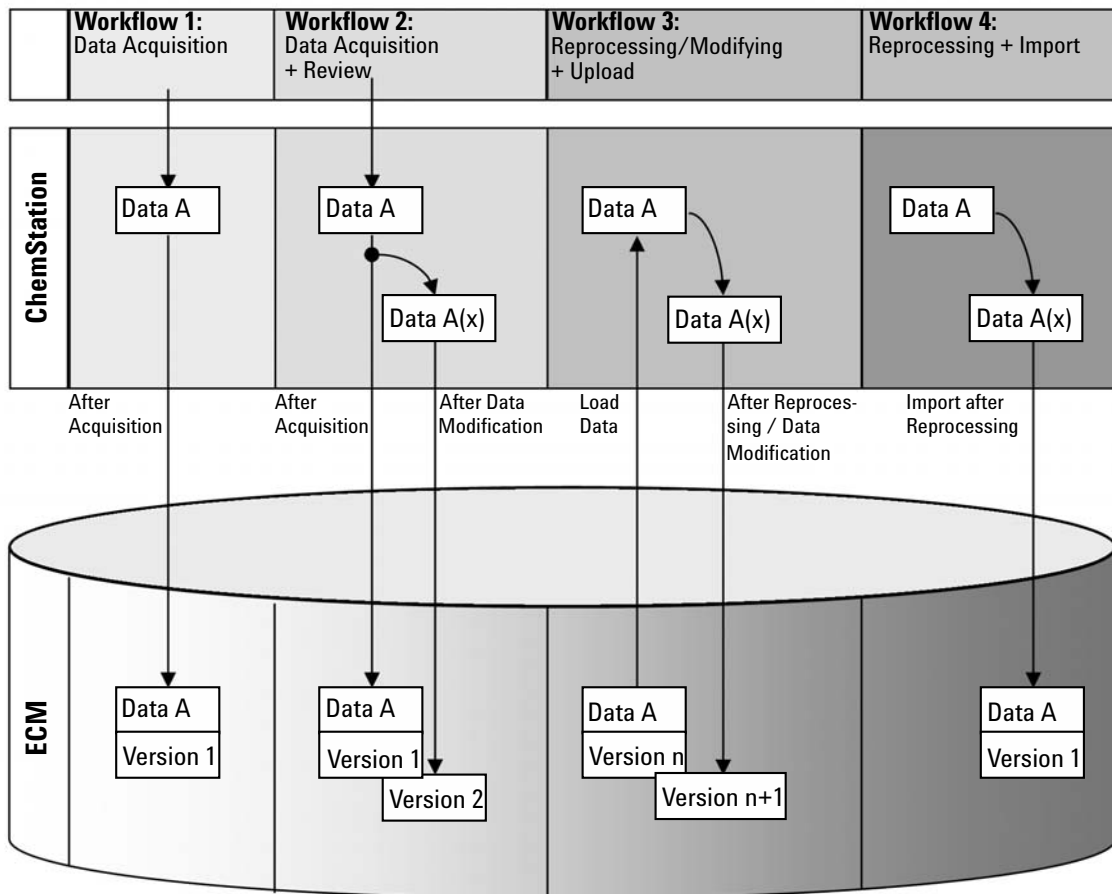
- Mandatory login/connection to ECM
- Configurable session locking
- Configurable ChemStation user roles and privileges
- Full data traceability through audit trails for methods and results
- Full data versioning

ChemStation OpenLAB Option requires the following components:

- ECM Server
- ChemStation OpenLAB Option installed on the ECM Server
- ECM Web Client installed on the ChemStation computer
- ChemStation with ChemStation OpenLAB Option installed on the ChemStation computer
- Connection between the ChemStation computer and the ECM Server

The main workflows for the transfer of raw data and methods/sequence templates are listed below. These workflows indicate the system activities in relation to the work processes.

Overview of data-related workflows



Workflow 1: Raw data acquisition and automatic transfer to ECM

- 1 Analytical raw data is acquired using ChemStation.
- 2 The raw data is automatically uploaded to ECM using the configured path definitions immediately after the single run/sequence is finished.
- 3 A new ECM data set is created in the defined ECM location.

Workflow 2: Offline revision during acquisition

- 1 Analytical raw data is acquired using ChemStation.
- 2 While the acquisition is still running, part of the data is changed using an offline ChemStation.
- 3 The raw data is automatically uploaded to ECM using the configured path definitions immediately after the single run/sequence is finished.
A new ECM data set is created in the defined ECM location.
- 4 After work in the offline ChemStation is finished, the changed data is also automatically uploaded to ECM.
Another new version of the ECM data set is created.

Workflow 3: Reprocessing data and automatic upload to ECM

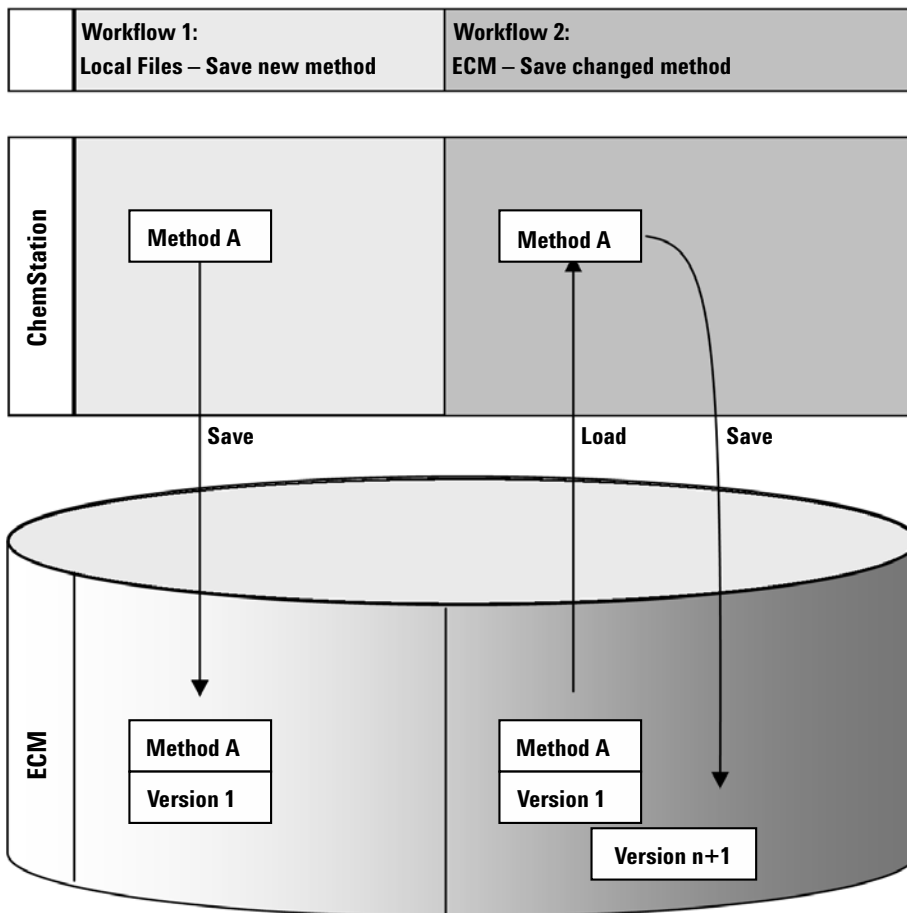
- 1 Existing analytical data is loaded from ECM into ChemStation.
- 2 The data is reprocessed in ChemStation.
- 3 The data is automatically uploaded to ECM. The location in ECM is defined by the original path definitions of the downloaded ECM data.
- 4 A new version of the data is created in ECM.

Workflow 4: Import after reprocessing

- 1 Existing analytical data is opened locally.
- 2 The data is reprocessed in ChemStation.
- 3 After reprocessing, the data is automatically uploaded to ECM. The location in ECM is defined by the current preferences in ChemStation.
- 4 A new version of the data is created in ECM.

For more details, and for additional workflows, refer to [“Data-related workflows”](#) on page 59

Overview of workflows for methods/sequence templates



Workflow 1: Uploading a new method

- 1 A new method or sequence template is created.
- 2 The method or sequence template is uploaded to ECM using the path selected by the user.
- 3 The version 1 of the method or sequence template is automatically created in ECM.

Workflow 2: Saving a changed method

- 1 An existing method or sequence template is loaded from ECM.
- 2 The changed method or sequence template is saved to ECM.
- 3 A new version of the method or sequence template is automatically created in ECM.

For more details, and for additional workflows, refer to [“Workflows for Methods and Sequence Templates”](#) on page 70

Data Storage in ECM

ECM provides a four-level data storage model with the structure of Location, Cabinet, Drawer, Folder. The Location, Cabinet, Drawer and Folder names comprise the path name (called either LCDF path or Remote Data Path) of the storage location. Data is stored at Folder level only.

The ECM program's content structure is similar to rooms filled with file cabinets. Each cabinet has multiple drawers, which then contain hanging folders. Finally, paper files are stored in the folders. The LCDF structure can be created using the ECM Web Client. In addition, it is possible to create additional Locations, Cabinets, Drawers, and Folders using the ChemStation Remote Data Path. In ChemStation, it is also possible to set predefined tokens for the Drawers and Folders.

In the ECM tree view, locations are denoted by a house icon. Inside each Location, Cabinets are denoted by the file cabinet icon. Inside each Cabinet, Drawers are denoted by the drawer icon. Finally, inside each Drawer, Folders are denoted by the folder icon. The entire content structure appears in the Content book.

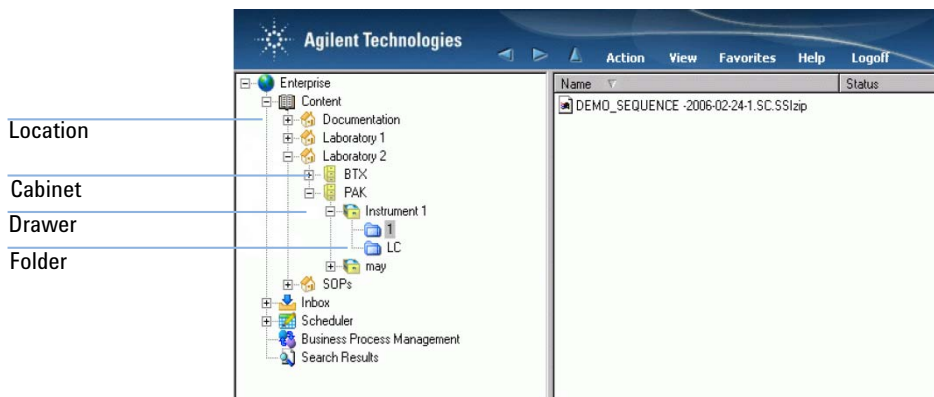


Figure 1 LCDF structure in ECM

Uploaded objects can be stored in the lowest (i.e. Folder) level only. It is not possible to upload data to other levels of the hierarchy.

21 CFR Part 11 Compliance

Effective August 20, 1997, the U.S. Food and Drug Administration (FDA) released and published a new rule to enable pharmaceutical companies to approve their results with electronic signatures and to transfer paper-trail documentation into electronic records. This rule is known as 21 Code of Federal Regulations Part 11 (referred to as 21 CFR Part 11) and applies to all industry segments regulated by the FDA.

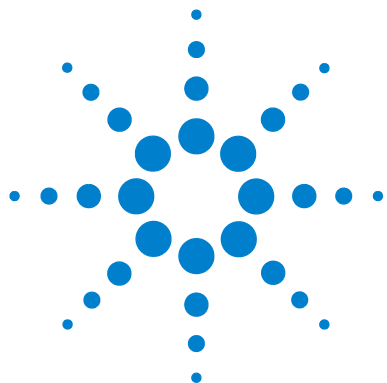
21 CFR Part 11 includes the US Federal guidelines for storing and protecting electronic records and applying electronic signatures. The intent of these guidelines is to ensure that electronic records subject to these guidelines are reliable, authentic, and maintained with high integrity.

ChemStation OpenLAB Option with ChemStation B.04.xx provides the necessary controls for managing system access, audit trail functions, versioning of ChemStation data, and electronic signature functions. Agilent OpenLAB ECM ensures secure record keeping and data archival. Agilent OpenLAB ECM is proven and has been deployed at many leading life sciences companies to satisfy compliance mandates for 21 CFR Part 11.

1

Introduction

21 CFR Part 11 Compliance



2 Installation

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This chapter describes the installation and configuration of ChemStation OpenLAB Option.



Prerequisites

Before you install Agilent ChemStation OpenLAB Option, make sure that the following prerequisites are met:

- The ECM Server software must be installed and configured as described in the *Enterprise Content Manager Installation Guide*. All server-related prerequisites, as well as the installation and configuration details, are described in the guide.

The ECM versions supported with ChemStation are:

- OpenLAB ECM Workgroup 3.3.1 - MS SQL Server 2005, with ECM 3.3.1 Hotfixes 1-5,
- OpenLAB ECM Enterprise with ECM 3.3.1 Hotfixes 31, 45, 47-54, 56-57, 59, and 70,
- OpenLAB ECM Workgroup 3.3.2 SP1 - MS SQL Server 2005,
- OpenLAB ECM Enterprise 3.3.2 SP1 - MS SQL Server 2005, or
- OpenLAB ECM Enterprise 3.3.2 SP1 - Oracle 10.2.0.1 or Oracle database server 10.2.0.4 with Oracle client 10.2.0.1
- Ensure that the minimum PC and operating requirements are met for ChemStation. Details can be found in the *Installing your ChemStation* manual for your respective instrument.
- Setting up the connection from ChemStation to the ECM Server requires the address of the ECM Server.

Compatibility

ChemStation Add-Ons

ChemStation OpenLAB Option is not supported in combination with the following ChemStation Add-Ons and features:

- ChemStore / Security Pack
- Purify
- Easy Access
- ChemStation **Unique Folder Creation OFF** (item is not accessible)

Installation and Configuration Tasks on ECM Server

You must execute the database script for ChemStation privileges on the ECM Server to implement ChemStation related users, roles and privileges within OpenLAB ECM. In addition, after installing the program, you must take care of several ECM settings.

Updating the ECM Database

A database script is provided on the *ChemStation DVD* that creates specific ChemStation privileges and ChemStation roles in ECM. The procedure depends on the ECM Database type (Oracle or SQLServer).

Prerequisites

You need the login data of the following users:

- A Windows user who can connect to the ECM Database.
- An ECM Database user who is authorized to access the ECM schema and to update the tables in this schema.

To update an Oracle ECM Database

- 1 Log on to a Windows computer that has *SQLPlus* installed.
- 2 Insert the *ChemStation DVD* in your DVD drive. Navigate to the folder ECM-DatabaseScript\Oracle.
- 3 If you have the password for the database user SYS, execute InstallOracle.cmd. Otherwise, execute InstallOracleNonSYS.cmd.
A command window opens.
- 4 You are prompted to enter several parameters. Type in the required data and press **Enter** to confirm each entry:
 - **Database name (host string):** The host string for your ECM Database.
 - **User name:** A user name is only requested if you executed InstallOracleNonSYS.cmd.

- **Path and filename of the log file:** An installation log file is created in the given location.
 - **Password for database user:** The password is not shown while typing.
 - **Schema/user name for ECM**
 - **Directories** where the data files, index files, and map files of the new database schema should be stored.
- 5 Review the data.
 - If something is wrong: press **Ctrl+C** to abort the installation.
 - 6 If everything is OK: Press **Enter**.
The installation begins. When the installation is finished, the text **Installation finished** is shown in the command window.
 - 7 Press any key to close the command window.
 - 8 Check the installation log file. It should only include messages about changing the database, no warnings or errors.

To update an SQLServer ECM Database

- 1 Log on to a client that has *SQLCmd* installed.
- 2 Insert the *ChemStation DVD* in your CD-ROM drive. Navigate to the folder EMC-DatabaseScript\SQLServer.
- 3 If you have the password for the database user SA, execute InstallSQL.cmd. Otherwise, execute InstallSQLNonSA.cmd.
A command window opens.
- 4 You are prompted to enter several parameters. Type in the required data and press **Enter** to confirm each entry:
 - **ECM Database Server:** Server name of the ECM Database Server.
 - **ECM Database Name**
 - **Database User Name:** Normally:
CYBERLABLOGIN
 - **Directory and Name for log file:** An installation log file is created in the given location.
- 5 Review the data.
 - If something is wrong: press **Ctrl+C** to abort the installation.

- 6 If everything is OK: Enter the password for the database user you provided before.

The installation begins. When the installation is finished, the text **Installation finished** is shown in the command window.

- 7 Press any key to close the command window.
- 8 Check the installation log file. It should only include messages about changing the database, no warnings or errors.

Updating roles in existing ECM Accounts

When updating the ECM Database, certain specific ChemStation roles and privileges have been created. If you create a new ECM Account, these roles and their privileges are automatically available in that new account. However, if you want to use ChemStation OpenLAB Option with an existing ECM Account, you must first update the roles in that specific account. The new ChemStation roles and their privileges will be available only after updating the roles for the existing account.

To make the new roles and privileges available in an ECM Account

NOTE

All system roles will be reset to default when performing **Reset Role**. If you made manual changes to a system role, these changes will be lost!

All other roles that were created manually will be deleted!

- 1 Open a browser window and connect to the ECM Web Server.
- 2 Log in to the ECM Account in which you want to update the roles.
- 3 Select the **Administration** tab.
- 4 Click **Account Administration**.
- 5 Double-click **Users / Groups / Roles**.
The **Account Administration** dialog opens.
- 6 Select the **Roles** tab.
- 7 Click **Reset Roles**.

The default ChemStation roles and the according ChemStation privileges (see [“ChemStation Roles in ECM”](#) on page 153) are now available in the current account and can be assigned to the users.

NOTE

The default ChemStation roles do not contain any ECM privileges! A ChemStation user who wants to access ECM must additionally be assigned the required ECM roles (see [“Assigning roles”](#) on page 26 and [“ECM related privileges concerning the ChemStation configuration”](#) on page 157).

Configuring users, roles and privileges

Concept of users, roles, and privileges

In ECM, you can either create specific ECM users or operate with the Windows users. Each user can be member of a specific group. The available groups depend on the ECM configuration.

You must assign a specific ECM role to each group. You can also assign roles to single users, however, for the sake of clarity, it is strongly recommended to assign roles only on the group level.

The roles are equipped with numerous specific privileges, which define what the users are allowed to view or do in ECM and in ChemStation.

NOTE

Once you created a new ECM user, group, or role, you can not delete it again. You can only deactivate the unused item.

Default roles and privileges

There are a number of default roles and privileges in ECM that are created during the installation of ECM and ChemStation OpenLAB Option. The following tables show an overview of these roles and privileges.

Name	Description
• Starting with “:CS”	Default ChemStation role. Can be restored by the Reset Roles function.
• Starting with “:”	Default ECM role. Can be restored by the Reset Roles function.

2 Installation

Installation and Configuration Tasks on ECM Server

Name	Description
• Starting with “ CS: ”	Privilege related to ChemStation For details on the ChemStation privileges, see “ Appendix ” on page 149.
• Starting with “ Content: ”	Privilege related to ECM
• Starting with “ System: ”	Privilege related to ECM

In addition, you can create your own roles in ECM, or grant further privileges to the default roles. For detailed information, refer to the ECM Administrator’s Guide.

Assigning roles

Users do not need any specific role in order to log in to ECM. However, in order for users to see a particular Location, Cabinet, Drawer, or Folder in the user interface, they must have the **:Reader** role as a minimum requirement. As a result, domain users with no global roles might not be able to view anything in the content unless they were granted the appropriate privileges.

You should grant the users of the ChemStation OpenLAB Option the **:Contributor** role. This can be done at the global level for the entire ECM Account, or individually for specific folders (see “[Roles and folders](#)” on page 91). The **:Contributor** role allows the ChemStation OpenLAB Option user to view and add content to ECM. The **:Contributor** role should be enhanced with the **Content: Add Folder** privilege. This allows ChemStation ECM users to add folders to the LCDF hierarchy.

NOTE

If the role does not include the **Add Folder** privilege, the users cannot add a new Remote Data Path (LCDF) in ChemStation.

In addition to the ECM roles, user of ChemStation OpenLAB Option must be assigned at least one of the ChemStation roles or another, customized role with according ChemStation privileges. You find a complete list of all ChemStation roles and all relevant privileges in the Appendix.

NOTE

If a ChemStation user has no ChemStation privileges in ECM, this user is not able to work with ChemStation OpenLAB Option!

Installation Tasks on the ChemStation Computer

ChemStation OpenLAB Option (G2189BA) is a separate installation package delivered on the *ChemStation DVD*. It can be initially installed with the ChemStation software, or added to an existing ChemStation. After installation, ChemStation OpenLAB Option is available for all ChemStation instances installed on the particular client PC.

Preparing the ECM Web Client

Preparations

You need to make sure there is an up-to-date version of the ECM Web Client installed on the ChemStation computer.

NOTE

If you use *Windows Vista*: Make sure the **User Account Control** feature is disabled before you connect to ECM!

To prepare the ECM Web Client

- 1 On the ChemStation computer: Open a browser window and connect to the ECM Web Server.
- 2 Log in to ECM.

All relevant hotfixes are automatically installed. You may be asked to restart the ChemStation computer during the installation.

Installing a new ChemStation with ChemStation OpenLAB Option

Before installing the software, verify that all prerequisites are met (see [“Prerequisites”](#) on page 20).

The installation is divided in the following steps:

- Installing the ECM API
- Installing ChemStation
- Adding instruments
- Providing license keys
- Configuring instruments

To install the ECM API

- 1 Insert the *ChemStation DVD* into the DVD drive.
- 2 In Windows Explorer, navigate to the folder [diskdrive]:\ECMAPI and double-click the file ECMAPIDeploy.mci.

The Agilent OpenLAB ECM API Installation wizard Opens.

- 3 Click **Next**.

- 4 Enter User Name and Organization. Select the option to install the API for **"Anyone who uses this computer (all users)"**. Click **Next**.
- 5 Select a destination folder where you want to install the ECM API (the default folder is C:\Program Files\Agilent Technologies\ECM API\1.0.24.1). Click **Next**.
- 6 Click **Install**.
- 7 After the installation has completed, click **Finish**.

To install ChemStation

- 1 Insert the *ChemStation DVD* into the DVD drive.
- 2 From the Start menu in the Task Bar, select **Start > Run**.
- 3 At the command line, type
[diskdrive] : \Setup For example: D:\Setup
The setup software checks if the following software components are available:
 - Microsoft .NET Framework 3.5 SP1
 - PDF-XChange 4.0
- 4 If there are missing components, additional dialogs open to install these components. Click **Install** to install the missing components. For the Microsoft .NET Framework also read and agree to the License Agreement.
After the missing components have been installed, the **Agilent ChemStation Setup Wizard** opens.
- 5 Click **Next**.
- 6 Select the check box to confirm the license agreement. Click **Next**.
- 7 Select a destination folder where you want to install the new ChemStation (the default folder is C:\Chem32). Click **Next**.
- 8 Click **Install**.
ChemStation is now being installed. This can take several minutes.
- 9 Click **Finish**.
The **Setup Wizard - Instruments** dialog opens. Proceed now with adding the instruments.

To add instruments

- 1 In the **Setup Wizard - Instruments** dialog, click the **Add** buttons to add the required instruments.

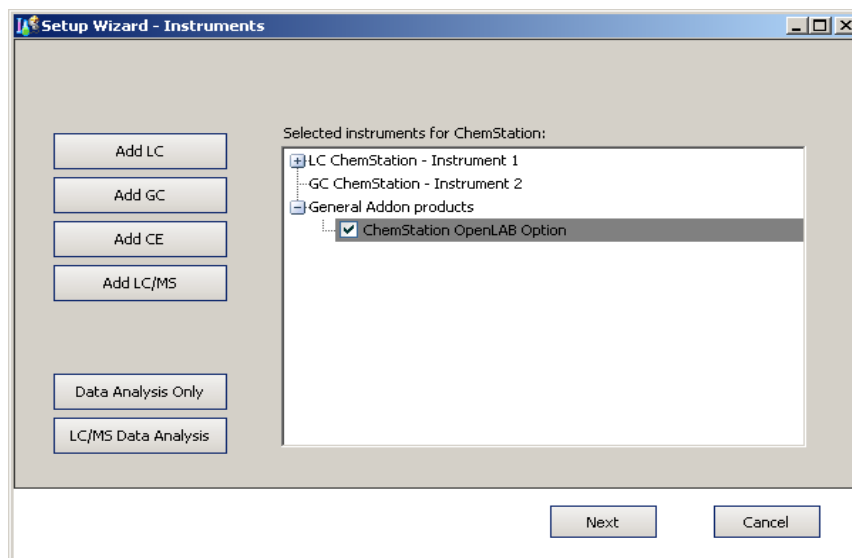


Figure 2 Setup Wizard - Instruments

- 2 Under **General Addon products**, select the **ChemStation OpenLAB Option** check box.
- 3 Click **Next**.
The **Setup Wizard - Licenses** dialog opens.
- 4 Proceed now with providing the license keys.

To provide license keys

- 1 In the **Setup Wizard - Licenses** dialog, enter a valid license key for ChemStation OpenLAB Option in the input field at the bottom.

NOTE

The applicable license product and license numbers are printed on your Software Certificate and Registration Packet.

NOTE

Note that any Windows user with administrative privileges can remove the G2189BA OpenLAB Option license and thus disable OpenLAB Option functionality from the ChemStation. It is therefore recommended that in a regulated environment ChemStation users work as Windows Users or Powerusers.

- 2 Click **Add** to add the license key to the list.
- 3 Provide valid license keys accordingly for all of the instruments shown in the list.

The software automatically recognizes which license is valid for which module.

- 4 Click **Next**.

The **ChemStation Administration Tool** dialog opens.

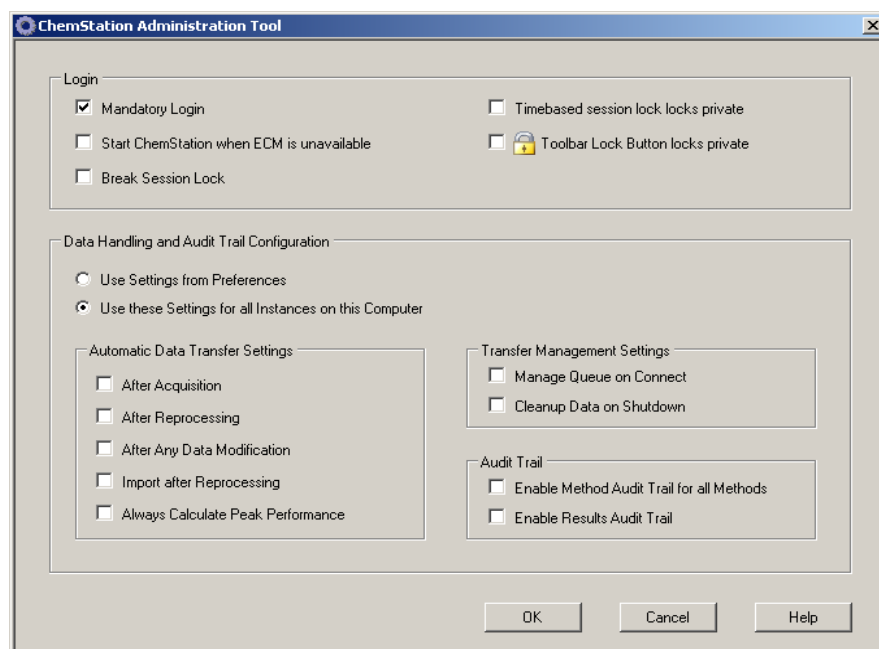


Figure 3 ChemStation Administration Tool

2 Installation

Installation Tasks on the ChemStation Computer

- 5 Select or clear the **Mandatory Login** check box, depending on whether the ECM login should be mandatory or optional in ChemStation (the settings will be used for all ChemStation instances that are installed on this computer). For more details on the login functions see [“User Permissions”](#) on page 38.

NOTE

You do not need to configure the other options in this dialog during the installation. You can configure these items anytime in ChemStation (see [“ECM Preferences”](#) on page 44 and [“Audit Trails and Logbooks”](#) on page 84) or by using the ChemStation Administration Tool directly (see [“ChemStation Administration Tool”](#) on page 92).

- 6 Click **OK**.
- 7 Click **Finish**.
The Configuration Editor opens.
- 8 Proceed now with configuring the instruments.

To configure instruments

You can configure the instruments in the Configuration Editor. For details see the manual *Installing your ChemStation*.

After the successful installation, ChemStation contains the new **ECM** menu and a number of other ECM interface elements (see [“Overview of new interface elements”](#) on page 41).

Adding ChemStation OpenLAB Option to an existing ChemStation

To add ChemStation OpenLAB Option subsequently

- 1 From the Start menu in the Task Bar, select **Start > All Programs > Agilent ChemStation > Add instrument**.
The **Setup Wizard - Instruments** dialog opens (see [Figure 2](#) on page 30).
- 2 Under **General Addon products**, select the **ChemStation OpenLAB Option** check box.
- 3 Click **Next**.
The **Setup Wizard - Licenses** dialog opens.

- 4** Enter a valid license key for ChemStation OpenLAB Option in the input field at the bottom.
- 5** Click **Add** to add the license key to the list.
- 6** Click **Next**.
The **ChemStation Administration Tool** dialog opens (see [Figure 3](#) on page 31).
- 7** Select or clear the check box **Mandatory Login**, depending on whether the ECM login should be mandatory or optional in all ChemStation instances on this computer.
- 8** Click **OK**.
- 9** Click **Finish**.
The Configuration Editor opens. As you have already configured the instruments, and have now added the OpenLAB Option, you can exit the Configuration Editor without any further actions.
- 10** Prepare the ECM Web Client and install the ECM API as described in [“Preparing the ECM Web Client”](#) on page 28.

Enabling users to start the ChemStation Administration Tool

The ChemStation Administration Tool is automatically installed as a part of ChemStation OpenLAB Option during the procedure described above.

The ChemStation Administration Tool offers you to change the transfer settings (see [“Automatic Data Transfer Settings”](#) on page 47) for all ChemStation instances on a computer in a single step. In addition, there are a number of functions which are helpful if the connection from the ChemStation client to the ECM Server is lost. As one of these functions is to switch off the mandatory ECM login, access to the ChemStation Administration Tool must be strictly limited.

During the Installation of ChemStation OpenLAB Option, the local user group **CSAdministrators** is automatically created. Only members of this group are allowed to run the ChemStation Administration Tool. The user who installs ChemStation, is automatically added to the **CSAdministrators** group. Additionally, the Windows group **Administrators** and the user who installs ChemStation are granted Full Control privileges on the Administration Tool program executable (Agilent.ChemStation.ECM.ECMAdmin.exe) itself, thus they are able to run the tool.

2 Installation

Installation Tasks on the ChemStation Computer

NOTE

See “[Administration of ChemStation Settings](#)” on page 92 for more details on the ChemStation Administration Tool.

To add a Windows user to the CSAdministrators group:

- 1 From the Start menu in the Task Bar, select **Start > Settings > Control Panel > Administrative Tools > Computer Management**.

The **Computer Management** window opens.

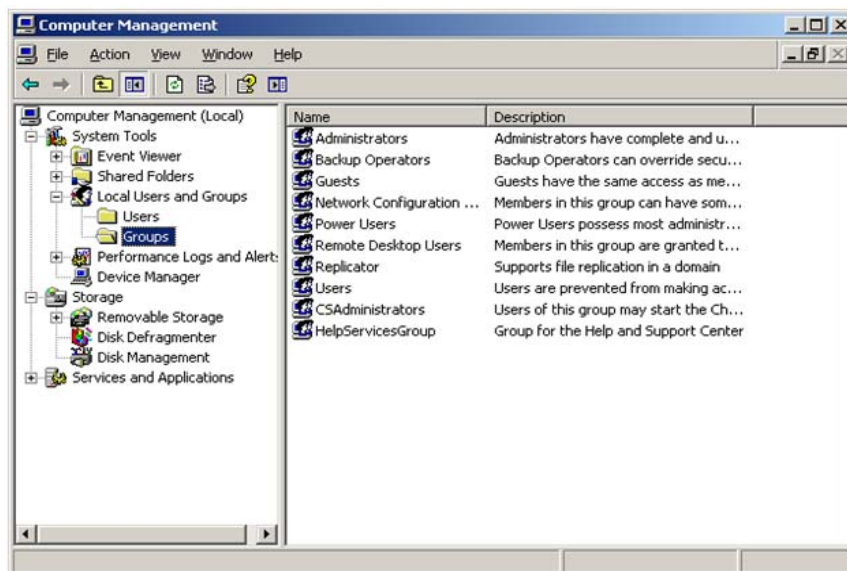
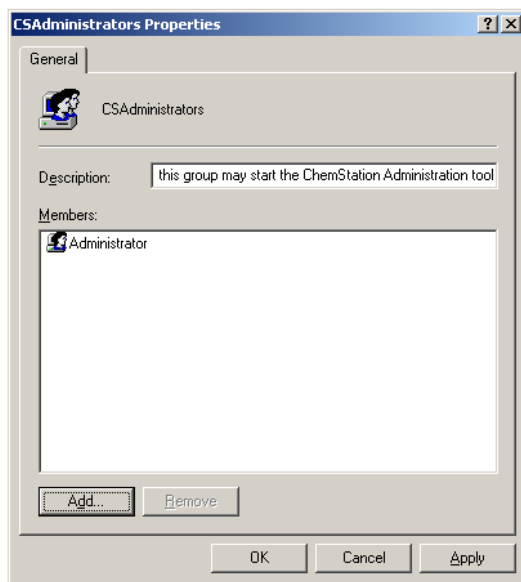


Figure 4 Computer Management window

- 2 Right-click the group **CSAdministrator** and select **Add to Group...** from the context menu.

The **Properties** dialog shows the users who are currently member of the group.



- 3 Use the **Add** button to add the required users.

After confirming with **OK**, the **Properties** dialog also contains the newly added users.

Uninstallation

To uninstall Agilent ChemStation

Windows XP:

- 1 From the Start menu in the Task Bar, select **Start > Settings > Control Panel > Add or Remove Programs**.
- 2 Select the **Agilent ChemStation** program and click **Remove**.
- 3 When asked for confirmation, click **Yes**.

To uninstall Agilent ChemStation

Windows Vista:

- 1 From the Start menu in the Task Bar, select **Start > Control Panel > Programs > Programs and Features**.
- 2 Select the **Agilent ChemStation** program and click **Uninstall**.
- 3 When asked for confirmation, click **Yes**.

The program is uninstalled. All files of the ChemStation folder (by default: C:\chem32) are removed. Only files that have been modified by the user (for example, methods, sequence templates, or data files) are not deleted.

To uninstall other ChemStation components

During the installation of ChemStation, a few additional components were installed. You can remove these components using the **Add or Remove Programs** function, with which you can also remove ChemStation.

The following components may have been installed together with ChemStation:

- PDF-XChange 4.0
- Microsoft .NET Framework 3.5 SP1



3 Basic Concepts of ChemStation OpenLAB Option

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This chapter describes how to log in to ECM in ChemStation, and explains the ECM-related user interface items and toolbars, as well as the main preference settings.



User Permissions

Log In/Log Out

To prevent unauthorized access to ECM or unauthorized use of ChemStation OpenLAB Option, ECM requires authentication with a user name and password. In addition, each user needs user privileges defining the accessible content.

The user administration is set up and managed on the ECM Server. For more details about login and user setup refer to the ECM User/Administrator's Guide.

Optional or mandatory

Depending on the configuration during the installation of ChemStation, the ECM login can be optional or mandatory. If it is mandatory, you must log in to ECM during the ChemStation startup. If it is optional, you can initially skip the login and then log in to ECM later.

If you are already logged in to ECM server in the online instrument session and start the offline session via the item **Reprocessing Copy** from the **View** menu, the user will be automatically connected to ECM with the same login information (silent login).

If you are not connected to ECM, all of the ECM functions are grayed out.

You can log in to ECM from the following ChemStation views:

- Method and Run Control
- Data Analysis

Once you have logged in to ECM, it is possible to upload data to ECM and simultaneously work on the local ChemStation file system.

The login is dependent on the instrument session; only one user can be logged in to ECM at any one time. If another user wants to log in, you must first log out.

User credentials

The **Login** dialog requires you to enter a set of valid authorization details in order to log in to ECM. The login information is ECM Server-specific and will be provided by the ECM administrator.

You need to enter the following login details:

- **Server URL:** the URL of the ECM Server
- **Account:** you can store content to the locations assigned in the specific account; one ECM Server may have several accounts.
- **Username:** the user name defined in the ECM Account, or your NT domain user name (depending on the user configuration in ECM)
- **Password:** the password provided by your administrator, which can be changed on request (for ECM 'built-in' users), or the password of your NT domain account, if you are logging in using your NT domain user name.
- **Log on to:** the domain administrating the ECM users

ChemStation Operator and ECM User

If you log in to ECM and have been authorized by the ECM system, the ChemStation operator name in the sample info (when running single samples) or the sequence parameters (when running a sequence) is overwritten by your ECM user name.

As long a user is logged on to ECM, the operator name is given by the ECM logon and cannot be overwritten. As soon as you log out of ECM, the ChemStation operator name defined by the ECM is removed, and is replaced by the entry "disconnected". While acquiring data to ECM, it is not possible either to log in or to log out of ECM. This prevents the operator name from being changed during data acquisition.

Session lock

If you leave the ChemStation computer for a certain period of time, you can lock ChemStation so that no other user can access the program. This is a safety feature to ensure that there is no unauthorized access to ChemStation. When you activate the session lock, you or another user must first provide a valid ECM login before continuing to work with ChemStation.

There are the following options to activate the session lock:




- *Privately* (**ECM > Lock Session > privately**): Only the user who activated the session lock, or a user with the **CS: Break Session Lock** privilege, can log in.
- *Non privately* (**ECM > Lock Session > non privately**): Any valid ECM user can log in. This is useful, for example, if there is a shift change, and the leaving personnel secures ChemStation until the personnel of the new shift starts work.
- *Toolbar Lock Button*: The toolbar lock button can be configured to lock the ChemStation session privately or non privately (see [“Login options”](#) on page 93).
- *Time based*: Depending on the ECM Account configuration, ChemStation is automatically locked after a given period of time without any user interaction (see **Inactivity Timeout** under [“Administration in ECM”](#) on page 89). If there is no activity in an ECM Web Client, the ECM Web Client is also locked after the given period of time. ChemStation and ECM Web Client are locked independently from each other.

The time based session lock can be configured to lock the ChemStation session either privately or non privately (see [“Login options”](#) on page 93).

OpenLAB Option User Interface in ChemStation

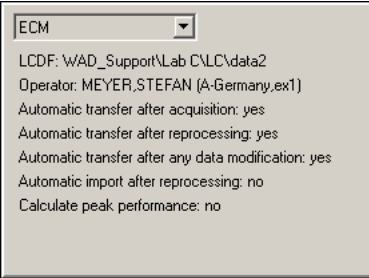
Overview of new interface elements

With the installation of ChemStation OpenLAB Option, the following new menus, menu items, and interface elements are available:

Menu	New elements	Description
Method	New command <ul style="list-style-type: none"> • Enable Audit Trail 	See “Method Audit Trail” on page 84
Sequence > Sequence Parameters, Sequence Parameters tab	New fields on the Sequence Parameters tab: <ul style="list-style-type: none"> • Remote Data Path 	See “Remote Data Path as Sequence Parameters” on page 54
Sequence > Sequence Parameters, Sequence Output tab	New fields on the Sequence Output tab: <ul style="list-style-type: none"> • OpenLAB Intelligence Reporter Template 	See “Template selection in Sequence Output” on page 124
Report	New command <ul style="list-style-type: none"> • Report History 	See “Report History” on page 86
View > Preferences 	New tabs in the Preferences dialog: <ul style="list-style-type: none"> • Transfer Settings • Audit Trail 	See “ECM Preferences” on page 44 and “Audit Trails and Logbooks” on page 84
ECM	Completely new menu	See “The ECM menu” on page 42
Toolbar (depending on the current view)  	<ul style="list-style-type: none"> • Shortcuts to several commands of the ECM menu • LCDF info 	<ul style="list-style-type: none"> • LCDF info in the Data Analysis view: shows the LCDF path of a file that has been stored to ECM. • LCDF info in the Method and Run Control view: drop down list showing the last ten LCDF paths as defined in the Preferences if the automatic upload After Acquisition is selected.

3 Basic Concepts of ChemStation OpenLAB Option

OpenLAB Option User Interface in ChemStation




Menu	New elements	Description
ECM related details in the System Diagram in Method and Run Control view (classic UI only).	Completely new details view	The following details are available: <ul style="list-style-type: none"> • LCDF • Operator • Automatic transfer after acquisition • Automatic transfer after reprocessing • Automatic transfer after any data modification • Automatic import after reprocessing • Calculate peak performance
		










The ECM menu

The **ECM** menu and its commands depend on the view that is currently active. See the following table for details.

NOTE

There is no **ECM** menu in the **Report Layout**, **Verification (OQ/PV)**, or **Diagnosis** view.

Command	Description	Available in ChemStation views
User-related commands:	See “User Permissions” on page 38 and “Session lock” on page 40.	<ul style="list-style-type: none"> • Method and Run Control • Data Analysis
 Log In ...  Log out Change User ...  Lock Session		
Update-commands: Update Methods ... Update Sequences Templates ...	Update all methods/sequence templates that are stored in the local file system with the current version from ECM (if existing in ECM). Local changes are overwritten.	<ul style="list-style-type: none"> • Method and Run Control

Command	Description	Available in ChemStation views
Cleanup Data	The Cleanup Data command deletes all data or sequence containers from the local file system that exist in ECM as well. Make sure you uploaded the latest version to ECM before you confirm this command. See “Cleanup Data on Shutdown” on page 49.	<ul style="list-style-type: none"> • Data Analysis
Manage Queue	With the Manage Queue command you can continue any interrupted data upload to ECM. See “Manage Queue on Connect” on page 49.	<ul style="list-style-type: none"> • Method and Run Control • Data Analysis
 Preferences	See “ECM Preferences” on page 44 for more details on the Preferences dialog.	<ul style="list-style-type: none"> • Method and Run Control • Data Analysis
Method-related commands:	See “Workflows for Methods and Sequence Templates” on page 70	<ul style="list-style-type: none"> • Method and Run Control • Data Analysis
 Load Method ...		
 Save Method		
Data-related commands:	See “Data-related workflows” on page 59	<ul style="list-style-type: none"> • Data Analysis
 Load Data ...		
 Save Data		
Save Data As ...		
Commands related to the sequence template:	See “Workflows for Methods and Sequence Templates” on page 70	<ul style="list-style-type: none"> • Method and Run Control
 Load Sequence Template ...		
 Save Sequence Template		
Commands related to OpenLAB Intelligence Reporter:	See “Interface Components Concerning OpenLAB IR” on page 124	<ul style="list-style-type: none"> • Data Analysis
 Start OpenLAB IR		
 Create OpenLAB IR Report		

ECM Preferences

The **Preferences** dialog contains two tabs that are relevant to ChemStation OpenLAB Option: the **Transfer Settings** tab and the **Audit Trail** tab.

NOTE

Several settings in the **Transfer Settings** tab and the **Audit Trail** tab may have been specified for *all* ChemStation instances on the computer via the ChemStation Administration Tool (see “[ChemStation Administration Tool](#)” on page 92). In this case, you cannot change the settings in the **Preferences** dialog.

On the **Transfer Settings** tab, you must specify the following preferences in order to automatically store ChemStation data to ECM:

- Remote Data Path
- Automatic Data Transfer Settings
- Transfer Management Settings

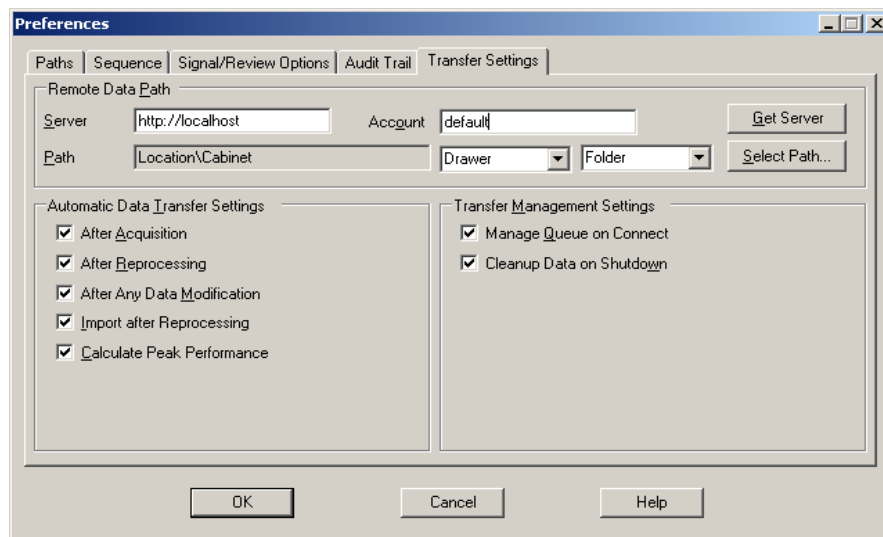


Figure 5 Transfer Settings tab in the Preferences dialog

All of these items can be specified independently for each instrument. Offline and online sessions are automatically synchronized.

On the **Audit Trail** tab, you can enable the Method Audit Trail and Results Audit Trail. For details on audit trails see “[Audit Trails and Logbooks](#)” on page 84.

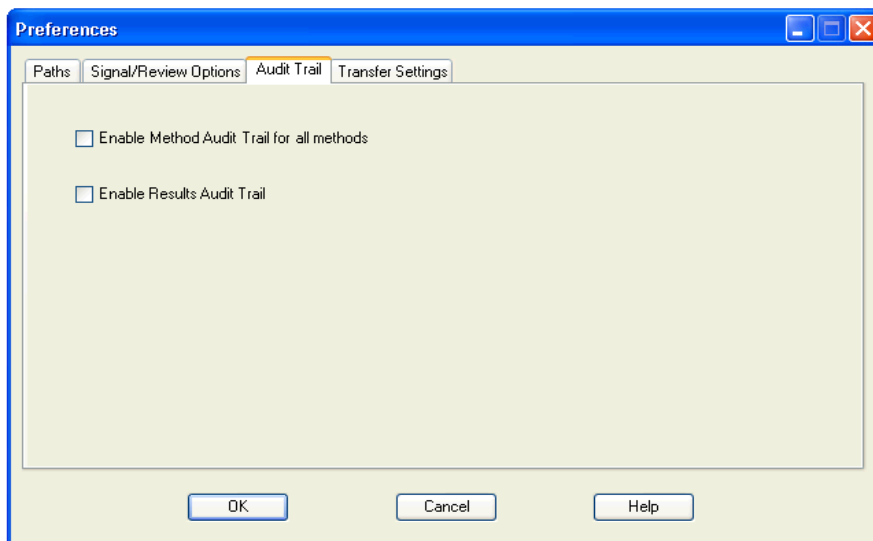


Figure 6 Audit Trail tab in the Preferences dialog

NOTE

You can change these settings for all ChemStation instances on the client PC in one single step by using the ChemStation Administration Tool (see “[ChemStation Administration Tool](#)” on page 92).

Remote Data Path

In ChemStation OpenLAB Option, the **Remote Data Path** needs to be specified in order to save the data to the correct location in ECM.

In the **Preferences** dialog, the **Transfer Settings** tab (see [Figure 6](#) on page 45) allows you to define the **Remote Data Path**. The **Remote Data Path** reflects the LCDF structure in ECM.

Server/Account

In the text fields **Server** and **Account**, you can specify the ECM Server and ECM Account that you want to use to store the ChemStation data.

At your first login from ChemStation to ECM, you must specify the server and account information. You can either enter the information manually, or you can click **Get Server** to fill the fields with the Server and Account where you are currently logged in. ChemStation then keeps the Server and Account information for future sessions.

If you log in to a different ECM Server later, you have to update the Server and Account information. You can click **Get Server** again to fill the fields with the current ECM Server name and the current ECM Account.

Path

To specify the Remote Data Path, you need to select a Location and Cabinet available in the ECM Browser. Click **Select Path** to select the required path in an ECM Explorer dialog.

NOTE

If no **Remote Data Path** is specified, a warning message will be shown at ChemStation startup.

For the Drawer and Folder, you can either keep the selected items, or you can select predefined tokens for an automatic path creation. When you use the predefined tokens in the Remote Data Path, the system automatically creates the items if they do not already exist in ECM.

NOTE

If you use tokens, make sure you have the required ECM privileges to create folders! Alternatively, another user who has the required privileges can create the necessary folders in advance.

Alternatively, the **Remote Data Path** can be specified as **Sequence Parameter** (see [“Remote Data Path as Sequence Parameters”](#) on page 54). Uploaded objects can be stored only at the Folder level.

Table 1 Remote Data Path items

ECM Data Path Item	Convention
Location	Fixed location to be selected in ECM
Cabinet	Fixed cabinet to be selected in ECM
Drawer	Drawer available in ECM Tokens: Instrument Name, Instrument Number, Operator
Folder	Folder available in ECM Tokens: Instrument Name, Instrument Number, Operator

Automatic Data Transfer Settings

In the **Preferences** dialog (**View > Preferences**), the **ECM** tab allows you to specify the automatic settings for the transfer of raw data. The transfer settings, as well as the Remote Data Path, are used to automatically upload data to ECM.

NOTE

If you are not logged in to ECM in ChemStation, the data cannot be automatically uploaded to ECM as specified in the transfer settings. The data is then queued in the Spooler Queue Manager (see [“Spooler Queue Manager”](#) on page 50).

NOTE

If you perform data acquisition from the **Diagnosis** view or **00/PV** view, the transfer settings are ignored. The analytical raw data is written to the ChemStation data file system as predefined in the diagnosis or verification methods.

After Acquisition

If you select this check box the data is automatically uploaded to ECM after an acquisition. The raw data files are written to the local ChemStation file system while the sequence is still running. When the complete sequence is finished, the raw data files are compressed to an SSIZip file which is then uploaded to ECM.

For more information, please refer to [“Workflow 1: Acquisition and automatic upload”](#) on page 59.

After Any Data Modification

If you select this check box, the sequence data container is automatically uploaded to ECM after you changed the data analysis parameters for a sample. The data is uploaded even if you do not reprocess the sequence.

For more information, please refer to [“Workflow 2: Offline review during acquisition”](#) on page 62.

After Reprocessing

If you select this check box, the sequence data container is automatically uploaded to ECM each time after you reprocessed the sequence.

For more information, please refer to [“Workflow 3: Reprocessing data and automatic upload”](#) on page 64.

Import after Reprocessing

If you select this check box, a sequence that is only stored locally is automatically uploaded to ECM after reprocessing.

For more information, please refer to [“Workflow 4: Import after reprocessing”](#) on page 68.

Calculate Peak Performance

This option influences the amount of transferred data. If you select this option, extended performance values (such as *noise* or *system suitability*) are always calculated, saved to ECM, and can be used in OpenLAB Intelligence Reporter. If the check box is cleared, the extended performance values are only available if you choose the ChemStation report styles **Performance** or **Extended Performance**.

For more information, please refer to [“Calculation of performance values”](#) on page 126.

Transfer Management Settings

Manage Queue on Connect

If the connection to ECM breaks down for any reason, a running data upload might be interrupted. In this case, the remaining data is written to an internal queue.

If you select the check box **Manage Queue on Connect**, ChemStation tries to upload the remaining data to ECM each time a connection to ECM is established (that is, each time a user logs on to ECM from ChemStation).

Alternatively, you can open the **Spooler Queue Manager** dialog (see “[Spooler Queue Manager](#)” on page 50) at any time with the **ECM > Manage Queue** command in the **Data Analysis** view.

Cleanup Data on Shutdown

If you select this check box, ChemStation checks the local file system at each shutdown. It deletes all local data and sequence files that are known to be stored in ECM as well. Methods and sequence templates remain on the local file system.

NOTE

If you select the **Cleanup Data on Shutdown** check box, you should also select the Automatic Data Transfer Settings **After Acquisition**, **After Reprocessing**, and **After Any Data Modification**. Otherwise, if the users forget to upload the data to ECM before closing ChemStation, data might be lost.

NOTE

Consider selecting the **Cleanup Data on Shutdown** check box when the system shall be compliant to 21 CFR Part 11. Using this function prevents unauthorized access to the local data files.

Alternatively, you can open the **Data Cleanup** dialog at any time with the **ECM > Cleanup Data** command in the **Data Analysis** view.

This dialog box lists all data sets related to ECM apart from the currently loaded data. The following columns are available:

- **Directory:** Location of the local file
- **ECM Information:** ECM server, account information, and LCDF path of the file in ECM
- **Last Modified:** Date/Time when the copy in ECM was last changed

- **Locally Modified:** Information whether the local copy has been modified
- **Local Version:** Version that was downloaded to the local directory

You can now manually select the data sets to be deleted from the local disk.

Alternatively, via a drop down list deselect all data sets, select all, select only single runs, select only sequence containers, select items older than today, or items older than a week.

After pressing **OK**, the local copies of the selected data sets are deleted.

Both automatic cleanup on shutdown and manual cleanup are only possible if the following conditions are fulfilled:

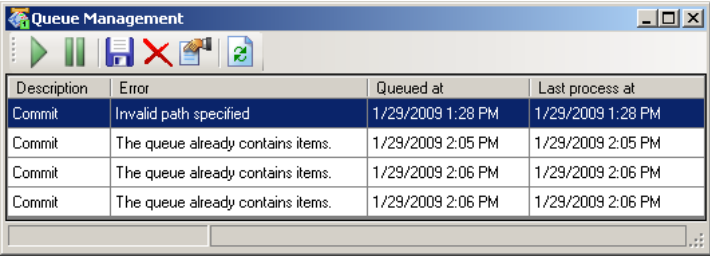
- the ChemStation user is logged on to ECM
- no other instance of the ChemStation instrument is open
- the spooler queue is empty

If one of these conditions is not fulfilled, automatic cleanup will not be performed and it is not possible to open the **Data Cleanup** dialog.

Spooler Queue Manager

The **Spooler Queue Manager** dialog is opened via **ECM > Manage Queue**. If you selected the check box **Manage Queue on Connect**, and there are interrupted transfers, the dialog is also opened when you start ChemStation.

With this dialog, you can manage the data transfers from ChemStation to ECM that were interrupted or could not be started for any reason. Each failed transfer job is listed in a separate line.



Description	Error	Queued at	Last process at
Commit	Invalid path specified	1/29/2009 1:28 PM	1/29/2009 1:28 PM
Commit	The queue already contains items.	1/29/2009 2:05 PM	1/29/2009 2:05 PM
Commit	The queue already contains items.	1/29/2009 2:06 PM	1/29/2009 2:06 PM
Commit	The queue already contains items.	1/29/2009 2:06 PM	1/29/2009 2:06 PM







Figure 7 Spooler Queue Manager

The following information is provided for each line:

- **Description:** Information on the version of the data that will be transferred. Two values are possible:
 - **Import:** No older version of the data exists in ECM at this time. The data has been newly created and will be uploaded as Version 1.
 - **Commit:** There is already at least one version of the data in ECM. The version number of the uploaded data will be increased by one.
- **Error:** Error that disrupted the data transfer. For details on the possible errors, see “[Error Messages in the Spooler Queue Manager](#)” on page 146.
- **Queued at:** Date when the unsuccessful transfer was queued in the Spooler Queue Manager.
- **Processed last at:** Date when the transfer was last attempted.

The toolbar offers you the following commands to manage the queue:

Table 2 Queue management toolbar


Icon	Tooltip	Description
	Process queue	Continue processing the transfer jobs. As long as there is no error, all pending transfer jobs will be processed in the order as they are shown in the list. This function is only active if you select the first line in the list.
	Stop processing	Stop processing the transfer jobs.
	Save selected item locally	Save the selected lines to a file. Only the displayed error, description, and dates are saved to the file. The respective data is not included!
	Delete selected item	Delete the selected transfer job from the queue. The concerned data will not be transferred to ECM.
	Properties	Display the Queue Management dialog box, which shows details of the items in the queue in either summary or detailed form.
	Refresh view	Update the display of the items in the list.

When items are selected from the queue or saved to the local disk, an audit trail entry will be added to Audit Trail of ECM.

NOTE

When items are deleted from the queue or saved to the local disk, they have not yet been uploaded to ECM.

Queue Management Details Dialog Box

The **Queue Management Details** dialog box is displayed when you click the  tool in the toolbar of the **Queue Management** dialog box. It shows the command-specific details of the commands in the **Queue Management** dialog box. The **Queue Management Details** tabs offer two views of the command details:

- Summary tab
- Details tab

In either tab, the tools in the toolbar allow you to navigate through the command details:



Displays the details of the first command in the list.



Displays the details of previous command in the list.



Displays the details of next command in the list.



Displays the details of last command in the list.

Summary tab

The **Summary** tab gives the following summary information about the selected item:

Command Description	The description of the item.
Created	The date and time when the item was added to the queue.
Changed	The date and time when the item was last processed.
Last Error	A description of the error that caused the item to be added to the queue.

Details tab

The **Details** tab gives detailed information about the selected item. You cannot edit the information in this list. The toolbar provides the following tools:



Sorts the properties by category.



Sorts the properties alphanumerically.



This tool is disabled under all circumstances in the ChemStation.

Remote Data Path as Sequence Parameters

Instead of specifying the **Remote Data Path** in the **Preferences** for all acquisition sequences to be run (see “[Remote Data Path](#)” on page 45), the remote data path can also be set directly in the sequence template. This allows to set up different remote paths for each sequence without having to modify the Preferences. The **Remote Data Path** for a sequence template is set up in the **Sequence Parameters** tab.

The screenshot shows the 'Sequence Parameters: Instrument 1' dialog box with the 'Sequence Parameters' tab selected. The dialog is divided into several sections:

- Data File:** Includes a 'Path' dropdown menu showing 'C:\Chem32\1\DATA\' and a 'Subdirectory' text field.
- Prefix/Counter:** Features radio buttons for 'Auto' (selected) and 'Prefix/Counter'. The 'Prefix' field contains 'SIG1' and the 'Counter' field contains '000001'.
- Part of method to run:** Includes a dropdown menu set to 'According to Runtime Checklist' and a checkbox for 'Use Sequence Table Information'.
- Wait:** A numeric field set to '0.00' followed by the text 'minutes after loading a new method.'
- Bar Code Reader:** Includes a checkbox for 'Use In Sequence' and two radio buttons for 'On a bar code mismatch': 'Inject anyway' and 'Don't inject'.
- Sequence Comment:** A large text area for entering comments.
- Remote Data Path:** Includes a checkbox for 'Use Preferences' (unchecked), a 'Path' text field containing 'WAD_Support\Lab C', and a 'Select Path ...' button.
- Shutdown:** Includes a checkbox for 'Post-Sequence Command/Macro' (unchecked) and a 'Not Ready Timeout' numeric field set to '0.00' followed by 'minutes.'
- Fraction Information:** Includes a 'Fraction Start Location' text field.

At the bottom of the dialog are 'OK', 'Cancel', and 'Help' buttons.

Figure 8 Sequence Parameters tab of the Sequence Parameters dialog

Use Preferences: When this checkbox is enabled, the **Remote Data Path** as specified in the **Preferences** will be used. Any LCDF path specified in the **Sequence Parameters** will be ignored for this sequence. When this checkbox is disabled, the **Remote Data Path** will be used as specified when the sequence template is used for data acquisition.





Path: To specify the **Remote Data Path**, you need to select a Location and Cabinet available in the ECM Browser. Click **Select Path** to select the required path in an ECM Explorer dialog. For the Drawer and Folder, you can either keep the selected items, or you can select predefined tokens for an automatic path creation. When you use the predefined tokens in the **Remote Data Path**, the system automatically creates the items if they do not already exist in ECM.

NOTE

If you use tokens, make sure you have the required ECM privileges to create folders! Alternatively, another user who has the required privileges can create the necessary folders in advance.

Compressed ChemStation File Formats

When ChemStation data is uploaded to ECM, the data is automatically packaged into an SSIZip file. Depending on the type of data, different packaging formats are used.

ChemStation data	Packaging format	Icon in ChemStation
Single Runs (*d file, ACQ.m and DA.M)	*.D.SSIZIP	
Sequence Container The sequence container contains recursively the whole sequence data stored in the sequence subdirectory: <ul style="list-style-type: none"> all *.d files along with ACQ.m and DA.M all methods *.m used during acquisition batch file *.b sequence logbook file *.log 	*.SC.SSIZIP	
Methods	*.M.SSIZIP	
Sequence templates	*.S or *.S.SSIZIP	

The packaging of ChemStation items is part of ChemStation OpenLAB Option and cannot be changed manually.

The packaging is automatically carried out when the data is uploaded to ECM. When the SSIZIP files are downloaded from ECM to ChemStation, they are automatically unpacked into the according directory in the ChemStation Explorer.



4 Working With ChemStation OpenLAB Option

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This chapter describes the basic workflows with ChemStation OpenLAB Option. There are four data-related workflows and two workflows for methods and sequence templates.



Transferring Data to or from ECM

ChemStation OpenLAB Option provides the ability to open and save different ChemStation items into their ChemStation contexts:

- Methods
- Sequence templates
- Single run data
- Sequence data

All of this data is stored in ECM as SSZIP containers (see [“Compressed ChemStation File Formats”](#) on page 56).

When the data is uploaded to ECM, local copies of the files still remain in the ChemStation file system. If an item is loaded from ECM back into ChemStation, it is automatically loaded into its original location.

Different options are available regarding the automatic upload of single run/sequence data to ECM. Loading back stored data from ECM to ChemStation, however, always requires a manual load action. Methods and sequence templates require always a manual upload to ECM as well as a manual load or update into ChemStation.

For downloading data from ECM, several **load** commands are available in the **ECM** menu. Depending on the current view, you can load different files from ECM. In the **Data Analysis** view, you can load single run data or sequence data. These data are automatically set to the status **checked out** in ECM. In the **Method and Run Control** view, you can load methods and sequence templates. These items are only retrieved and not checked out.

The following workflows are examples that represent typical tasks done with ChemStation OpenLAB Option.

Data-related workflows

Workflow 1: Acquisition and automatic upload

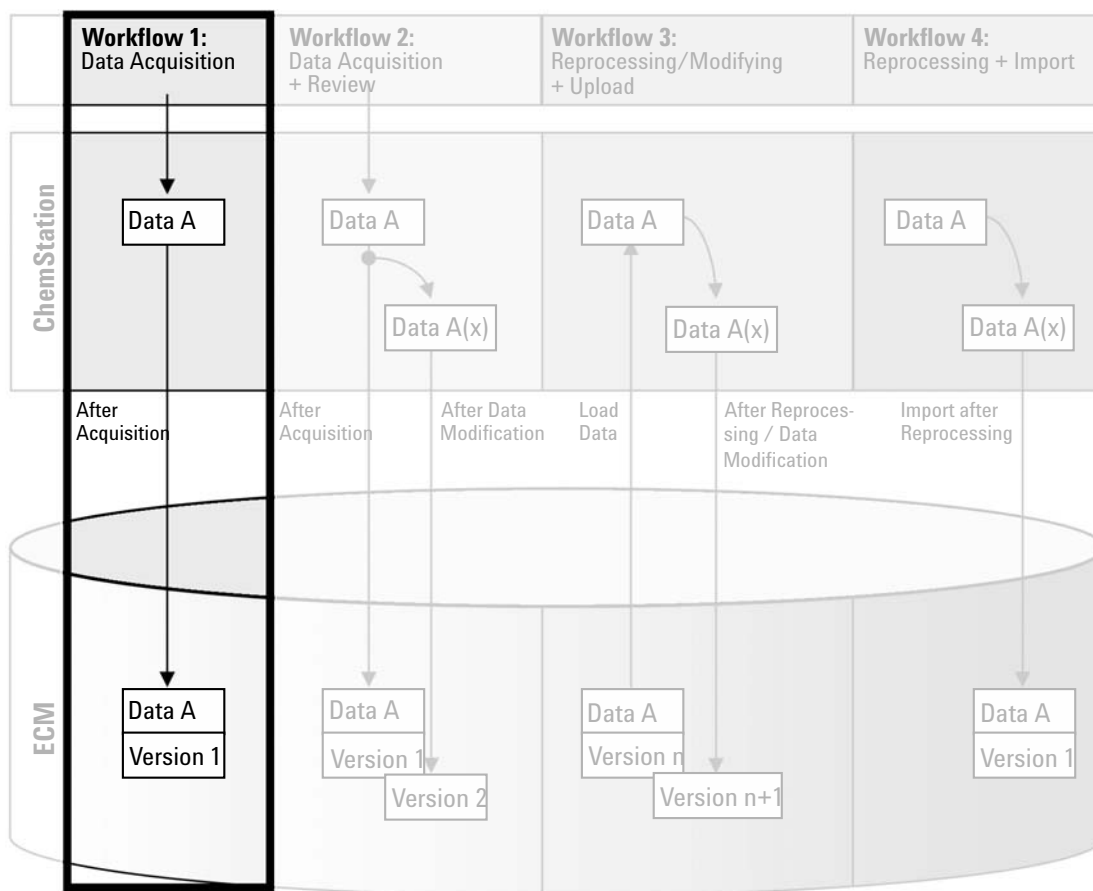


Figure 9 Acquisition and automatic upload

The workflow *Acquisition and automatic upload*, see [Figure 9](#) on page 59, illustrates how raw data is uploaded to ECM directly after the acquisition is finished. The raw data is initially stored locally. After completing the acquisition, the data is automatically uploaded to ECM.



To save data to ECM automatically after completion of a single run or sequence:

- 1 Log in to ECM in an online ChemStation.
- 2 Load a sequence template.

Your ECM user name is automatically inserted as operator name into the sequence template.
- 3 In the **Data Analysis** view, click **View > Preferences**.
- 4 On the **Transfer Settings** tab, configure the following settings:
 - **Remote Data Path:** Select the ECM location that you want to use for the sequence data upload.
 - Select the **After Acquisition** check box.
- 5 Configure the sequence parameters and the sequence table.
- 6 Start the acquisition.

While the acquisition is running, the raw data, method definition, and a copy of the sequence template are locally stored on the ChemStation computer.

After the sequence is finished, all data is automatically uploaded as an *.SC.SSIZIP* file to ECM to the previously defined LCDF path. The local copy of the data remains on the ChemStation computer. The file name of the sequence container is determined by the settings in the sequence template (for more details on the sequence template settings, refer to the manual *Understanding Your ChemStation*). After uploading the sequence container the sequence icon in the ChemStation Navigation Pane changes

from  to . The LCDF path of the sequence container is shown in the ChemStation toolbar.

NOTE

The color of the **Sequence Data** icon in the Navigation Pane allows to track the modification status of the data:



: The sequence container is stored in ECM and has not been modified locally



: The sequence container is stored in ECM and has been modified locally

NOTE

The upload process may take some time when large amounts of data are uploaded. During this time ChemStation is busy and the user cannot perform tasks in ChemStation. Please wait until the upload is completed.

Workflow 2: Offline review during acquisition

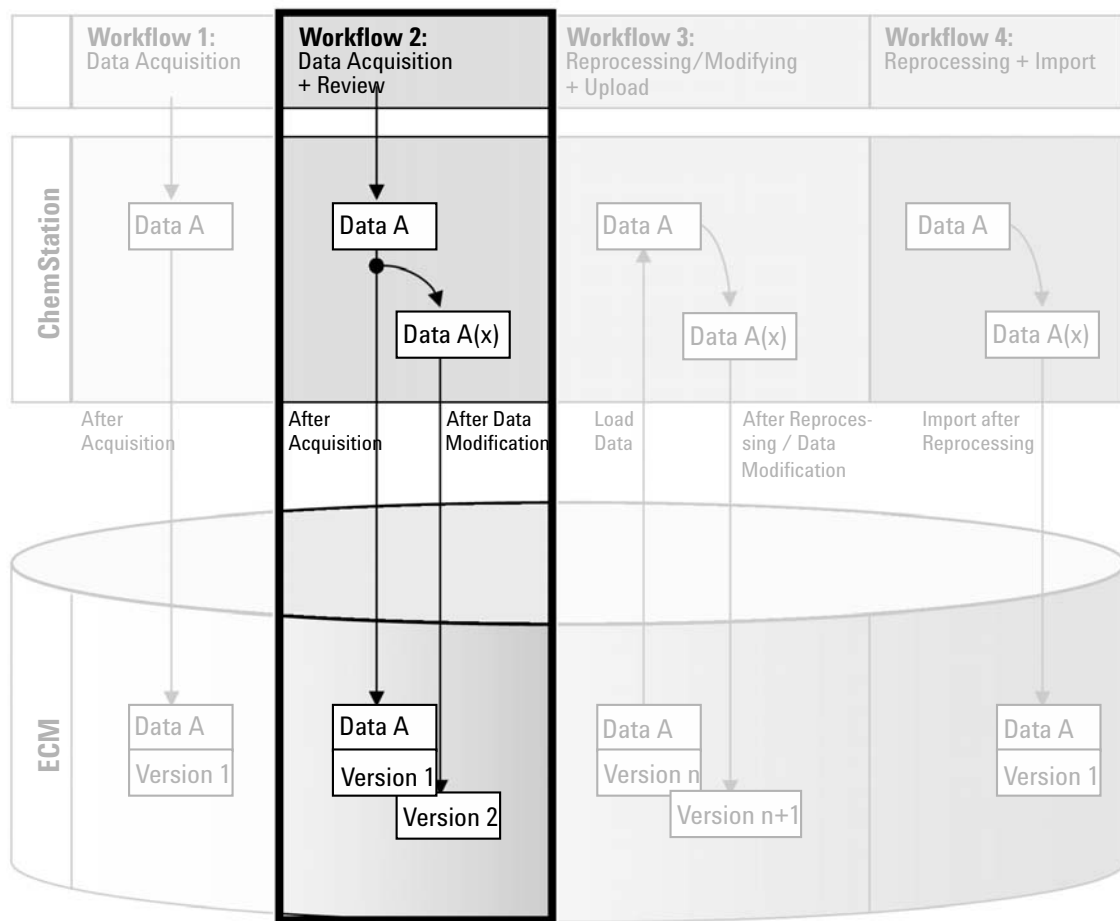




Figure 10 Offline review during acquisition

The workflow *Offline revision during acquisition*, see [Figure 10](#) on page 62, illustrates how raw data is reviewed while the acquisition is still running. Directly after the acquisition is finished, the original raw data is automatically uploaded to ECM. After the review, the changed data is again uploaded to ECM. When the data is uploaded the second time, a new version is created.

To save data to ECM automatically after changing the data:

- 1 Log in to ECM in an online ChemStation.
- 2 Load a sequence template.
Your ECM user name is automatically inserted as operator name into the sequence template.
- 3 In the **Data Analysis** view, click **View > Preferences**.
- 4 On the **Transfer Settings** tab, configure the following settings:
 - **Remote Data Path:** Select the ECM location that you want to use for the sequence data upload.
 - Select the **After Acquisition** check box.
 - Select the **After Any Data Modification** check box.
- 5 Start the acquisition.
While the acquisition is running, the raw data, method definition, and a copy of the sequence template are stored locally on the ChemStation computer.
- 6 Open an offline ChemStation and change some data analysis parameters for one of the already finished samples. Save your changes locally.
- 7 After the acquisition has been finished, two things will happen:
 - The original raw data is automatically uploaded as an *.SC.SSIZIP* file, *Version 1*, to ECM to the previously defined LCDF location. The LCDF of the new sequence is shown in the toolbar in the online ChemStation.
The file name of the sequence container is determined by the settings in the sequence template (for more details on the sequence template settings refer to the manual *Understanding Your ChemStation*).
The sequence icon in the ChemStation Navigation Pane changes from  to .
 - The **ECM forced upload** dialog opens in the online ChemStation. Click **OK** to confirm that you finished all work in the offline instance. As soon as you confirm this dialog, the changed data is uploaded as *Version 2* to ECM.
A local copy of the changed data remains on the ChemStation computer.

NOTE

For both versions (the one after acquisition and the one from the parallel offline review) the ECM operator is the user who has run the acquisition, even if another user has performed the review in the Offline ChemStation.

Workflow 3: Reprocessing data and automatic upload

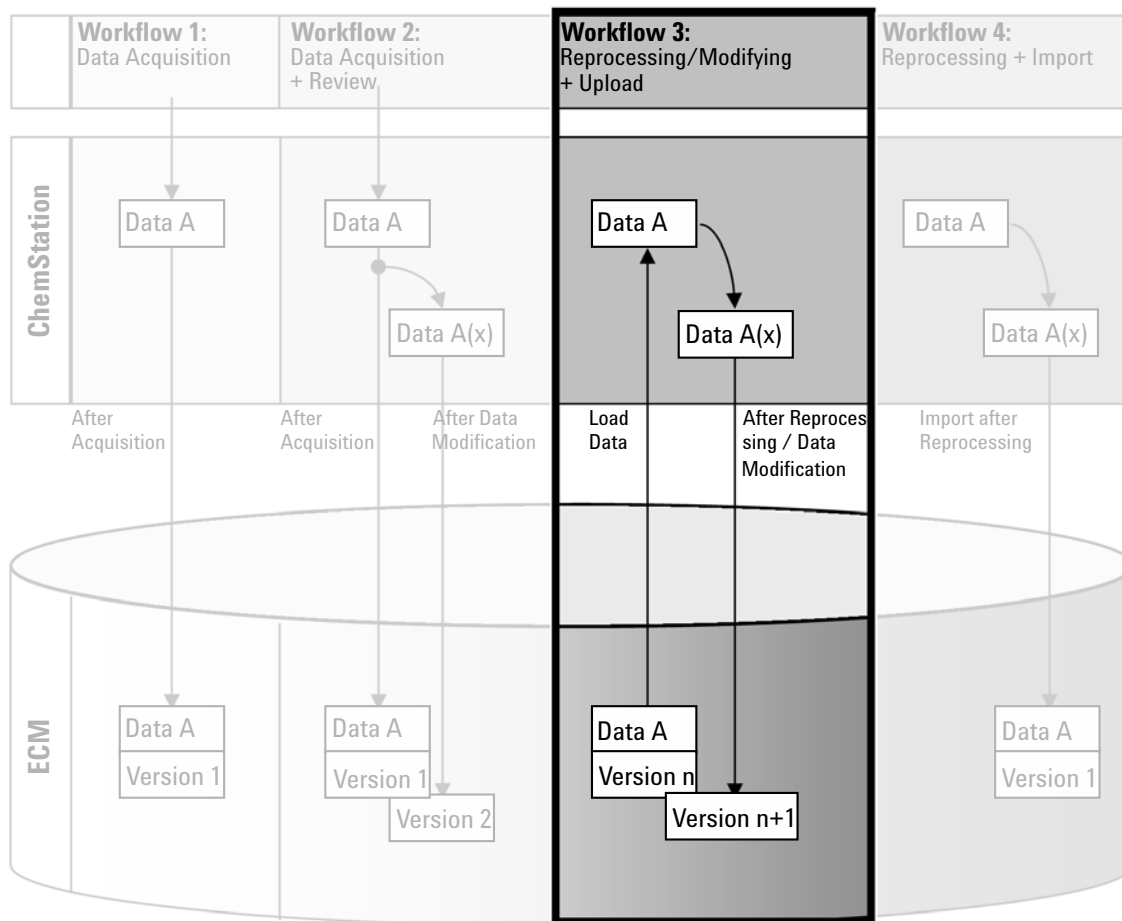


Figure 11 Reprocessing data and automatic upload

The workflow *Reprocessing data and automatic upload*, see [Figure 11](#) on page 64, illustrates how data is reprocessed and then automatically uploaded. This workflow applies to data that has been previously stored in ECM. A new version of the data is created in ECM for the reprocessed or changed data.

To save data to ECM automatically after reprocessing:

- 1 Log in to ECM in ChemStation (online or offline).
- 2 Select **ECM > Load Data** to download a sequence from ECM.

The **ECM Desktop Open** dialog opens. Navigate to the ECM folder to load the data of your choice and select one of the following packaged files:

- Single run data: *.D.SSIZIP files
- sequence data: *.SC.SSIZIP files

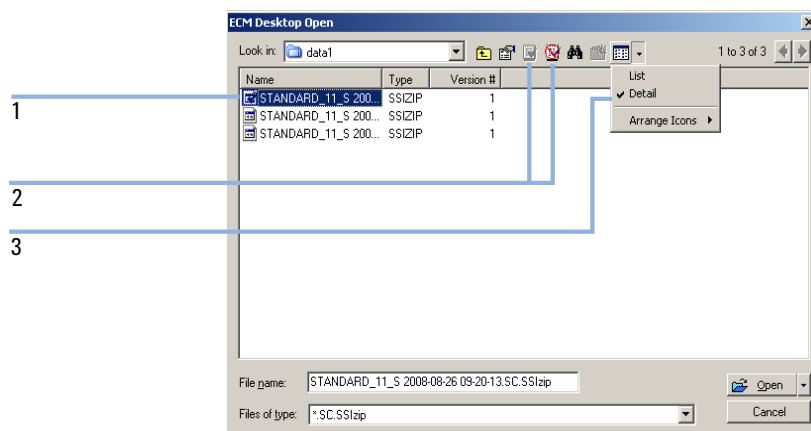



Figure 12 ECM Desktop Open dialog

If the item is checked out, it is marked with a blue or red icon (see marker 1):

 (blue icon): the item has been checked out by you (current user)

 (red icon): the item has been checked out by another ECM user

You can load any checked out item. However, if an item has been checked out by another ECM user, the other user must check in the item before you can save it back to ECM.

4 Working With ChemStation OpenLAB Option

Data-related workflows

To check out or check in an item, you can use the respective icons available in the **ECM Desktop Open** dialog (see marker 2). You can only check out the latest version of an item.

In order to see more details regarding the type and version of the available items, select the **Detail** view (see [Figure 12](#) on page 65, marker 3). To open an older version of an item, select the **Open Revisions** command from the **Open** menu (see [Figure 13](#) on page 66). This opens the **File Versions** dialog, where all available versions of the item are listed (see [Figure 14](#) on page 67).

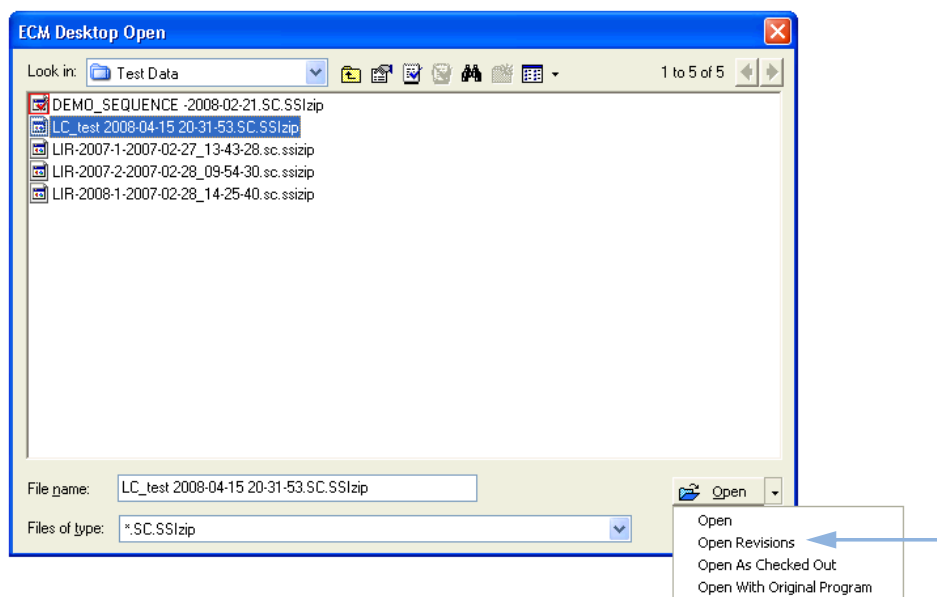


Figure 13 Open Revisions command

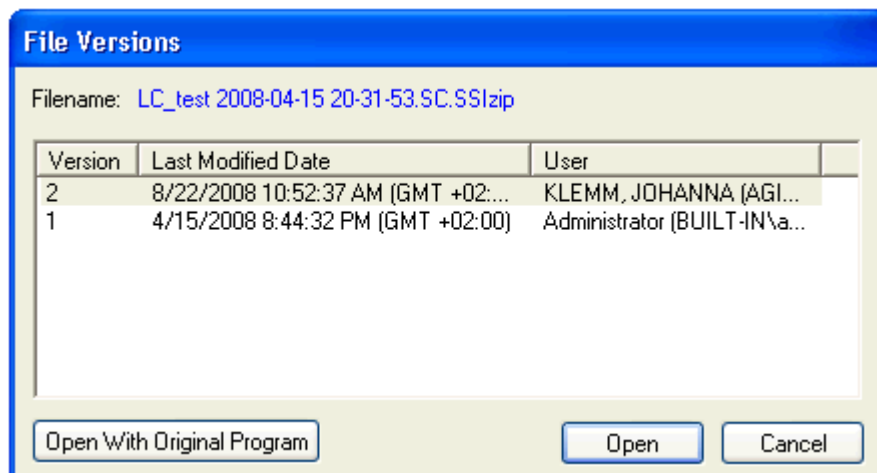


Figure 14 File versions dialog

- 3 Select **Open** in either dialog to download the item to ChemStation.

If the item was not already checked out, it is automatically checked out of ECM when you load it to ChemStation.

The LCDF path of the data is shown in the ChemStation toolbar.

- 4 In the **Data Analysis** view, click **View > Preferences**.
- 5 On the **Transfer Settings** tab, configure the following settings:
 - Select the **After Reprocessing** check box.
 - Select the **After Any Data Modification** check box.
- 6 Modify or reprocess the sequence data.

After the reprocessing is finished, the sequence data is uploaded with its original name to its original LCDF path. The version number is increased by one.

The local copy of the reprocessed data remains on the local file system of the ChemStation computer.

Workflow 4: Import after reprocessing

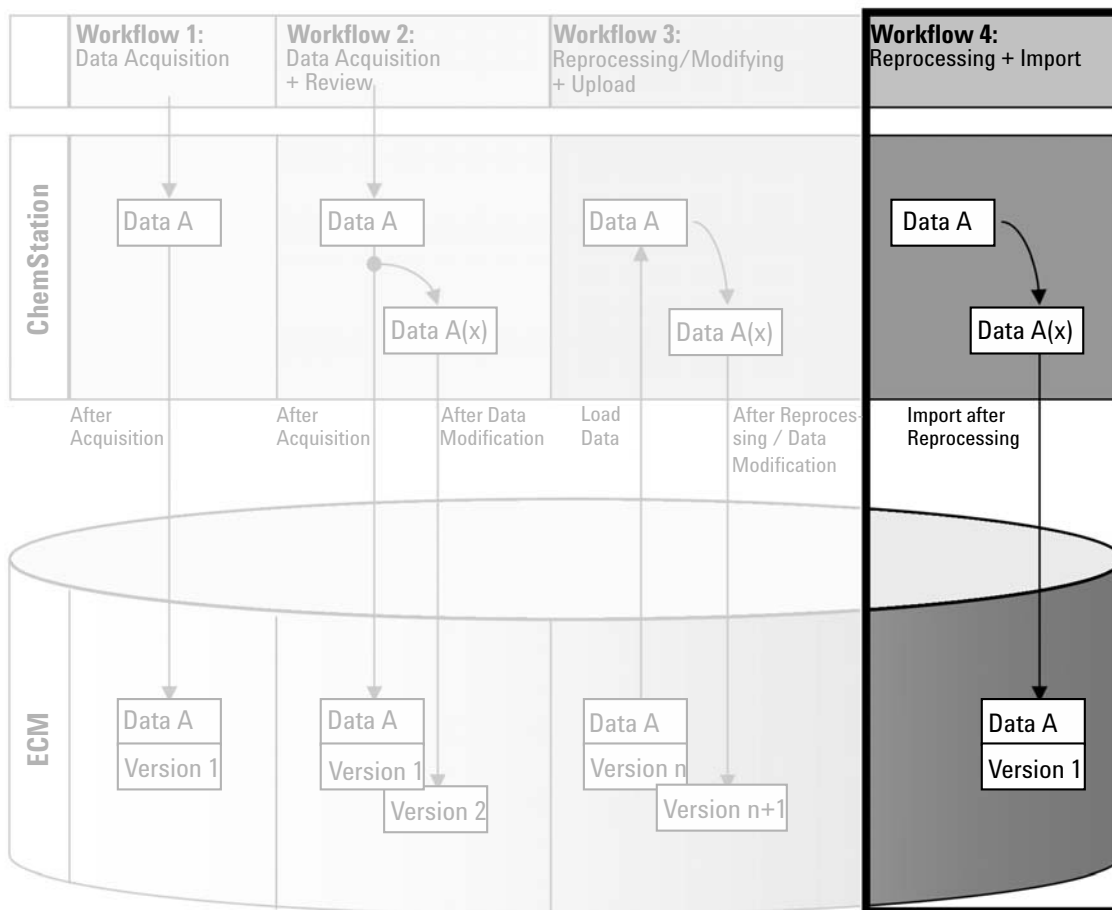


Figure 15 Import after reprocessing

The workflow *Import after reprocessing*, see [Figure 15](#) on page 68, illustrates how locally saved data is reprocessed and then automatically imported in ECM.

To save data to ECM automatically after reprocessing:



- 1 Log in to ECM in an offline ChemStation.

- 2 From the local file system, open a sequence that has never been saved to ECM before.
- 3 In the **Data Analysis** view, click **View > Preferences**.
- 4 On the **Transfer Settings** tab, configure the following settings:
 - **Remote Data Path:** Select the ECM location that you want to use for the sequence data upload.
 - Select the **Import after Reprocessing** check box.
- 5 Reprocess the sequence data.

NOTE

The data will not be uploaded if you only modify it. You need to reprocess the sequence data.

The sequence data is uploaded as a new *.SC.SSIZIP* file, version 1, to the previously defined LCDF path in ECM. The file name of the sequence container is determined by the settings in the sequence template (for more details about the sequence template settings refer to the manual *Understanding Your ChemStation*).

The sequence icon in the ChemStation Navigation Pane changes from  to .

The local copy of the reprocessed data remains on the local file system of the ChemStation computer.

Workflows for Methods and Sequence Templates

Workflow 1: Local files – Save new method

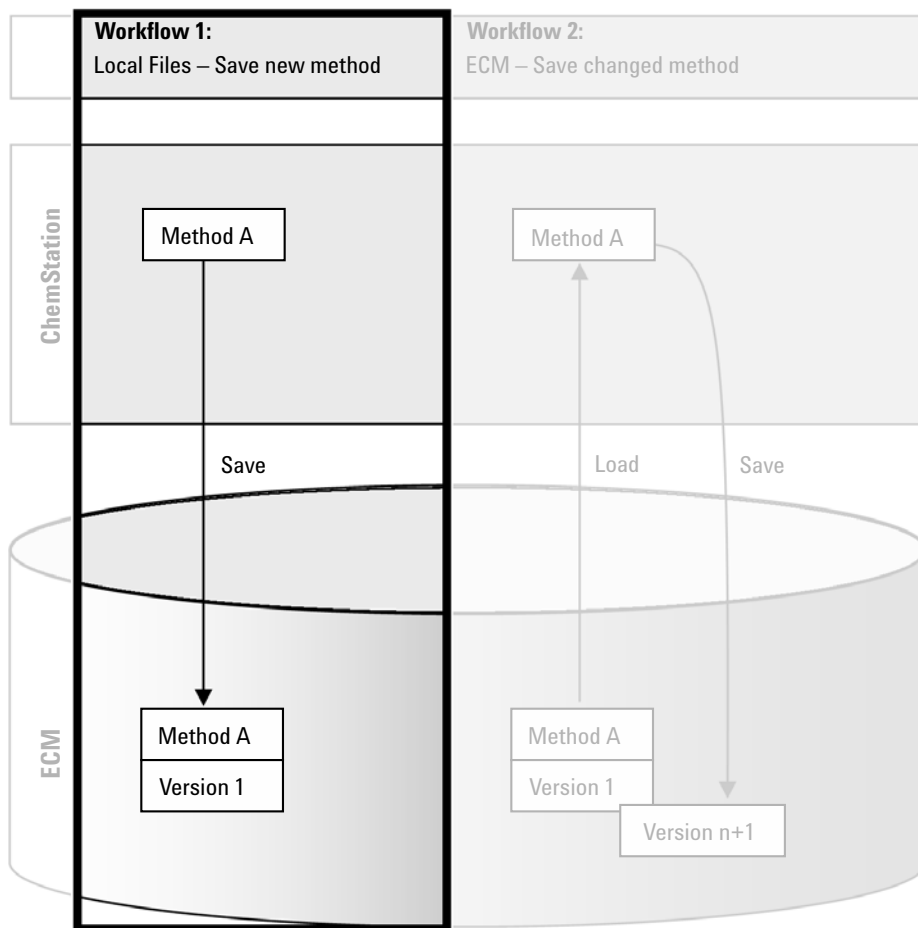


Figure 16 Local files - Save new method





The workflow *Local files - Save new method*, see [Figure 16](#) on page 70, illustrates how newly created or locally stored methods or sequence template can be manually uploaded to ECM.

To upload a new method or sequence template:

- 1** Log in to ECM in an offline ChemStation.
- 2** In ChemStation, load the method/sequence template or create a new one.
- 3** In the **Method and Run Control** view, click **ECM > Save Method** or **ECM > Save Sequence Template**, respectively.
The **ECM Save** dialog opens.
- 4** Navigate to the Remote Data Path of your choice to upload the method/sequence template.
You can only upload items into a Folder, not into a Location, Cabinet, or Drawer.
- 5** If necessary, save the item using a different name. the original name is used by default, but you can modify the name.
- 6** Click **Save**.
The **Add File** dialog opens.
- 7** Enter a reason for the upload and click **OK**. The reason is then shown in the ECM Audit Trail (see [“ECM Audit Trail”](#) on page 86).

The progress of the upload is displayed in a window until the item is uploaded to ECM.

After finishing the upload, the SSIZIP file is available in ECM as version 1. The file is saved to the Remote Data Path defined in the Preferences (see [“Remote Data Path”](#) on page 45).

The method icon in the ChemStation Navigation Pane changes from  to . The icon for a sequence template changes from  to  accordingly.

Workflow 2: ECM – Save changed method

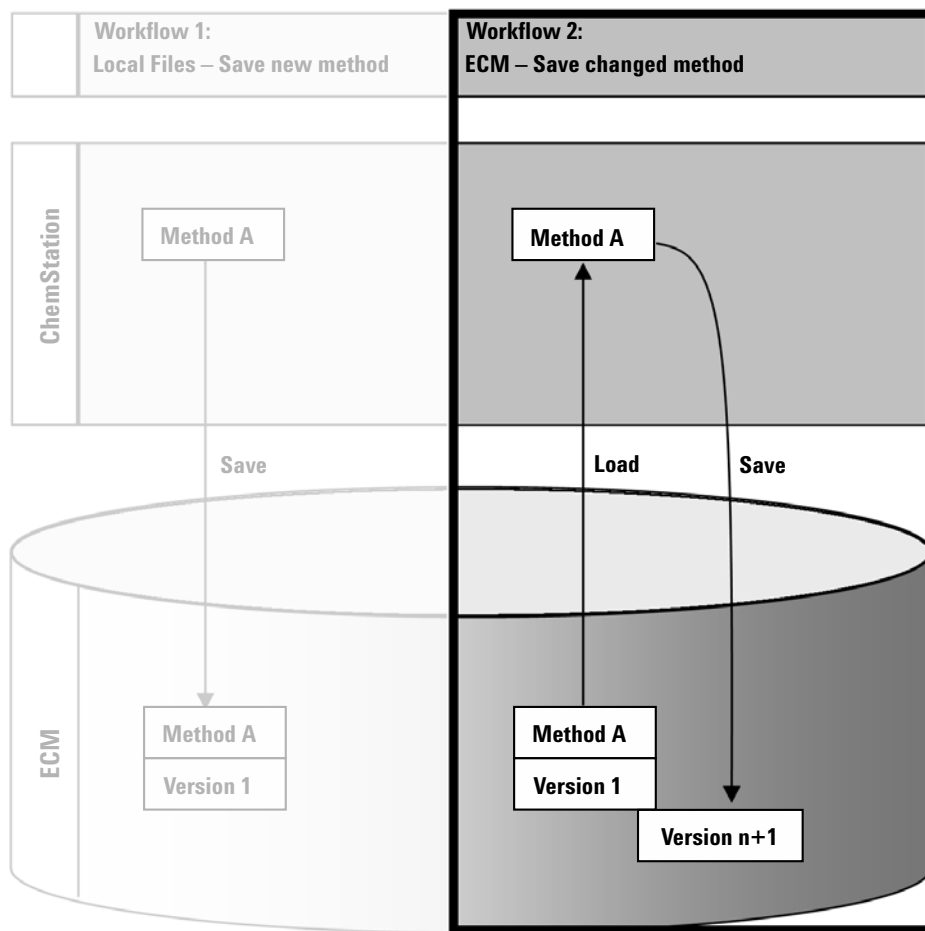


Figure 17 ECM - Save changed method

The workflow *ECM - Save changed method*, see [Figure 17](#) on page 72, illustrates how methods or sequence templates that are already stored in ECM are edited and saved under the same name as a new version.

- 1 Log in to ECM in ChemStation.
- 2 Load a method or sequence template.

- Open a method/sequence template from your local PC. Choose a method/sequence template that has been uploaded to ECM before. ECM

Methods are indicated by , ECM sequence templates by  in the ChemStation Navigation Pane.

– or –

- Select **ECM > Load Method** or **ECM > Load Sequence Template** respectively to download a method/sequence template from ECM.

If you use one of the **Load** commands, the **ECM Desktop Open** dialog will open. Navigate to the ECM folder to load the method (*.M.SSIZIP) or sequence template (*.S or *.S.SSIZIP) of your choice.

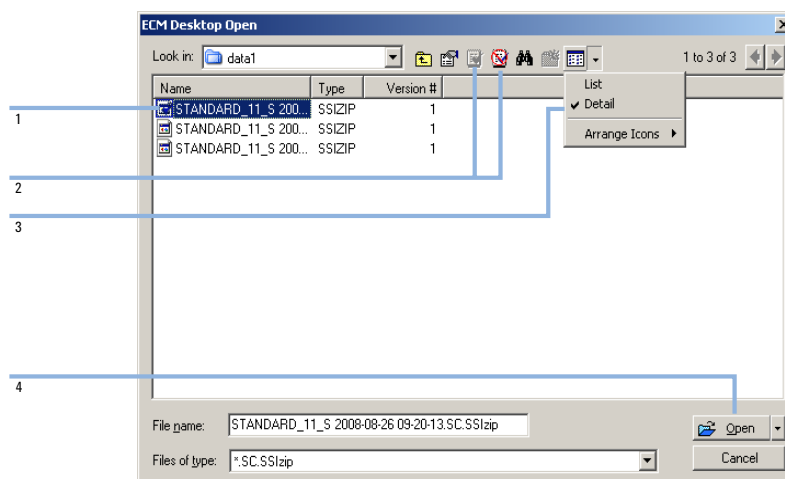




Figure 18 ECM Desktop Open dialog

If the item is checked out, it is marked with a blue or red icon (see [Figure 18](#) on page 73, marker 1):

 (blue icon): the item has been checked out by you (current user)

 (red icon): the item has been checked out by another ECM user

You can load any checked out item. However, if an item has been checked out by another ECM user, the other user must check in the item before you can save it back to ECM.

4 Working With ChemStation OpenLAB Option

Workflows for Methods and Sequence Templates

To check out or check in an item, you can use the according icons available in the **ECM Desktop Open** dialog (see [Figure 18](#) on page 73, marker 2). With these icons, you can only check out the latest version of an item.

In order to see more details regarding the type and version of the available items, select the **Detail** view (see [Figure 18](#) on page 73, marker 3). To open an older version of an item, select the **Open Revisions** command from the **Open** menu (see [Figure 19](#) on page 74, marker 1). This opens the **File Versions** dialog, where all available versions of the item are listed (see [Figure 20](#) on page 75).

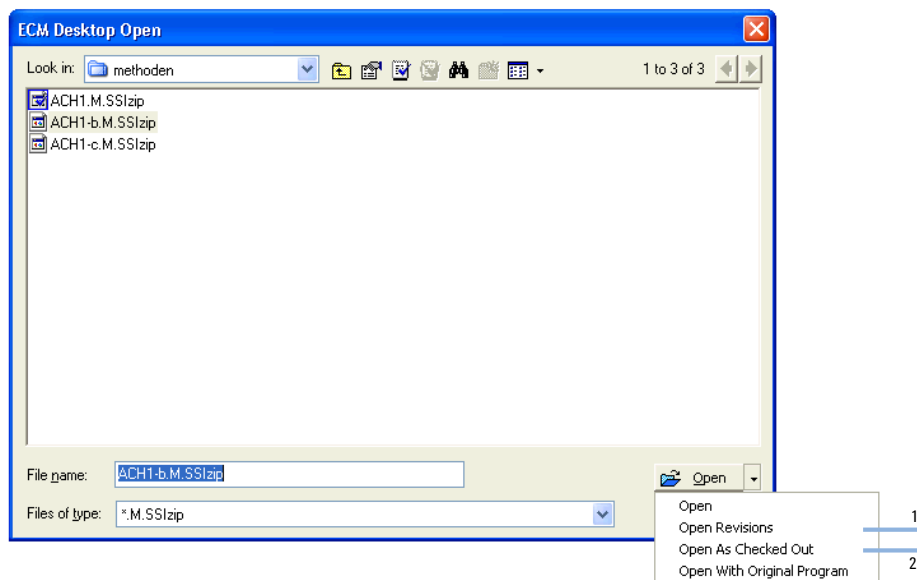


Figure 19 Open Revisions command

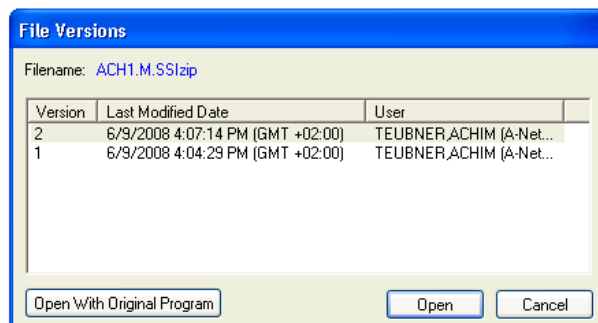


Figure 20 File versions dialog

- 3 Select **Open** in either dialog to download the item to ChemStation. In order to prevent other users from modifying the item, it is possible to select the **Open As Checked Out** command to mark the item as checked out from ECM (see [Figure 19](#) on page 74, marker 2).


NOTE

Unlike the data files, the methods and sequence templates are not automatically checked out of ECM! In order to modify those items in ChemStation, you should check them out from ECM manually. Otherwise, there is no guarantee that you are working on the latest version.

If the file already exists on the ChemStation computer in the specified location, you must choose a different download location.

The LCDF path of the loaded method/sequence template is shown in the ChemStation toolbar in ChemStation.

- 4 Make some changes to the method/sequence template.

The modified method is indicated by 

, a modified sequence templates by  in the Navigation Pane.

- 5 Select **ECM > Save Method** or **ECM > Save Sequence Template** respectively to save the changed method/sequence template.

NOTE

If you have not checked out the item before loading it from ECM, and another ECM user has checked out the item in the meantime, you cannot proceed with the upload back to ECM. A warning message is displayed, and it is not possible to save the item back to ECM until the other user has released the checked out item.

- 6 When the **Add File** dialog opens, enter a reason for the upload and click **OK**. The reason is then shown in the ECM Audit Trail (see “[ECM Audit Trail](#)” on page 86).

The progress of the upload is displayed in a window until the item is uploaded to ECM.

The *.M.SSIZIP/.S* file is uploaded with its original name to its original LCDF path (the path is shown as a tooltip of the method/sequence template in ChemStation). The version number is automatically increased by one.

Updating the Local Master Method or Sequence Template

If a master method or sequence template is updated in ECM (i.e. a new version is created), it is possible to update the local copies with the following update procedure.

- 1 Make sure the master method or sequence template to be updated is currently not loaded. The currently loaded method or sequence template is not available for update.
- 2 Select **ECM > Update Methods ...** or **Update Sequence Templates ...**

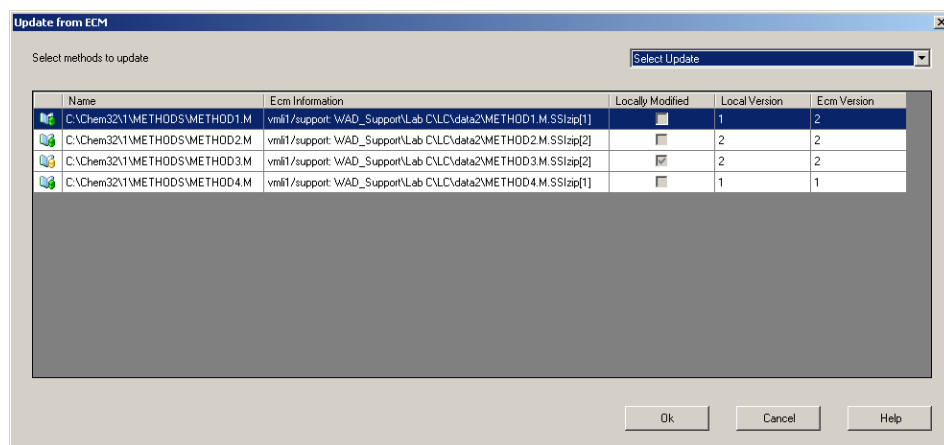


Figure 21 Update Methods dialog box

The **Update from ECM** dialog box is displayed.

The dialog box lists all methods that are connected to ECM. The following columns are available:

- **Name:** Path and Name of the local copy of the method/sequence template.
 - **ECM Information:** ECM server, account information, and LCDF path of the file in ECM.
 - **Locally Modified:** A check box indicating whether the local copy was modified.
 - **Local Version:** Version number of the local copy of the method/sequence template.
 - **ECM Version:** Version number of the file in ECM.
- 3** You can now manually select the methods that are to be updated. Alternatively you can via the drop down list deselect all methods, select all methods, select to those methods with a higher version number in ECM, or select all methods that have been modified locally.
- After pressing OK, the selected local methods/sequence templates are updated with the version in ECM.

4 Working With ChemStation OpenLAB Option

Workflows for Methods and Sequence Templates



5 Administration Regarding 21 CFR Part 11 Compliance

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This chapter explains the purpose of 21 CFR Part 11 and its implementation in ChemStation with ChemStation OpenLAB Option.



Introduction to 21 CFR Part 11

Effective August 20, 1997, the U.S. Food and Drug Administration (FDA) released and published a new rule to enable pharmaceutical companies to approve their results with electronic signatures and to transfer paper-trail documentation into electronic records. This rule is known as 21 Code of Federal Regulations Part 11 (referred to as 21 CFR Part 11) and applies to all industry segments regulated by the FDA.

The impact of this rule on current work practices and data handling in the pharmaceutical industry has been much higher than expected. *“The industry wanted to have a rule on electronic signatures, but what they got was a rule on electronic records.”* (Martin Browning, former FDA inspector, during a validation seminar in Washington D.C.)

21 CFR Part 11 places high emphasis on the implementation of all measures to protect and secure electronic records. Notwithstanding the uncertainties and the changes that 21 CFR Part 11 requires in the behavior of both the pharmaceutical industry and the vendors of chemical analysis equipment, it is well worth implementing in today’s laboratories because it can help the industry with one of the most important issues in pharmaceutical research-bringing new drugs on the market faster.

The major benefits of this shift towards electronic data management are in the potential productivity increase for the industry. The industry can decrease its data output on paper, speed up the data review and approval process, and benefit from new automation technology based on computerized system control, for example, in manufacturing or dissolution drug release testing.

In addition to this rule on electronic records, other general requirements for computerized systems are brought to the auditor’s attention. These rules cover the basic requirements of validation which are limiting data access and ensuring data integrity and data traceability.

It is, of course, the industry that must ensure that its work practices support the FDA rules, but most of the requirements also affect the chemical analysis systems and suppliers of these systems.

21 CFR Part 11 Requirements

To fulfill the FDA rules and guidelines for compliant electronic records and computerized systems, it is important to understand the basic aspects of secure data handling.

- *Data security*: physical protection of data by limiting access to the system and preventing unauthorized access.
- *Data integrity*: protecting raw data and metadata and preventing these from unauthorized modification, and linking raw data and results to reproduce the original results at any time, for example, in an audit situation, and document each new result copy.
- *Audit traceability*: documenting who did what to the results and when, and tracing the user adding new reanalyzed versions to the original raw data.

General Aspects of Data Security in Computerized Networks – Open Versus Closed Systems

Before discussing details of data security in a chromatographic system, some general aspects of data security in a computerized network need to be considered.

It is generally known that data transfer over a public network can be accessed by unauthorized external persons, “hackers”, who gain access either for personal amusement or intentional fraud.

If an electronic identification comprising user ID and a password is used to approve confidential or important data, users must be sure that their signatures are unbreakably linked to the data and that nobody can copy this signature or get access to the passwords. In a public system, this would require additional encryption technology, for example, a private/public key combination of data encryption. In contrast, if a computerized system is protected from unauthorized access, users can be sure that their signatures are private and are not accessible to unauthorized individuals.

The FDA also distinguishes between these two scenarios and defines them as *open* and *closed* systems. A *public* network system can therefore only be viewed as an open system and a protected network as a closed system, if it fulfills additional requirements.

5 Administration Regarding 21 CFR Part 11 Compliance

Introduction to 21 CFR Part 11

In FDA terms, *“closed system means an environment in which access is controlled by persons who are responsible for the content of electronic records on the system”* (11.3.5). The evidence of a system being a closed system is not a one-time check but an ongoing process of executing and documenting the system controls that make sure that the system is closed. In contrast, in an open system, *“those persons being responsible for the content of electronic records do not control the system access.”*

As a result, open systems require additional encryption technology for all data transfer over the network.

ChemStation OpenLAB Option is designed for and supported in closed systems.

Overview of Configuration Steps Required for Part 11

If you want to configure ChemStation OpenLAB Option to be compliant with 21 CFR Part 11, you need to go through the following checklist:

- LCDF structure on the ECM Server prepared according to your needs
See [“Data Storage in ECM”](#) on page 16.
- ChemStation OpenLAB Option installed on the ECM Server
See [“Updating the ECM Database”](#) on page 22.
- ECM Roles/Users/Groups configured
See [“Configuring users, roles and privileges”](#) on page 25.
- ECM Account configuration with active audit trail and mandatory reason
See [“To enable the ECM Audit Trail”](#) on page 87 and [“Account configuration”](#) on page 89.
- Password policy realized in ECM (including E-mail Notification)
See [“To configure the password settings for an ECM Account according to the password policy”](#) on page 90.
- E-Signatures prepared (messages and privileges)
See [“Using electronic signatures”](#) on page 96.
- ChemStation with ChemStation OpenLAB Option and mandatory ECM login
See [“Installing a new ChemStation with ChemStation OpenLAB Option”](#) on page 28.
- Automatic Data Transfer Settings and Transfer Management Settings activated
See [“ECM Preferences”](#) on page 44.
- Audit trail active for methods and results
See [“Method Audit Trail”](#) on page 84 and [“Results Audit Trail”](#) on page 85.
- Emergency Plan available, based on options of the Administration Tool
See [“ChemStation Administration Tool”](#) on page 92.

Audit Trails and Logbooks

In order to comply to 21 CFR Part 11, ChemStation OpenLAB Option offers various audit trails and logbooks to document all activities associated with methods, results, reports, or with ECM files generally. These audit trails and logbooks track all changes that are made to any file, including data acquisition, re-analysis, and long-term archiving.

The audit trails are stored in separate files, which are stored together with the sample or method data. The audit trail files are archived together with the other data in the according SSZIP files. The ECM logbooks are available only directly in ECM.

Method Audit Trail

Each method has a Method Audit Trail. By default, this Method Audit Trail contains only the comments that you must provide each time when you save a method. As there is no control on the provided text, there is no guarantee that the method changes are reproducible.

With regards to 21 CFR Part 11, ChemStation OpenLAB Option makes it possible to generate a more detailed Method Audit Trail. If the function is activated, the Method Audit Trail contains not only the user comments, but also each individual changed parameter with its old and new value. All changeable data analysis parameters are tracked. This means that you can reproduce exactly which value has been changed to what, when, and by whom.

To enable the Method Audit Trail for all methods

This is required if you want to comply to 21 CFR Part 11.

- 1 Select **View > Preferences**
- 2 In the **Audit Trail Status** dialog, select **Enable Audit Trail for this method** and click **OK**.

Once enabled, the Method Audit Trail cannot be disabled.

NOTE

You can also use the ChemStation Administration Tool to enable the Method Audit Trail for all methods (see [“ChemStation Administration Tool”](#) on page 92).

To enable the Method Audit Trail only for the currently open method

You can also activate the Method Audit Trail only for one method. This might be useful, for example, when you finished the development of new method and want to track all further changes.

- 1 Select **Method > Enable Audit Trail**
- 2 On the **Audit Trail** tab, select **Enable Method Audit Trail for all methods**.

To view the Method Audit Trail for the currently open method in ChemStation

- 1 Select **Method > Method Audit Trail**.

To remove the detailed Method Audit Trail

Once a method is enabled for the detailed audit trail, you cannot disable it again. The only way to get rid of an existing Method Audit Trail is to save the method under a different method name. In this case, the only hint in the new method's audit trail is a comment about the method being based on another method.

Results Audit Trail

Manual integration events are not saved in the method. Therefore, the Method Audit Trail contains no information on manual integration events. These events are only saved in the data file. Nevertheless, they have an influence on the results. Manual integration events are therefore saved as part of the Results Audit Trail.

If activated, this Results Audit Trail is added to the existing Data File Logbook (file name RUN.LOG). By default, the Data File Logbook only contains the acquisition parameters and reprocessing information for each sample. The Results Audit Trail additionally tracks the changes of all data analysis parameters for a sample.

To enable the Results Audit Trail

If you enable the Results Audit Trail, the relevant changes are tracked for *all* samples, independent of the sequence they belong to and independent of the user who carries out the change.

- 1 Select **View > Preferences**
- 2 On the **Audit Trail** tab, select **Enable Results Audit Trail**.

To view the Results Audit Trail for the loaded sample in ChemStation

- 1 In the **Data Analysis** view, select **View > Current Data File Logbook**.

Report History

If you create a ChemStation report, you can display the report on the screen, send it to a printer, or save the report as a specific file (*report.pdf*). These report outputs may easily be lost or overwritten, especially when you create several reports after each other.

With ChemStation OpenLAB Option, ChemStation automatically tracks any report that was generated. In order to reproduce an old or overwritten report, select **Report > Report History**. Here, you can see all reports created for the current data file since the installation of ChemStation OpenLAB Option. You can also export or print this history.

ECM Audit Trail

Audit Trail is a record showing who accessed the system and what operations he or she performed during a given period of time.

You can view file-related, system administration, folder administration, and scheduler-related entries. For example, you can see when a file was added and who added it.

For each operation, ECM asks the user for a reason. This reason is also shown in the ECM Audit Trail. For automatic uploads there are default reasons given by the system. The reason entry may be optional or mandatory, depending on

the ECM configuration (see “[Account configuration](#)” on page 89). If the system is configured to be compliant to 21 CFR Part 11, providing a reason is mandatory.

To enable the ECM Audit Trail

You can enable the ECM Audit Trail only for a complete ECM Account. To activate the ECM Audit Trail, you must select the check box **Enable audit trail for this account** when creating a new account.

There is no possibility to activate the ECM Audit Trail afterwards for an existing account, or to deactivate the ECM Audit Trail again.

NOTE

If the system shall be compliant to 21 CFR Part 11, the ECM Audit Trail must be enabled.

To view the ECM Audit Trail for a specific file

- 1 In ECM, right-click the respective file and select **Properties** from the context menu.
- 2 In the **File Properties** dialog, select the **Audit Trail** tab.

All actions related to this specific file are listed here, together with the date, ECM user name who performed the action, and a reason provided by the according user.

To view the ECM Audit Trail for all files

- 1 In ECM, select the **Administration** page.
- 2 In the Navigation Pane, select the **Activity Log > Audit Trail** node.

All actions related to any ECM file are listed here, together with the file name, date, ECM user name who performed the action, and a reason provided by the according user.

You can search the entries, for example, for a specific date or date range, or for entries related to specific categories (Files, Folders, System, Scheduler, or Instrument). Also you can print the entries or export them to a file.

ECM System Log

The System Log is a record that shows changes to the system, including configuration changes, e-mail notifications, and additions or changes of Locations, Cabinets, Drawers, or Folders.

You can view file-related, system administration, folder administration, or Scheduler-related entries. For example, you can see when a Location was added and by whom.

The System Log is always active; you do not need to enable it.

To view the ECM System Log

- 1 In ECM, select the **Administration** page.
- 2 In the navigation pane, select the **Activity Log > System Log** node.

All general actions related to ECM are listed here, together with the date, ECM user name who performed the action, and a reason provided by the respective user. Depending on the ECM Account administration, the reason may be optional or mandatory (see “[Account configuration](#)” on page 89).

You can search the entries, for example, for a specific date or date range, or for entries related to specific categories (Files, Folders, System, Scheduler, or Instrument). Also you can print the entries or export them to a file.

Administration in ECM

When you install ChemStation OpenLAB Option, you need to carry out certain basic configuration tasks in ECM (see [“Installation and Configuration Tasks on ECM Server”](#) on page 22). In addition, there are several other settings in ECM that are relevant with regard to 21 CFR Part 11. These settings are described in the following section.

Account configuration

To configure the ECM Account

- 1 In ECM, select the **Administration** page.
- 2 In the Navigation Pane, select the **Account Administration** node.
- 3 Double-click the **Configuration** item.

The **Account Administration** dialog opens.

The screenshot shows the 'Account Administration' dialog box with the 'Configuration' tab selected. The dialog is divided into several sections:

- Security:** Includes checkboxes for 'Lockout users after:' (with a text box for 'unsuccessful login attempts') and 'Inactivity timeout:' (with a text box for 'minutes'). There is also a 'Minimum password length:' field with the value '6'.
- System email addresses:** Includes text boxes for 'System administrator email:' and 'Archive administrator email:'.
- File upload options:** Includes a checked checkbox for 'Require entry in Reason fields.'
- Network logon:** Includes a note 'This user is responsible for obtaining the User and Group Lists from the domains.', a 'Username:' field with the value 'company\User' and an example 'Example: domain\username', and a 'Password:' field with masked characters.
- Cluster configuration:** Includes buttons for 'Application Service ...' and 'File Transfer Server ...', and a 'Transfer protocol:' field with the value 'HTTP'.

At the bottom right, there are 'OK' and 'Cancel' buttons.

5 Administration Regarding 21 CFR Part 11 Compliance

Administration in ECM

Setting	Description	21 CFR Part 11 Requirements
Lockout	If a user tries too often to log in with invalid user credentials, he is locked out of the system and cannot log in any more – not even with valid user credentials. You can define the number of allowed login attempts.	You should limit the number of allowed login attempts to three.
Inactivity Timeout	If a user does not perform any action in ChemStation for the given period of time, he is automatically logged out. The same applies to the ECM Web Client.	You should specify a timeout.
System administrator email	The e-mail address you provide here will automatically be notified when a user was locked out after too many unsuccessful login attempts.	You should provide an e-mail address.
Minimum Password Length	If users change their passwords, they must choose a password with at least the given number of characters. The default setting is 5.	You should require a minimum password length of at least 5 characters.
Require entry in Reason fields	In each ECM Audit Trail or System Log entry the users can enter a specific reason for the action. If this check box is selected, the entry is mandatory.	The ECM Audit Trail and System Log reasons must be mandatory.

Users/Groups/Roles

To configure the password settings for an ECM Account according to the password policy

NOTE

21 CFR Part 11 requires that company/the laboratory has a password policy.

- 1 In ECM, select the **Administration** page.
- 2 In the navigation pane, select the **Account Administration** node.
- 3 Double-click the **Users/Groups/Roles** item.

The **Account Administration** dialog opens.

21 CFR Part 11 does not define any specific rules for the password settings. However, your company must have defined a password policy. You may consider the following settings:

- User cannot change password
- User must change password after next login

Note that the minimum password length is defined in the ECM Account configuration (see “[Account configuration](#)” on page 89).

Roles and folders

ECM allows you to assign specific roles to users or user groups. This can be done at the global level for the entire ECM Account, or individually for specific folders. For example, a specific user group may have the **Contributor** role for folder A, but at the same time have only the **Reader** role for folder B.

Preparations

If you want to assign roles at the folder level, you must first enable this feature in ECM. The setting is valid for the complete ECM Account.

To enable roles for folders:

- 1 In ECM, select the **Administration** page.
- 2 In the navigation pane, select the **Account Administration** node.
- 3 Double-click the **Users/Groups/Roles** item.
The **Account Administration** dialog opens.
- 4 On the **Roles** tab, select the required role and click **Edit**.
- 5 Select the **Available in folder access tab** check box.

Administration of ChemStation Settings

ChemStation Administration Tool

The ChemStation Administration Tool offers a number of functions which are helpful if the ECM Server is down and the connection from the ChemStation client to the ECM Server is lost. As one of these functions is to switch off the mandatory ECM login, the access to the ChemStation Administration Tool is strictly limited. The ChemStation Administration Tool can only be started by users who are a member of the local user group **CSAdministrators** (see [“Enabling users to start the ChemStation Administration Tool”](#) on page 33).

To start the ChemStation Administration Tool:

- 1 From the Start menu in the Task Bar, select **Start > All Programs > Agilent ChemStation > ChemStation Administration Tool**.

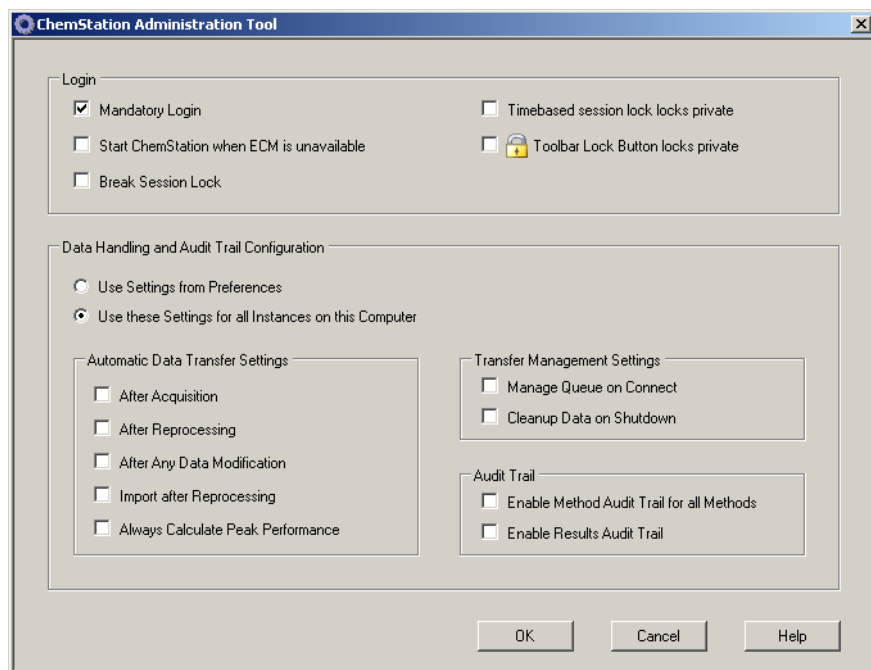


Figure 22 ChemStation Administration Tool

Login options

The following check boxes are relevant in case of an emergency, that is, if the ECM Server is down:

- **Mandatory Login:** If you clear this check box, all ChemStation instances on this client can be started without an ECM login. If the ECM login used to be mandatory and the ECM Server is down, clearing this check box can be used to make ChemStation accessible again.

NOTE

Be aware that, as a consequence, the privileges of the ChemStation users are now unlimited. The users have access to all ChemStation functions.

- **Start ChemStation when ECM is unavailable:** If you select this check box, the ChemStation can be started when the ECM server is unavailable even if **Mandatory Login** is enabled. The Login dialog at startup of ChemStation can be cancelled. With this option selected, any user can continue to work in ChemStation in case the server is down without contacting a user who has access to the Administration Tool.

NOTE

Be aware that, as a consequence, the privileges of the ChemStation users are now unlimited. The users have access to all ChemStation functions.

- **Break Session Lock:** If you select this check box, a locked ChemStation can be accessed by any user just by clicking **Cancel** in the **Login** dialog. If a ChemStation is currently locked and the ECM Server is down, selecting this check box is the only possibility to regain access to the current ChemStation session.

NOTE

Be aware that, as a consequence, the user who regained access to ChemStation now has unlimited access to all ChemStation functions.

The following check boxes allow you to configure the timebased session lock and the ChemStation toolbar Lock Button:

- **Timebased session lock locks private:** If you select this check box, the time based session lock will lock the ChemStation sessions privately. Otherwise, the timebased session lock will be non private.

- **Toolbar Lock Button locks private:** If you select this check box, the ChemStation toolbar lock button will lock the ChemStation session privately. Otherwise, a non-private lock will be applied.

Data Handling and Audit Trail Configuration

The ChemStation Administration Tool offers to conveniently configure all ChemStation instances on a client at the same time with the same settings. By default, the option **Use instance specific settings** is selected, so that the settings are not overwritten.

To change the settings for all ChemStation instances

- 1 Select the option **Use these settings for all instances on this computer**.
- 2 Select the required check boxes. The settings are the same as in the **Preferences** dialog (see “[ECM Preferences](#)” on page 44).
- 3 Click **OK**.

Electronic Signature

Electronic signatures provide a means to sign documents as equally binding as a handwritten signature. In addition, electronic signatures are reproducible, because they are recorded in a secure, time stamped audit trail. Manipulation is prevented by enabling only users with specific privileges to sign electronically.

An electronic signature contains the user name (full name), date, and time when the signature was applied, the location where the signing occurred, and a user-configurable definition associated with the signature. The signature is always related to the complete SSIZIP container, not to a single file inside the container.

CFR 21 Part 11 requires that companies, especially ones that employ any type of approval process, use electronic signatures. With the help of the Agilent OpenLAB Business Process Manager (BPM) module, you can create highly automated review or approval processes including e-mail notification.

Preparation

Privileges

An ECM user needs to have the privilege **Content: File Signatures** in order to be able to sign electronically. This privilege is, for example, assigned to the ECM default role: **:Approver**.



Reasons for the signature

With each signature the ECM users must either select a given reason or, if they are allowed to, provide their own reason.

To configure the reasons for signatures:

- 1 In ECM, select the **Administration** page.
- 2 In the navigation pane, select the **Account Administration** node.
- 3 Double-click the **Electronic Signature** item.

The **Account Administration** dialog opens.

- 4 To provide a new reason, enter the required text into the **Reasons** field and click .
- 5 To delete an existing reason, select the reason in the **Default reasons** list and click .
- 6 If you want to allow users to provide their own reason with a signature, select the **User can specify reason** check box.

NOTE

If you clear this check box, the users can only select one of the given default reasons.

- 7 If necessary, adjust the timeout settings:
 - The **Signature screen timeout** defines, how long an e-signature dialog will stay open if no signature is submitted. The default setting is 5 minutes.
 - The **Consecutive signature timeout** is relevant if an ECM user carries out several successive e-signatures. If the next e-signature takes place within the given timeout interval, the **location** and the **reason** provided in the first e-signature will be pre-filled in the next dialog. The default setting for the consecutive signature timeout is 5 minutes.

Using electronic signatures

To apply an electronic signature

- 1 Right-click the required SSZIP container and select **Electronically Sign > Electronic Signature** from the context menu.

The **Electronic Signature** dialog opens.

NOTE

The other command in the context menu, **Electronically Sign > Acrobat Plug-In Signature**, works only for PDF documents and only if you purchased the according plugin. It enables you to add signatures directly inside PDF documents.

- 2 Enter your ECM user credentials (username, password, and domain).


- 3** Enter your current location. With this information, the location from where you provide the signature is reproducible.
- 4** Select a reason for the signature from the **Default reason** drop-down list.
- Or -
Select the **User specified** check box and enter a different reason into the text field. Note that this option is only available if the ECM Account is configured accordingly.
- 5** Click **Sign**.
The file is now signed electronically. The e-signature is shown in the file properties in the **eSig** tab. The e-signature is also included in the ECM Audit Trail.

To view electronic signatures

The user preferences in ECM can be configured in such a way that the number of e-signatures applied to a file is shown by default in the ECM content display, together with the file name and status.

The electronic signature itself is shown in the file properties in the **eSig** tab, and it is also part of the ECM Audit Trail.

To adjust the user preferences:

- 1** In ECM, select the **Administration** page.
- 2** In the navigation pane, select the **Account Administration** node.
- 3** Double-click the **User Preferences** item.
- 4** Click **Modify...** to modify the column settings.
- 5** Select **# of signatures** and click  to add this property to the selected columns.
- 6** Click **OK**.

The number of e-signatures is then shown on every content page in ECM.

5 Administration Regarding 21 CFR Part 11 Compliance

Electronic Signature



6 Custom Fields

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This chapter explains the purpose and usage of custom fields in ChemStation.



About Custom Fields

ChemStation provides numerous fields in which you can enter information on a sequence, specific samples, or the expected compounds. These fields are sufficient for many standard analysis tasks. However, for some specific tasks you may need to save additional information on the samples or compounds. In this case, you can define the so-called *custom fields*.

Custom fields are available for sample information and for compound information. The custom fields definition is saved as part of the method definition. When you define custom fields, you can define a suitable field name and data type for the additional information, according to your needs.

After you have defined the custom fields, you can enter the actual values in the sequence table of the current sequence. These values will be shown on ChemStation reports and are available also for OpenLAB Intelligence reports. In OpenLAB Intelligence reports, the values can even be used for calculations or statistical evaluations.

In addition, you can use custom fields to flag all samples related to a specific project or study. This flag is then used by OpenLAB Intelligence Reporter to find all results related to this specific project or study.

Setting Up Custom Fields

The custom fields definition is part of the method. You can define up to ten custom fields related to the samples, and up to ten custom fields related to the compounds. Also, you can import the custom fields definitions from another, existing method.

To define new custom fields

- 1 Select the **Method and Run Control** view.
- 2 Load the required method.
- 3 Select **Method > Custom Fields Setup**.

The **Set up Custom Fields definitions** dialog opens. It contains two sections, one for sample custom fields, and one for compound custom fields.

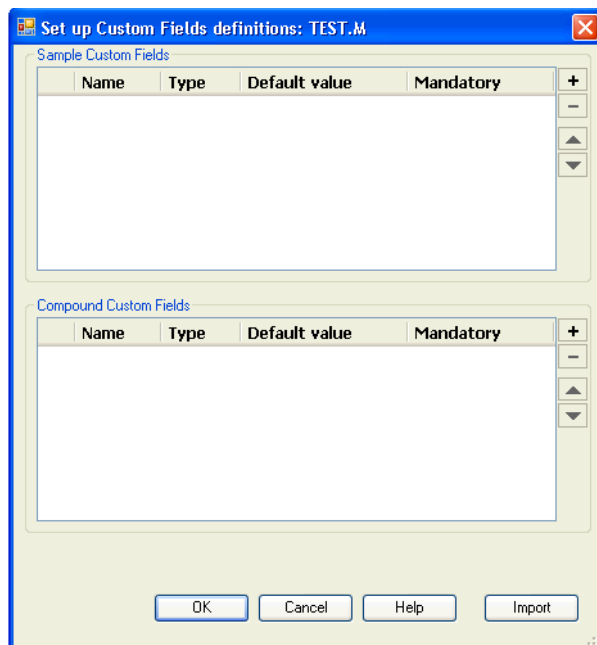






Figure 23 Set up Custom Fields definitions dialog

- 4 Click  to add a new custom field in the according section.
- 5 Enter a suitable name for the new custom field (for example, *Color*).

NOTE

If you create sample custom fields named **Project** or **Study**, these custom fields will be reported twice in the .acaml file: in the regular custom fields section, and also in the projects/study mapping. This enables OpenLAB Intelligence Reporter to find all results related to a specific project or study.

- 6 Select a suitable data type (for example, *TEXT*).
- 7 If appropriate, enter a default value (for example, *Blue*).
- 8 If appropriate, select the **Mandatory** check box to ensure that the custom field is always filled.

If you make a custom field mandatory, you should also provide a default value.
- 9 If required, click  to delete a selected custom field.
- 10 If required, adjust the order of the custom fields with the *Up*  and *Down*  buttons.

To import custom fields from an existing method

- 1 Make sure the method with the custom fields is available in your local file system.
- 2 Load the target method (the one to which you want to import the custom fields definition).
- 3 Select **Method > Custom Fields Setup**.
- 4 Click **Import**. A dialog opens where you can select the source method from the local file system.
- 5 Click **OK**.

Specifying Custom Fields Values

The specific values of the predefined custom fields depend on the actual sequence. Therefore, the values are specified in the sequence table.

To provide sample custom fields values

- 1 In the **Method and Run Control** view, load the required sequence.
- 2 Select **Sequence > Sequence Table** to open the sequence table.
- 3 Click **Custom Fields**.

The **Set up Custom Fields values** dialog opens. The **Sample Custom Fields** tab is active. Each predefined custom field is shown in a separate column. Mandatory custom fields are marked with (*) in front of the field name.

The lines correspond to the lines in the sequence table.

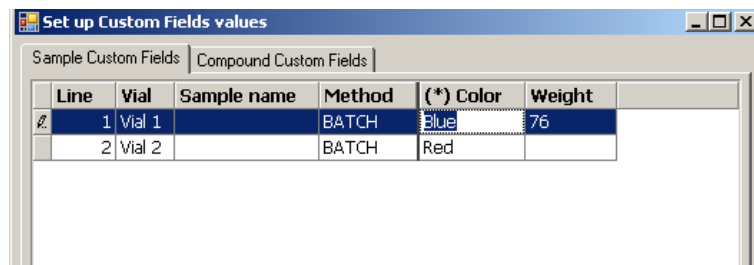


Figure 24 Set up Custom Fields values - Sample Custom Fields

- 4 Enter the required values for each sample and custom field.

NOTE

You can only start a sequence after the mandatory fields have been completed.

To provide compound custom fields values:

- 1 Select the **Compound Custom Fields** tab.

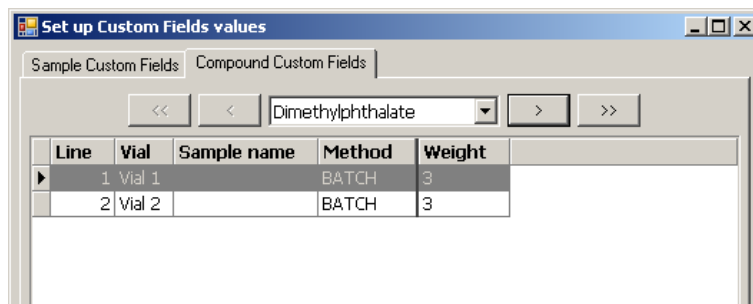


Figure 25 Set up Custom Fields values - Compound Custom Fields

NOTE

This tab is only available if compounds have been set up in the method's calibration table.

- 2 Select the required compound from the drop-down list at the top, or click **<<**, **<**, **>**, or **>>** to navigate to the required compound.
- 3 Enter the required values for each sample and custom field.
- 4 Select the other compounds and provide the values accordingly.
- 5 Click **OK**.

Reporting of Custom Fields

Custom fields values are always saved to ECM and are therefore always available in OpenLAB Intelligence Reporter. However, they are not automatically shown in ChemStation reports. If you want to display the custom fields in your ChemStation reports, you must first adjust the report options.

To display custom fields in ChemStation reports

- 1 Select the **Data Analysis** view.
- 2 Select **Report > Specify Report**.
- 3 Select the check boxes **Add Sample Custom fields to Sample info** and **Add Compound Custom fields**.
- 4 Click **OK**.

The custom fields and the according values are then displayed on ChemStation reports (see examples below).

Data File C:\CHEM32\1\DATA\TEST 2008-04-07 16-09-40\002-0201.D

```
=====
Acq. Operator   :                               Seq. Line :    2
Acq. Instrument : Instrument 1                   Location  : Vial 2
Injection Date  : 4/7/2008 4:12:16 PM           Inj       :    1
                                                Inj Volume : 5 µl
Sequence File   : C:\Chem32\1\DATA\TEST 2008-04-07 16-09-40\TEST.S
Method          : C:\Chem32\1\DATA\TEST 2008-04-07 16-09-40\BATCH.M
Last changed    : 4/7/2008 4:09:19 PM
```

Sample-related custom fields:

Name	Value
Color	Red
Weight	

Figure 26 Sample custom fields

6 Custom Fields

Reporting of Custom Fields

```
3  2.568      0.0000   0.00000  0.00000 Biphenyl
4  5.846      0.0000   0.00000  0.00000 o-Terphenyl
```

```
Totals :                      0.00000
```

```
1 Warnings or Errors :
```

```
Warning : Calibrated compound(s) not found
```

```
=====
```

```
Compound-related custom fields:
```

```
Corr. Exp. RT [min]:0.747021   Dimethylphthalate
```

```
-----|-----
Name                                     |Value
```

```
-----|-----
Weight                                 3
```

```
Corr. Exp. RT [min]:1.021871   Diethylphthalate
```

```
-----|-----
Name                                     |Value
```

```
-----|-----
```

Figure 27 Compound custom fields

Reprocessing with Custom Fields

It is possible to modify the values of the custom fields during reprocessing. When you prepare the reprocessing, you can edit the custom fields values in the Sequence Table in the *Data Analysis* view. For more information on editing custom fields values, see [“Specifying Custom Fields Values”](#) on page 103.

After an acquisition, you can only edit the values of existing custom fields, that is, custom fields that were defined in the method used for the acquisition. You can not add new custom fields afterwards, even if the method used for reprocessing contains different custom fields than the original method.

6 Custom Fields

Reprocessing with Custom Fields



7

Treatment of ChemStation Legacy Data and Data Migrated from ChemStore

Introduction 110

Sequence Container Migration 111

Conversion of Data Migrated from ChemStore 113

This chapter provides information on migrating legacy ChemStation sequence data to sequence container format, in order to be able to upload these data sets to ECM.



Introduction

When ChemStation OpenLAB Option is installed, **Unique Folder Creation** can not be switched off. All sequence data sets that are acquired are therefore stored as sequence container. Please refer to the manual *“Getting Started with New ChemStation Workflow”* for more details on working with **Unique Folder Creation**.

The sequence container format of sequences is essential for upload to ECM. Therefore ChemStation legacy sequence data acquired with ChemStation prior to B.02.01 or while **Unique Folder Creation** was off, have to be migrated to sequence container format before they can be uploaded to ECM.

Legacy ChemStore data that have been migrated to ECM can also be converted to be reviewed in the Navigation Table.

Sequence Container Migration

ChemStation provides a tool to migrate non-container data to sequence container format. To successfully perform this task, it is required that the original sequence file is still available. It must contain all the necessary sequence lines and follow the original data file naming scheme to reprocess all the data files of the sequence. In addition, all the methods in the Method column of the sequence table have to be available.

To perform migration,

start the **Sequence Container Migration** from the **Sequence** menu in **Data Analysis** view.

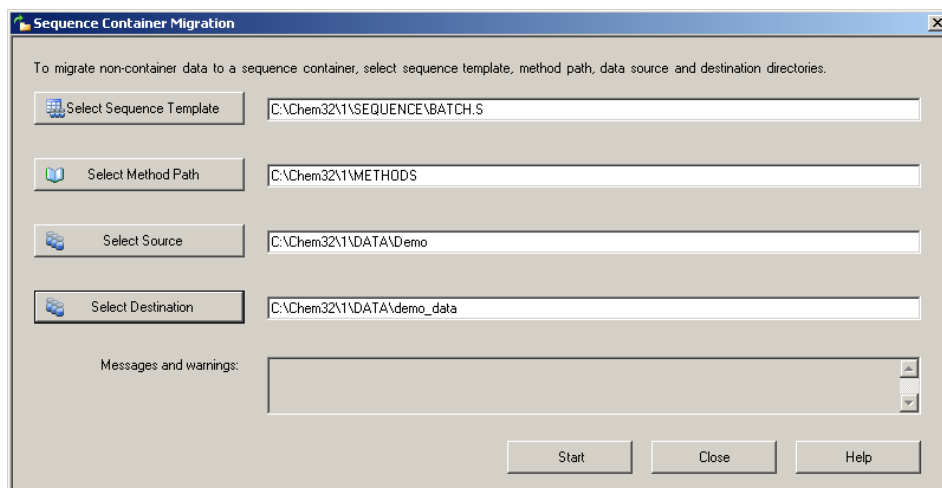


Figure 28 Sequence Container Migration

Fill in the following required fields (see [Figure 28](#) on page 111):

Select Sequence Template: Select the sequence file .S that contains the sequence table that matches the data set to be migrated.

Select Method Patch: Select the directory where the methods are located that are referenced in the sequence table.

Select Source: Select the directory that contains the data files to be migrated.

7 Treatment of ChemStation Legacy Data and Data Migrated from ChemStore

Sequence Container Migration

Select Destination: Specify the path and name of the sequence container to be created. You may select an existing folder or create a new one.

When all fields are filled in, the migration can be started.

The following steps will be performed:

- The sequence container directory will be created.
- The sequence template will be copied to the container. It will also be converted to a state where it is able to reprocess data files in **Data Analysis** view.
- The methods referenced in the sequence table are copied from the specified method path to the container folder.
- The data files, the sequence logbook, and the batch file are copied from the data source directory to the destination directory.
- According to the information in the sequence table, a copy of the corresponding method is copied to each data file as DA.M.

When the container migration is completed, a success message is displayed in the **Messages and Warnings** field. Otherwise a warning message indicates any problem during migration. Details about the warning can be obtained by double-clicking the warning message.

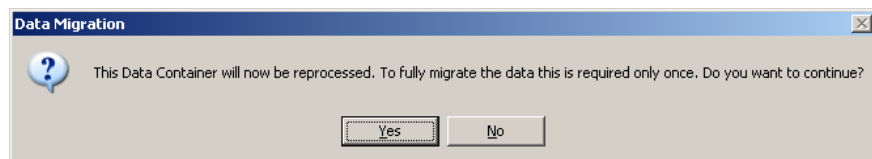
Conversion of Data Migrated from ChemStore

When ChemStore sequence data have been migrated to ECM, they are already available in the form of .sc.szip files and thus ready to be downloaded into ChemStation Data Analysis view. However, such sequence containers have to be converted to be ready for review in the Navigation Table.

The conversion process is started automatically after downloading the data from ECM:

- 1 Select **ECM > Load Data** and select the data set you want to view in ChemStation.

A message is displayed that the sequence data will be reprocessed. Press **Yes** to continue.



NOTE

If you press **No**, the local copy of the data set will be deleted immediately.

- 2 When asked to save the sequence file, press **Yes**.

In order to prevent printing reports for the reprocessing step for conversion, the **Sequence Output** settings of the sequence are changed in the following way:

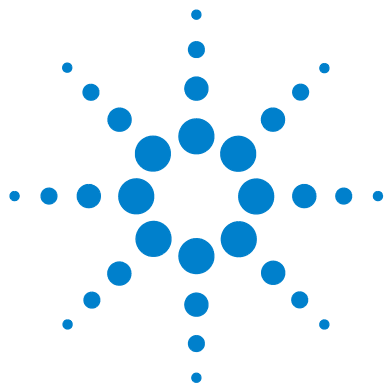
- **Print sequence summary report:** on
- **Report to printer:** off
- **Report to file:** off
- **Report to PDF:** off
- **Report to HTM:** off
- **Print individual report for each run as well:** off

- 3 Now you can review or reprocess the sequence data.

If the sequence container is uploaded to ECM after conversion (either automatically after reprocessing or manually), the new versions of the sequence can be loaded into ChemStation without further conversion steps later on.

7 Treatment of ChemStation Legacy Data and Data Migrated from ChemStore

Conversion of Data Migrated from ChemStore



8 Interface to OpenLab Intelligence Reporter

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Template selection in Sequence Output [124](#)

Automatic Creation of OpenLAB Intelligence Report at the End of the Sequence [125](#)

OpenLAB IR commands in the ECM menu [125](#)

Calculation of performance values [126](#)

This chapter provides information on the integration of OpenLAB Intelligence Reporter in Agilent ChemStation.



Introduction

Agilent OpenLAB Intelligence Reporter provides advanced reporting functions for any chromatographic data generated by Agilent ChemStation or Agilent OpenLAB ICM. The reports are based on the standardized ACAML 1.1 or 1.2 data, which is automatically generated by ChemStation (B.02.01.SR1 or higher, with ChemStation OpenLAB Option).

OpenLAB Intelligence Reporter enables you to generate knowledge by creating various types of intelligent reports:

- Sequence reports with summary calculations and statistics
- Reports of complex tests with condensed information, for example by visualizing key results or by presenting trend charts
- Reports presenting decision-based results (for example, with flagged outliers, or with results automatically sorted by pass/fail criteria)

You can either use OpenLAB Intelligence Reporter to report the results currently shown in ChemStation, or you can define the required data in the Reporter Client.

NOTE

For more detailed information on OpenLAB Intelligence Reporter, please see the OpenLAB Intelligence Reporter documentation.

ACAML version

ChemStation stores all data in the ACAML format (ACAML = Agilent Common Analytical Markup Language), which results in .acaml files. There is one .acaml file for each sequence or single run. When the data is uploaded to ECM, the .acaml file is part of the SSIZIP sequence container. OpenLAB Intelligence Reporter uses the data provided in these .acaml files.

In ChemStation B.04.02, the ACAML schema is updated from version 1.1 to 1.2. This version 1.2. of the ACAML schema is only supported by OpenLAB Intelligence Reporter revision A.02.01.

Data flow - example

When using ChemStation together with ECM and OpenLAB Intelligence Reporter, data is transferred at different times from the ChemStation client to the ECM Server and back. There are several possible scenarios for the data flow, depending on the workflow you follow.

As an example, the following figure shows the data flow for creating a single sequence report.

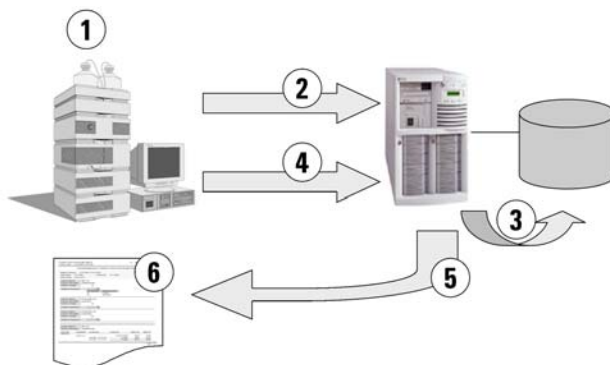


Figure 29 Example: Data flow for creating a single sequence report

1 In ChemStation:

- You select a report template for the OpenLab Intelligence Reporter in the Sequence Output.
- If the report is to be created automatically at the end of the sequence, you select **Preview at end of sequence** in the Sequence Output.
- You select the Automatic Data Transfer Setting **After Acquisition**.
- You start the sequence.

2 After the acquisition, all data is automatically transferred to ECM.

3 The result data and metadata is automatically extracted from the .acaml files into the Reporting Database.

4 In ChemStation: You trigger the creation of the report by clicking **Create OpenLAB Intelligence Report**. If **Preview at end of sequence** was selected in the Sequence Output, the report is created automatically without additional user interaction.

- 5 The previously selected report template is automatically applied to the new sequence data. The resulting report is transferred to the ChemStation client computer.
- 6 The resulting OpenLAB IR report is shown in ChemStation.

Prerequisites

If you want to use OpenLAB Intelligence Reporter, the following prerequisites must be met:

- OpenLAB ECM is installed.
- OpenLAB Intelligence Reporter is installed.
- ChemStation OpenLAB Option is installed.
- The chromatographic data has been uploaded to ECM.

Typical reporting workflows

Depending on the scenario, there are different workflows when working with OpenLAB Intelligence Reporter. Typically one of the following workflows applies:

- **Single Sequence OpenLAB Summary Report** (see [“To create a Single Sequence OpenLAB Summary Report”](#) on page 123)

A single sequence is acquired in ChemStation, and the data is reviewed in ChemStation first. The OpenLAB summary report is created for this single sequence only.

- **Multiple Sequence Summary Report**

Multiple sequences are acquired over time (days to weeks). A user subsequently searches for these sequences, and creates a summary report for the selected sequences.

- **Study/Project Summary Report**

A large number of sequences (10's to 100's) are acquired over time (weeks to months). A user searches for *all* data for these sequences and creates a complex study summary report based on these data.

NOTE

Only the *Single Sequence Summary Report* can be directly generated from ChemStation. For the other two reporting workflows, you need to perform all tasks in OpenLAB Intelligence Reporter. See the OpenLAB Intelligence Reporter documentation for more details.

NOTE

When printing an *Intelligence Report* directly in the ChemStation only a report based on the latest version of the data can be created. For reports based on earlier versions the report template has to be modified, or the report has to be created in the OpenLAB Intelligence Reporter software.

Example reports

The reports generated by OpenLAB Intelligence Reporter can include a wide variety of information, such as:

- Custom calculations (e.g. summary calculations, statistics, and complex tests)
- Decision-based result presentation (flag outliers, automatically sort results by pass/fail criteria, etc.)
- Search-based report content selection
- Condense information by visualizing key results (e.g. in trend charts)

In addition, interactive reports can be based upon specific parameters, such as a date range, or the reports can contain expandable detail information.


See the following figures as an example.

8 Interface to OpenLab Intelligence Reporter

Introduction

Sequence Summary Report ChemStation

Report Creation Date: 5/2/2008 5:08:30 PM



Agilent Technologies

Sequence Name: LIR-2008-1-2007-02-28_14-25-40

Location: \WAD_Location\Laboratory 2\Data\LIR Data

Rev: 1

Sequence Description: Third Sequence for Agilent OL Reporting

Acquired by: R. Honsberg **Acq Date:** 2/28/2007 3:42:40 PM

Reprocessed by: R. Honsberg **Rep. Date:** 3/1/2007 9:08:04 AM

Acq. Instrument: AT1200

Line #	Sample Name Data File Name	Type Calib Lvl	Vial# Multipl.	Num Inj Dil Fact	Injection Date/Time Sample Amount	Analysis Method Manually Int Y/N
1	Solvent 1DA-0101.D	Control	P1-D-01 1	1	2/28/2007 1:26:00 PM 0	XSR_MDA.M No
2	SS Resolution 1FA-0201.D	Control	P1-F-01 1	1	2/28/2007 1:31:01 PM 0	XSR_MDA.M No
3	SS RSD 1 1FB-0301.D	Control	P1-F-02 1	1	2/28/2007 1:36:05 PM 0	XSR_MDA.M No
4	Standard L1	Calibration	P1-F-04 1	1	2/28/2007 2:05:27 PM	XSR_MDA.M

Results Calibration Standards for Level: 1

#	Name	Inj#	Datefile	des-hyd cis tramadol (C) DAD1 A, Sig=270.8 Ref=508,100			TRAMADOL DAD1 B, Sig=254.10 Ref=450,100			trans-trama DAD1 A, Sig	
				RT	Area	Amount (I)	RT	Area	Amount (I)	RT	Area
4	Standard L1	1	1FD-0401.D	2.52	0.68	0.8156	1.57	206.54	999.922	1.43	
10	Standard L1	1	1FD-1001.D	2.52	0.67	0.8079	1.57	206.58	1000.0276	1.43	
16	Standard L1	1	1FD-1601.D	2.52	0.68	0.819	1.57	206.27	998.9758	1.43	
22	Standard L1	1	1FD-2201.D	2.52	0.65	0.7964	1.57	206.33	999.4256	1.43	
Average				2.52	0.67	0.8098	1.57	206.43	999.5877	1.43	
Stand. Dev				0	0.01	0.01	0	0.15	0.4851	0	0.01
Min				2.52	0.65	0.7964	1.57	206.27	998.9758	1.43	0.49
Max				2.52	0.68	0.819	1.57	206.58	1000.0276	1.43	0.52

Results QC Samples

#	Name	Inj#	Datefile	des-hyd cis tramadol (C) DAD1 A, Sig=270.8 Ref=508,100			TRAMADOL DAD1 B, Sig=254.10 Ref=450,100			des-hyd trans tramadol (B)	
				RT	Area	Amount (I)	RT	Area	Amount (I)	RT	Area
2	SS Resolution	1	1FA-0201.D	2.52	4.41	5.4052	1.63	0.5	1.678	2.64	3.27
3	SS RSD 1	1	1FB-0301.D	2.52	0.67	0.8085	1.57	205.84	997.0556	2.65	0.52
		2	1FB-0302.D	2.52	0.66	0.7946	1.57	205.85	997.1232	2.64	0.5

Figure 30 Multi-sequence summary report

- (1) Report header with company logo
- (2) Sequence information
- (3) Sequence table
- (4) Results for calibration standards

- (5) Statistical calculations
- (6) Results for quality control samples, grouped by sample name

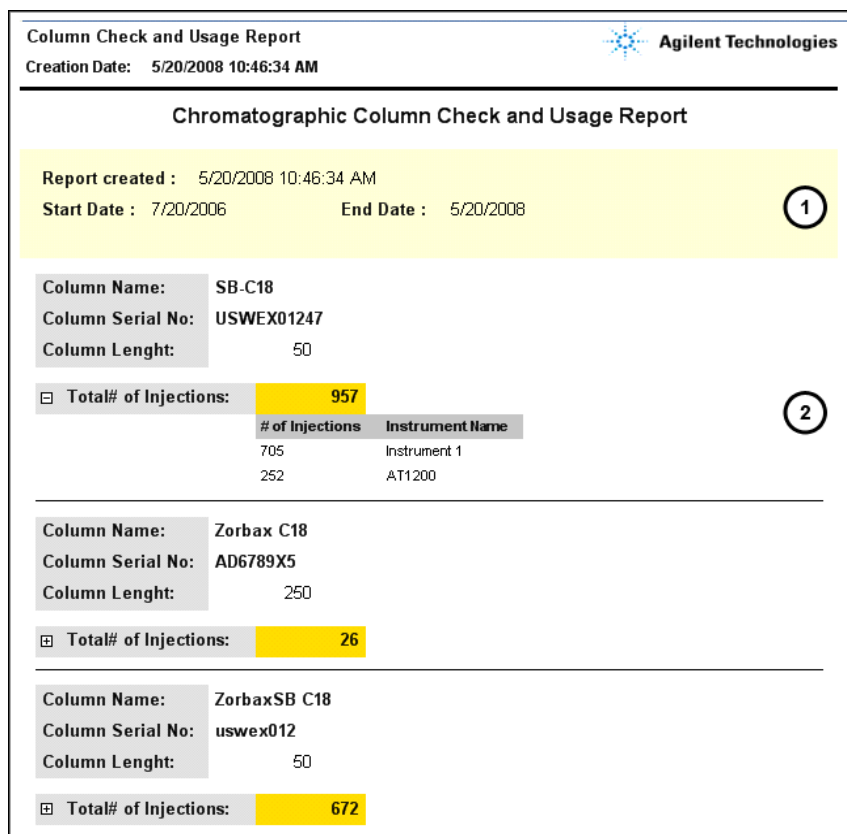


Figure 31 Interactive column usage report

- (1) User parameters (here: **Start Date** and **End Date**) as selected by the user
- (2) Expandable detail information

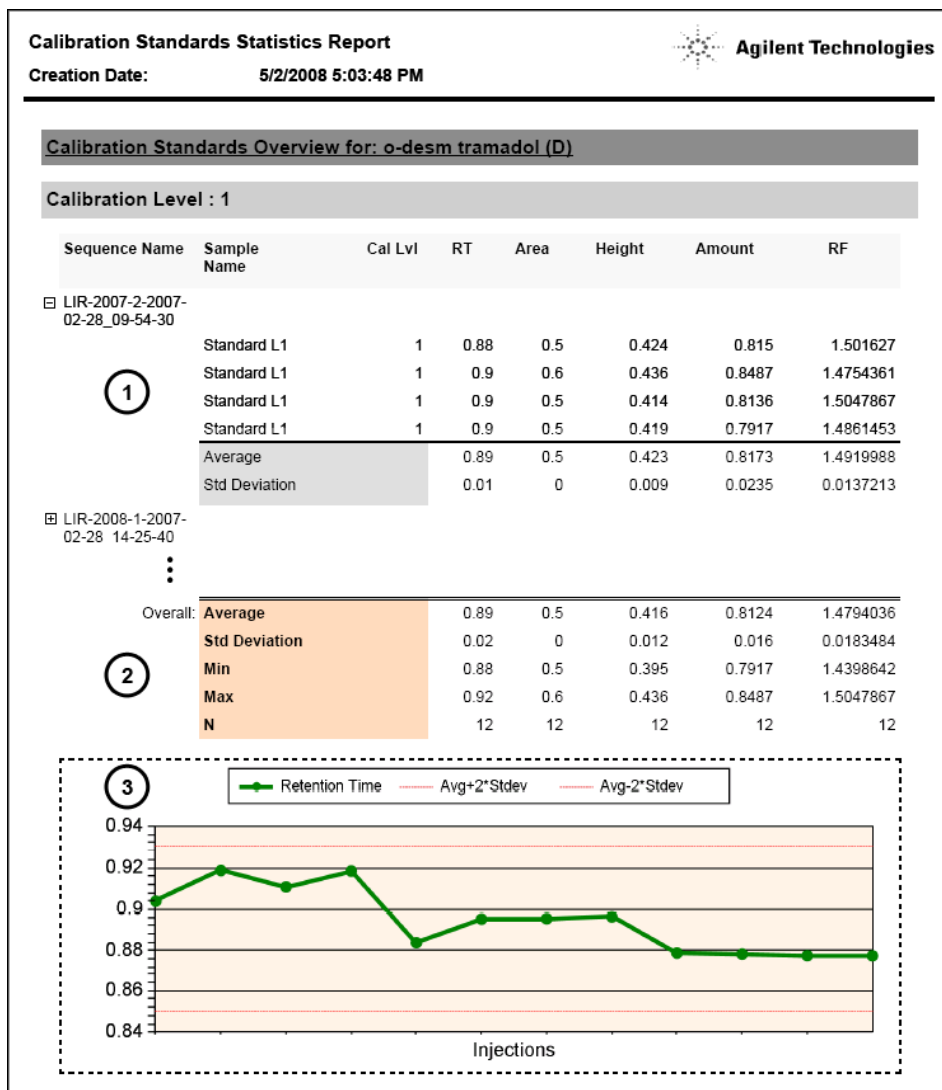


Figure 32 Cross sequence statistics with trend chart

- (1) Expandable detail information on each sequence
- (2) Overall statistics
- (3) Trend chart

To create a Single Sequence OpenLAB Summary Report

- 1 Prepare the data in ChemStation. There are different ways of preparing the data (see “[Data-related workflows](#)” on page 59). For example, run a sequence with the Transfer Setting **After Acquisition**.

NOTE

Make sure the data has been uploaded to ECM.

- 2 In the **Data Analysis** view, load the relevant data set.
- 3 Under **Sequence > Sequence Output**, select a suitable OpenLAB IR template.
- 4 Select **ECM > Create OpenLAB Intelligence Report**.

The resulting OpenLAB IR report is opened with the data of the current sequence.

Interface Components Concerning OpenLAB IR

If OpenLAB Intelligence Reporter is installed, several new interface components are available in ChemStation. These components are described in the following.

Template selection in Sequence Output

Under **Sequence > Sequence Output**, you can select an **OpenLAB Intelligence Report Template** for the currently loaded sequence. This setting is optional.

- If you select a specific report template:
When you create a report, OpenLAB Intelligence Reporter automatically uses the given report template. The resulting report is shown in OpenLAB Intelligence Reporter without any further inquiry.
- If you do not select any specific report template:
When you create a report, OpenLAB Intelligence Reporter opens with the relevant data already selected, but without applying any specific report template to the data. You must open a suitable report template manually in the OpenLAB IR Reporter Client.

NOTE

On an ECM installation with multiple accounts, projects from *all* accounts are visible in the **Projects** menu of OpenLAB Intelligence Reporter! Ensure that you select a project belonging to the ECM Account you are working on.

This is not an issue when selecting a template directly from ChemStation, as you select the template from the LCDF structure of the specific ECM Account you are working on.

Depending on the options selected in the OpenLAB IR Reporter Client, the report is either generated automatically after loading the template or must be generated manually.

The link to the selected report template is stored in the sequence parameters. Thus, when you create the report the next time, the report template will be automatically applied.

You can select a different report template in OpenLAB Intelligence Reporter at any time. The setting in the Sequence Output in ChemStation is only used as a default setting.

Automatic Creation of OpenLAB Intelligence Report at the End of the Sequence

Under **Sequence > Sequence Output**, you can select **Preview at end of sequence** for the currently loaded sequence template. This setting is optional. It requires that an OpenLAB Intelligence Report Template is also selected.

With this setting enabled, the OpenLAB Intelligence Report will be created automatically at the end of sequence acquisition or sequence reprocessing based on the selected template.

OpenLAB IR commands in the ECM menu

In the **ECM** menu, there are two commands related to OpenLAB Intelligence Reporter:

- **Start OpenLAB IR**



This command opens OpenLAB Intelligence Reporter. No data is passed from ChemStation to the Reporter Client. You can select the required data directly in the Reporter Client.

- **Create OpenLAB IR Report**



After acquiring or reprocessing sequence data, you can create a report in OpenLAB Intelligence Reporter as soon as the data has been uploaded to ECM. The report is based specifically on the current sequence, that is, the sequence that is currently loaded in the **Data Analysis** view in ChemStation.

NOTE

You must first upload the sequence data to ECM before you create a report. Only data that is available in ECM can be used by OpenLAB Intelligence Reporter to generate a report.

Calculation of performance values

In ChemStation, certain specific values, such as *noise* and *peak performance* values, are not necessarily calculated and uploaded to ECM. If these values are not uploaded to ECM, you can not use them in your reports.

Under **ECM > Preferences**, there is the check box **Calculate Peak Performance**. This check box is cleared by default.

- If you select **Calculate Peak Performance**:

Values such as *noise* and *peak performance* values are always calculated. They are uploaded to ECM together with the other sequence data. You can use the values in your reports.

- If you do not select **Calculate Peak Performance**:

Values such as *noise* and *peak performance* values are only calculated if you choose the ChemStation report styles **Performance** or **Extended Performance**. As a consequence, there is no guarantee that these values always exist in ECM, and you can not generate reliable OpenLAB IR reports containing this type of information.



9

Attribute Extraction Services for ChemStation Data

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ACAML Filter [131](#)

ChemStation XML Attribute Extraction Service [132](#)

ChemStation Filter [133](#)

This chapter provides an overview of the available ECM Attribute Extraction Services (AES) for ChemStation data. The AES extract metadata information from the ChemStation data files. These metadata make the ChemStation data searchable. For detailed information, refer to the ECM documentation.



Attribute Extraction Services for ChemStation Data

ECM Attribute Extraction Services (AES) provides the following AES for the extraction of metadata from ChemStation data files:

- The *ChemStation XML* filter extracts peak, compound and result data from the result.xml file generated by the XML export routine in ChemStation revision A.10.02 and later.
- The *ChemStation* filter extracts basic sample and run data from the header of the channel files (*.ch), *.uv and *.txt files generated by all ChemStation revisions.

AES need to be installed by an ECM Administrator on the ECM Server; in addition, the filters need to be enabled for the system. The keys of an AES that are to be applied to a ChemStation file need to be selected for the respective LCDF structure. These are ECM administration tasks, and are described in the Enterprise Content Manager Administrator's Guide and the ECM online help.

The metadata can be queried using various search types in ECM. The ECM Search functionality is also available within ChemStation. When opening a file from ECM, the **ECM Open** dialog allows you to search for files of interest using the 'magnifying glass' icon, see [Figure 33](#) on page 129.

Using the Quick Search, you can search through various alphanumeric fields by entering a search key, such as an operator name. On the upcoming search page, you select the **Advanced** tab where, depending on the enabled filter packages, various keys are enabled, see [Figure 34](#) on page 129.

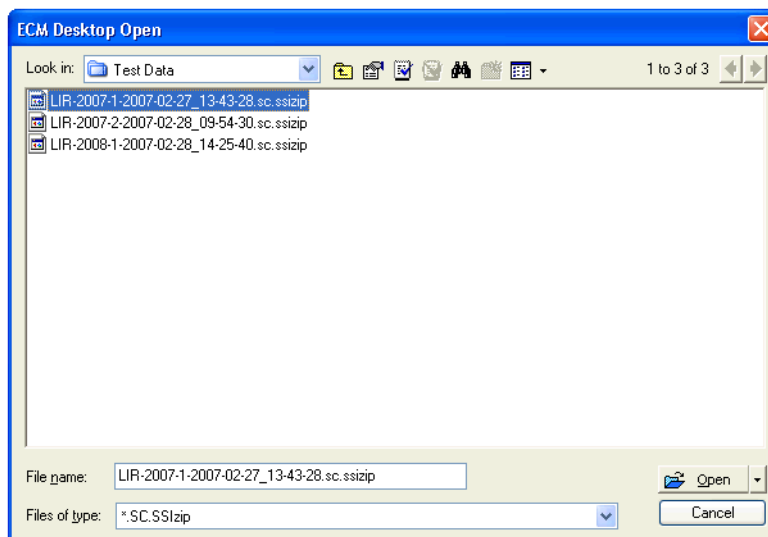


Figure 33 Search options

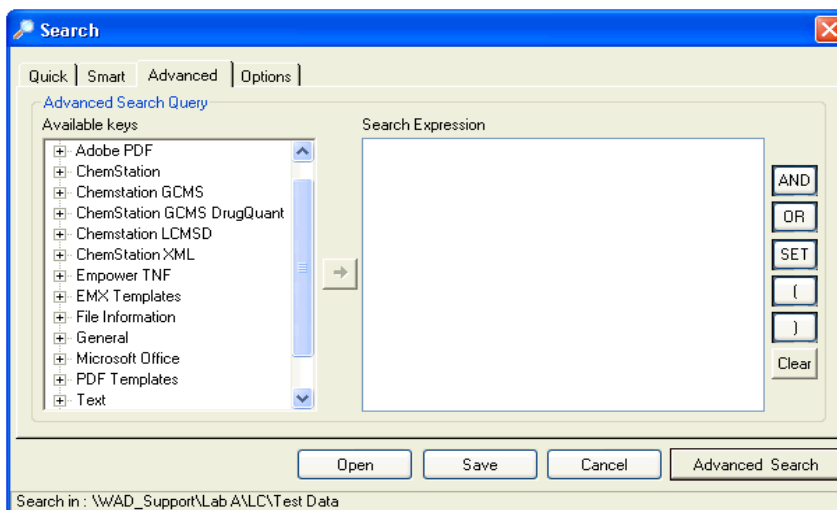


Figure 34 Filters available in search options

In the **Search** dialog, you can specify the available keys, and it is possible to define a search expression by combining two or more of the available keys using boolean operators. For detailed information regarding the use of the

9 Attribute Extraction Services for ChemStation Data

Attribute Extraction Services for ChemStation Data

various search algorithms, refer to the online help of your ECM system or the Enterprise Content Manager Administrator's Guide, as well as the AES-related manuals.

ACAML Filter

The ACAML Filter extracts information from the ACAML files that are also used for the OpenLAB Intelligence Reporter (see [“Interface to OpenLab Intelligence Reporter”](#) on page 115). The ACAML files are always created when acquiring or reprocessing data when the OpenLAB Option is installed.

Please note that the ACAML filter is only available for ECM 3.3.2 SP1.

ChemStation XML Attribute Extraction Service

The AES for ChemStation XML extracts key information from the following categories of the result.xml generated by ChemStation Rev. A (revision A.10.02 and later) and ChemStation Rev. B (revision B.01.01 and later) per data file. Note that ChemStation must be configured to generate the result.xml file, see the ChemStation XML Connectivity Guide.

- Acquisition (for example, instrument name, method information)
- Chromatogram (for example, derivative order, detector name)
- Custom
- Module
- Peaks (for example, peak name, amount, retention time, compound name)
- Sample (for example, calibration method, LIMS ID)
- Signal/noise

ChemStation Filter

The AES for ChemStation extracts attributes from *.ch, *.uv, and *.txt files created by the 16-Bit ChemStation (Rev A.x.x) or 32-Bit ChemStation (Rev B.x.x). It extracts key information from the header of ChemStation *.ch and *.uv data files (for example, sample name, method file, instrument model). From the report.txt file, it extracts key information (for example, sample name, acquisition method, analysis method). In addition, the service extracts information on support files from the category Content.

An ECM Scheduler Add-in for Agilent ChemStation enables the ECM Scheduler to automatically upload data generated by ChemStation to ECM.

9 **Attribute Extraction Services for ChemStation Data**

ChemStation Filter



10 Using Print Services in ChemStation

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This chapter gives a brief overview of how to install and configure the Print Services. This enables you to automatically upload ChemStation reports to ECM in a PDF format.



ECM Print Services

ECM Print Services are print management systems that transfer human readable electronic documents to ECM. They can be used to print ChemStation reports to ECM in PDF format.

When you add and configure a print service, it appears as an available printer on your computer. When you print with ECM Print Services, a PDF file is created and automatically uploaded to the ECM system. In addition, you can also set up the system to print additional hard copies to a conventional printer.

ECM Print Services can be installed for ECM Server revision 3.3.1 or later.

The *ECM Print Service* consists of two components:

- The *ECM Print Service Manager*, where you add and manage printers for the ECM Print Service.
- The *ECM Print Service*, which monitors a folder on your local disk drive. When a print service receives a print job, the print driver prints to a file in the monitor folder. Then the ECM Print Service intercepts the file and uploads it to ECM. In order for a file to be uploaded to the ECM program, it must have the file extension *.pdf.

Setting Up ECM Print Services

Installing ECM Print Services

The installation and setup of ECM Print Services requires following steps. The installation details are given in the ECM Print Services documentation.

- 1 Connect to the ECM Server revision 3.3.1 and select the **Administration** tab.
- 2 In the **Download** section of the **Administration** tab, select **ECM Print Services** for ECM and run the installation. Follow the instructions given by the installation wizard.
- 3 After the installation, the ECM Print Services icon is available in the task bar and the Anyuni PDF Convert is available as printer (see **Start > Settings > Printers and Faxes > Anyuni PDF Converter**).
- 4 Double-click the ECM Print Services icon. The **ECM Login** dialog opens.
- 5 Enter the required user credentials and click **Login** to proceed for configuration.

Configuring ECM Print Services for use with Amyuni PDF Converter

- 1 Create a monitor folder on your ChemStation ECM Client system. The folder should not be placed in the Chem32 directory.
- 2 Right-click the ECM Print Services icon in the task bar and select **Configure Printers**.

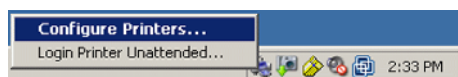


Figure 35 ECM Print Service icon

- 3 Log on to the **ECM Print Services**.
- 4 Select the **Add Printer** icon to add a printer with the following details:
 - **Type:** PDF Converter
 - **Name:** Specify a unique name, e.g. **Chem1 Print**
 - Define the printer security options in accordance with your organization's security policies.
- 5 Click **Add** to continue. Depending on your PC configuration, a message regarding the **Browse for Folder** dialog is shown. Exit that message with **OK**.
- 6 In the upcoming **Browse for Folder** dialog, select the monitor folder for the ECM print service.
- 7 The printer has now been created successfully and is available in the **ECM Service** dialog.
- 8 Right-click the ECM Print Service icon in the task bar and select **Configure Printers**, see [Figure 35](#) on page 138.
- 9 Open the printer configuration by marking your specific printer and select the **Configuration** tab. For details, refer to the ECM Print Services online help.
 - **ECM:** you need to specify the ECM (LCDF) data path where the uploaded files will be stored after transfer.
 - **Settings:** Transfer-specific settings.

- **Hardcopy Printers:** It is also possible to get a hardcopy printout.
- **Email:** It is possible to enable e-mail notification.

- 10** Click **Apply** to apply the configuration to the ECM Print Service and leave the dialog box with **OK**.
- 11** Leave all printer-related dialog boxes with **OK**.
- 12** In ChemStation, it is now possible to specify the newly configured printer in the **File** pull-down menu under **Printer set up**. It is possible to select the ECM Print Service as specific printer; if the printer has been marked as default printer in the Windows Settings, it will be already defined as default printer in ChemStation.

To set the printer to 'unattended mode'

Typically, when you print to an ECM Print Service, a dialog box asks you to confirm the upload location in ECM as well as some other settings for each report. If you are planning to print a whole sequence of reports, you can confirm these settings once for the series and then run the printer in unattended mode for a specified time. The duration of the unattended mode is set in the Configuration of the ECM Print Service during setup, but can be modified at any time.

- 1** Right-click the toolbar icon ECM Print Service and select **Login Printer Unattended**.

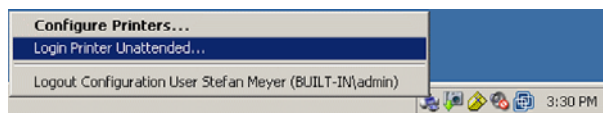


Figure 36 Define Logon for Print Service

- 2** Select the printer that you want to operate in unattended mode.
- 3** Confirm the job settings once and click **OK**.

Configuring ECM Print Services - Adobe Distiller

- 1 Create a monitor folder on your ChemStation computer. The folder should not be placed in the Chem32 directory.
- 2 Select the **Add Printer** icon to add a printer with the details:
 - **Type:** Adobe Distiller
 - **Name:** Specify a unique name, e.g. Chem1 Print
 - Define the printer security options in accordance with your organization's security policies.
 - In the upcoming **Add Port** dialog, choose **Add Port** and select the specified monitor folder on the ChemStation computer.
- 3 Click **Add** to continue and browse for the monitor folder for the ECM print service.
- 4 Open the printer configuration by marking your specific printer and select the **Configuration** tab.
 - **ECM:** you need to specify the ECM data path where the uploaded files will be stored after transfer.
 - **Settings:** Transfer specific settings.
 - **Hardcopy Printers:** It is also possible to get a hardcopy printout.
 - **Email:** It is possible to enable e-mail notification.

HINT

For details, refer to the ECM Print Services online help.

- 5 Click **Apply** to apply the configuration to the Print Service and leave the dialog box with **OK**.
- 6 Depending on the Acrobat Distiller version in use, additional configuration settings are necessary. A message requests you to perform certain tasks.
Example for Adobe Distiller Rev. 6.00:
In **Start > Settings > Printers** open the properties of the newly added printer. Select **Print Preferences**.
 - In the Adobe PDF Conversion Settings, deselect **View Adobe PDF results**.

- In the Adobe PDF Output Format, select the monitored path of the ChemStation computer.
 - Select **Edit** for the default settings. On the upcoming **Adobe PDF Settings** dialog, deselect **optimize for fast Web View** and save the settings.
- 7 Exit all printer-related dialog boxes with **OK**.
 - 8 In ChemStation, it is now possible to specify the newly configured printer in the **File** pull-down menu under **Printer set up**. It is possible to select the ECM Print Service as specific printer; if the printer has been marked as default printer in the Windows Settings, it will be already defined as default printer in ChemStation.

To set the printer to 'unattended mode'

Typically, when you print to a Print Service, a dialog box asks you to confirm the upload location in ECM as well as some other settings for each report. If you are planning to print a whole sequence of reports, you can confirm these settings once for the series and then run the printer in unattended mode for a specified time. The duration of the unattended mode is set in the configuration of the ECM Print Service during setup, but can be modified at any time.

- 1 Right-click the ECM Print Services toolbar icon and select **Login Printer Unattended**, see [Figure 36](#) on page 139.
- 2 Select the printer that you want to operate in unattended mode.
- 3 Confirm the job settings once and click **OK**.

Working with ECM Print Services in ChemStation

When you use the ECM Print Service in ChemStation, any report printed using the Print Services is converted to a *.pdf file, placed in the monitored folder, and transferred by the print service to the specified location in ECM. During conversion to PDF, the name supplied by the system is fixed. It is defined as follows:

- single runs: [datafile name].pdf
- sequence runs: [sequence name]_ [datafile name].pdf
- sequence summary reports: SSR_[sequencename].pdf

The maximum file length for this automatically generated report name is 30 characters; longer files names are truncated. If, due to the truncation, filenames are the same, the existing file is overwritten.

NOTE

Be aware that when you specify the sequence pattern and datafile name in the sequence setup, the complete *.pdf file name may not exceed 30 characters.



11 Troubleshooting

General Problems [144](#)

ECM Server is not Available [144](#)

Alerts and Error Messages at ChemStation Startup [145](#)

Error Messages in the Spooler Queue Manager [146](#)

The chapter gives some elementary troubleshooting hints.



General Problems

ECM Server is not Available

If the ECM Server is not available while working with ChemStation, there are two possible scenarios.

ECM Server is not available before/during login

If the ECM Server is not available while logging in to ECM from ChemStation, the user cannot be authenticated by the ECM system. Login is aborted and there will be no access to the ECM functions in ChemStation; all ECM-related menu items will be grayed out.

For further troubleshooting, please contact your ECM administrator.

ECM Server is not available after login

If the ECM Server connection is interrupted after login to ECM from ChemStation, the user has been authenticated by the ECM system. In this case, ChemStation knows the current logged-in user.

When the ECM Server becomes unavailable, ChemStation automatically tries to reestablish the user login.

The ECM Load and Save functions are accessible, but an alert informs the user about the interrupted connection to the ECM.

While acquiring data, the automatic transfer of data to ECM cannot be completed. The user is notified by an error message, and must manually upload the data as soon as the connection is reestablished (**ECM > Manage Queue**).

As soon as the ECM Server is available again, all ECM tasks are available without restarting the application. A new login is not required.

For further troubleshooting, please contact your ECM administrator.

Alerts and Error Messages at ChemStation Startup

Your Transfer Settings/Remote Data Path seems to be set to default

At every startup, Agilent ChemStation checks whether all necessary information is provided for transferring data to ECM. This message is shown if the Remote Data Path is not set or is incomplete.

Probable cause

- 1** The Remote Data Path is not set or is incomplete.

Suggested actions

Make sure that the information on ECM Server, ECM Account, and a complete LCDF path is provided in the Transfer Settings (**ECM > Preferences > Transfer Settings**).

Error Messages in the Spooler Queue Manager

Account Mismatch

Probable cause

- 1 Account setting in Preferences differs from current connection (or offline).

Suggested actions

Correct the Transfer Settings and connect to ECM.

Host Mismatch

Probable cause

- 1 ECM Server in Preferences differs from current connection (or offline).

Suggested actions

Correct the Transfer Settings and connect to ECM

The queue already contains items

Probable cause

- 1 There are items in the queue that have been queued before the current item.

Suggested actions

Process queue in the correct order. If necessary, export items that can't be resolved.

Invalid license ID or license has expired.

Probable cause

- 1 Server license timeout.

Suggested actions

Log out and log in again.

You do not have permission to create a new Drawer/Folder.

Probable cause

- 1** You do not have appropriate privileges to create the Drawer or Folder.

Suggested actions

Ask an administrator to give you the corresponding privileges or to create the needed directories.

You do not have permission to add files.

Probable cause

- 1** You do not have appropriate privileges to save files to the specified location in ECM.

Suggested actions

Ask an administrator to give you the corresponding privileges.

Unable to upload (filename). This file is currently checked out to another user and may not be updated. (error -1).

Probable cause

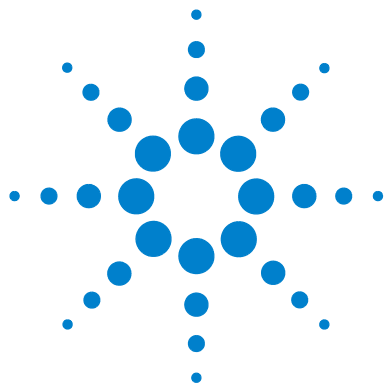
- 1** Another user has checked out the file.

Suggested actions

The other user has to check in the file before you can upload the file.

11 Troubleshooting

Error Messages in the Spooler Queue Manager



12 Appendix

ChemStation Privileges in ECM [150](#)

ChemStation Roles in ECM [153](#)

ECM related privileges concerning the ChemStation configuration [157](#)



ChemStation Privileges in ECM

Privilege	Description
CS: Audit Trail	Run: Enable the audit trail for a specific method
CS: Batch	Run: Enables all operations in Batch view
CS: Break Session Lock	Run: Unlock a ChemStation session locked by other users
CS: Calibration	Edit: Create and modify the calibration table; change calibration settings
CS: Command Line	Run: Turn on / off the command line
CS: Companion	View: Access to Companion view (GC ChemStation only)
CS: Control	View: Access to Method and Run Control view
CS: Data	Edit: Interactive saving of data to ECM Delete: Delete data files in ChemStation Explorer
CS: Data Analysis	Run: Access to Data Analysis view
CS: Diagnostic	View: Access to Diagnosis view
CS: Full Menu	Run: Enable the ChemStation Full Menu
CS: Instrument Configuration	Edit: Modify instrument configuration parameters
CS: Instrument Setup	Edit: Modify instrument method parameters
CS: Integration Events	Edit: Modify Integration Events + perform Auto Integration
CS: Ion Labels	Edit: Edit options for Ion Labels (LC/MS-only)
CS: Logbook	Edit: Save the current logbook Delete: Clear the current logbook

Privilege	Description
CS: Manage Transfer Queue	Run: Access to the following items of the Spooler Queue Manager <ul style="list-style-type: none"> • Save selected item locally • Delete selected item • Properties
CS: Manual Integration	Run: Perform manual integration
CS: Method	Edit: Save method changes (includes <i>Update Sequence/Master Method</i> in Data Analysis view) Delete: Delete a method in ChemStation Explorer
CS: Method Properties	Edit: Modify Run Time Checklist and Method Information
CS: Print Report	Run: Print/preview a report
CS: Recalibration	Run: Perform interactive recalibration
CS: Report	Edit: Modify report calculation/print style +edit Instrument Curves dialog
CS: Report Layout	View: Access to Report Layout view
CS: Report Template	Edit: Save a report template
CS: Reprocess	Run: Reprocess a sequence
CS: Retention Time Lock	Edit: Access to the Retention Time Lock menu (GC only)
CS: Retention Time Search	Edit: Access to Retention Time Search menu (GC only)
CS: Run	Run: Start acquisition (single sample or sequence)
CS: Sequence	Edit: Save sequences Delete: Delete sequences in ChemStation Explorer
CS: Sequence Summary	Edit: Modify sequence summary report and extended statistics settings
CS: System Suitability	Edit: Edit noise ranges and performance limits

12 Appendix

ChemStation Privileges in ECM

Privilege	Description
CS: Transfer Preference	Edit: Edit the Transfer Settings in the Preferences
CS: Tune	View: Access to Tune view (LC-MSD ChemStation only)
CS: Verification	View: Access to Verification (OQ/PV) view

ChemStation Roles in ECM

Please note: the default ChemStation roles do not contain any ECM privileges.

Table 3 Default CS Administrator privileges

Privilege	View	Edit	Delete	Add	Run
CS: Audit Trail					X
CS: Break Session Lock					X
CS: Command Line					X
CS: Control	X				
CS: Data		X	X		
CS: Data Analysis	X				
CS: Diagnostic	X				
CS: Full Menu					X
CS: Instrument Setup		X			
CS: Logbook		X	X		
CS: Manage Transfer Queue					X
CS: Manual Integration					X
CS: Method		X	X		
CS: Method Properties		X			
CS: Print Report					X
CS: Report Layout	X				
CS: Report Template		X			
CS: Sequence			X		
CS: Transfer Preferences		X			

Table 4 Default CS Analyst privileges

Privilege	View	Edit	Delete	Add	Run
CS: Batch					X
CS: Calibration		X			
CS: Control	X				
CS: Data		X			
CS: Data Analysis	X				
CS: Full Menu					X
CS: Instrument Setup		X			
CS: Integration Events		X			
CS: Logbook		X			
CS: Manual Integration					X
CS: Method		X	X		
CS: Method Properties		X			
CS: Print Report					X
CS: Recalibration					X
CS: Report		X			
CS: Report Layout	X				
CS: Report Template		X			
CS: Reprocess					X
CS: Run					X
CS: Sequence		X	X		
CS: Sequence Summary		X			
CS: System Suitability		X			

Table 5 Default CS Lab Manager privileges

Privilege	View	Edit	Delete	Add	Run
CS: Audit Trail					X
CS: Batch					X
CS: Break Session Lock					X
CS: Calibration		X			
CS: Command Line					X
CS: Companion	X				
CS: Control	X				
CS: Data		X	X		
CS: Data Analysis	X				
CS: Diagnostic	X				
CS: Full Menu					X
CS: Instrument Configuration		X			
CS: Instrument Setup		X			
CS: Integration Events		X			
CS: Logbook		X	X		
CS: Manage Transfer Queue					X
CS: Manual Integration					X
CS: Method		X	X		
CS: Method Properties		X			
CS: Print Report					X
CS: Report		X			
CS: Report Layout	X				
CS: Report Template		X			
CS: Reprocess					X
CS: Run					X

Table 5 Default CS Lab Manager privileges

Privilege	View	Edit	Delete	Add	Run
CS: Sequence		X	X		
CS: Sequence Summary		X			
CS: System Suitability		X			
CS: Transfer Preferences		X			
CS: Tune	X				
CS: Verification	X				

Table 6 Default CS Operator privileges

Privilege	View	Edit	Delete	Add	Run
CS: Control	X				
CS: Data		X			
CS: Print Report					X
CS: Run					X
CS: Sequence		X			
CS: Sequence Summary		X			

ECM related privileges concerning the ChemStation configuration

The privileges described in the following table must be assigned to at least one of your roles in order to become active.

Table 7 List of ECM related privileges

Privilege	View	Edit	Delete	Add	Run	Description
Content: File	X			X		<ul style="list-style-type: none"> Minimum privilege for ChemStation to access ECM Privileges to view ECM Properties in ChemStation
Content: File Filtering		X				<ul style="list-style-type: none"> Minimum privilege for ChemStation to access ECM Privilege to add files manually to an ECM folder
Content: File Revisions	X					<ul style="list-style-type: none"> Privilege to view revisions in ChemStation
Content: File Type [XLS]		X		X		<ul style="list-style-type: none"> Privilege to add and check in files with an .xls extension
Content: Folder	X	X		X		<ul style="list-style-type: none"> Minimum privilege for ChemStation to access ECM Privilege to view ECM Properties in ChemStation
Content: Folder Access Properties		X				<ul style="list-style-type: none"> Privilege to view and change any folder property tab
Content: Rekey File					X	<ul style="list-style-type: none"> Privilege to rekey files in ECM e.g. with XML Filters
System: Advanced Search					X	<ul style="list-style-type: none"> Privilege to use the Advanced Search in ChemStation
System: Audit Trail	X					<ul style="list-style-type: none"> Privilege to view ECM Properties in ChemStation

12 Appendix

ECM related privileges concerning the ChemStation configuration

Table 7 List of ECM related privileges

Privilege	View	Edit	Delete	Add	Run	Description
System: Filtering Configuration	X					<ul style="list-style-type: none">• Privilege to view or change the filtering configuration• Privilege to use attribute extraction services and to manage user-defined attributes
System: indexing Configuration	X					<ul style="list-style-type: none">• Minimum privilege for ChemStation to access ECM• Privilege to view ECM Properties in ChemStation
System: Quick Search					X	<ul style="list-style-type: none">• Privilege to use Quick Search in ChemStation
System: Super Object	X					<ul style="list-style-type: none">• Privilege is mandatory for OLIR
System: Project	X					<ul style="list-style-type: none">• Privilege to view projects in OLIR
System: Project Access	X					<ul style="list-style-type: none">• Privilege to access projects in OLIR

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In This Book

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