Agilent ChemStation Security Pack for AD, GC, LC, CE, LC-MSD, and CE-MSD



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Manual Part Number

G2183-90006

Edition

02/09

Printed in Germany

Agilent Technologies Hewlett-Packard-Strasse 8 76337 Waldbronn, Germany

Software Revision

This guide is valid for revision B.04.0x of the Agilent ChemStation Security Pack for AD, GC, LC, CE, LC-MSD, and CE-MSD software.

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In This Guide...

This book describes the Agilent ChemStation Security Pack for AD, GC, LC, CE, LC-MSD, and CE-MSD techniques. The Security Pack is an add-on module for the Agilent ChemStation and helps you meet the requirements of the U.S. Food and Drug Administration's (FDA) ruling on electronic records and signatures, CFR 21 Part 11.

1 Introduction

The first chapter provides an overview of Security Pack and 21 CFR Part 11–FDA's final rule for electronic records and electronic signatures.

2 Prerequisites, Configuration, and Installation

This chapter shows you how to setup the Security Pack in ChemStation.

3 A Brief Tour

Refer to this chapter for getting an introduction to the main concepts behind Security Pack.

4 Access Level and Batch Review Interface Changes

This chapter includes a description of the changes that have been made in operator mode and batch review mode.

5 Data Reanalysis

Use this chapter as a guidance for reanalyzing your data.

6 Administrator Tasks and Reference

This chapter provides an overview of administrative tasks.

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Introducing Security Pack

Security Pack revision B.04.0x is built upon the ChemStation B.04.01. It is an add-on module to the Agilent ChemStation for GC, LC, CE, LC-MSD, CE-MSD and A/D targeted to support the compliance requirements for 21 CFR Part 11.

Security Pack provides changes to the ChemStation result management.

- It provides logon and locking procedures for each individual application.
- It offers a fully automated result and meta data versioning—each time a new result is calculated and displayed, the Security Pack stores this result with a new version number in the database.
- It protects data directory with NTFS permission rights.

Security Pack changes the operator privileges of the ChemStation operator user level and adds the ChemStore C/S relational database for result management and data storage.

The changes on the ChemStation are discussed and explained in this manual; for a description of the ChemStore C/S product, please refer to the *Agilent ChemStore C/S Concepts Guide*.

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. Besides all uncertainties and 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 faster to market.

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 has to make sure that its work practices support the FDA rules, but most of the requirements also affect the chemical analysis systems and suppliers of these systems. This manual outlines how a chromatographic data handling system can help the industry to comply with the FDA rules. Security Pack meets the demands on data security, data integrity, and audit-trail using either a standalone Microsoft[®] Access database or a server-based Oracle[®] database.

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 and meta data 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 an 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.

The Security Pack is designed for and supported in a closed system only.

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.

1 Introduction

21 CFR Part 11



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Prerequisites

PC Hardware

The Security Pack does not require a large amount of resources from the computer, the minimum requirements for the PC are the same as for ChemStore C/S. Refer to the *ChemStore C/S Installation Guide* for details about minimum hardware requirements.

Operating System

Security Pack requires Windows XP with Service Pack 3, Windows 2003 R2 server with Service Pack 2, or Windows Vista with Service Pack 1. Additionally, the hard drive on which the ChemStation Plus system is installed must use the NTFS format. Format the hard drive prior to the installation of the Security Pack.

Client Configuration

The following section will discuss how Security Pack ties into the Windows security tools and how the default setup configures the security settings under Windows. For further information on the administration of both, the Windows permissions and the database, please refer to Chapter 6, "Administrator Tasks and Reference," starting on page 73.

Security Pack utilizes the Windows group security concept to add full compliance with 21 CFR Part 11 to ChemStation Plus. The section "Windows User Management" on page 17 briefly outlines this concept and section "Minimum Requirements for Windows User Administration" on page 17 explains an easy configuration that is fully sufficient for a standalone system.

However Agilent recommends to customize the Windows security configuration according to the needs in the laboratory. Sections "Minimum Requirements for Windows User Administration" on page 17 and "Windows Group Policies" on page 18 briefly outline how these features built into the Microsoft Windows operating system can be used to make ChemStation Plus easier to use.

Windows User Management

The core part of the Windows user management in standalone usage is the group concept. Each Windows user is a member of a group. These groups then are assigned certain permissions, like logging on to a computer, installing software, access to certain files, etc.

Each user has its own profile, where the layout of their desktop, the applications they see in the start menu, and other things are stored.

System policies can be used to further customize the security settings. Using system policies usually requires a Windows domain, where the policies will be maintained centrally.

Minimum Requirements for Windows User Administration

As the user identification required by 21 CFR Part 11 for electronic records is done by the ChemStation plus Security Pack, the Windows user management can be simplified. It is sufficient to divide users in two groups:

- Operators, that normally use the ChemStation plus system and do not need to change database connections or do backups.
- Administrators, that do database backups and change database connections.

One user configuration example would use only one generic Windows user log-on for all users sharing one computer. Security Pack manages the system security and the user identification. This generic user only needs to be a member of the Windows user group *Users*. This user must not be a member of the Windows user group *Power Users* or *Administrators*.

NOTE

When using Windows systems that are not purchased from Agilent, it is necessary to grant specific permissions on operating system folders used by the application. The configuration should be done according to the document 'Configure and Maintain your Agilent ChemStation computer' (P/N G2170-90132). An electronic version of this documented is located on your ChemStation installation CD.

For the administrators, we recommend personalized Windows user accounts, to track their actions. All users with this job description must be a member of either the Windows user group *Power Users (Windows XP only)* or *Administrators*. Chapter 6, "Administrator Tasks and Reference," starting on page 73 provides further details on the security settings chosen to prevent unauthorized deletion of data.

NOTE

If your Windows networked environment is structured in domains, each domain user group must be explicitly listed as a member of the local user group for Security Pack to work properly. The domain user group must not be member of the *Power Users* group (Windows XP only).

Windows Group Policies

Windows operating systems include numerous commands and settings that control and manage the entire computer system. One example is the control panel that allows for installation and removal of applications, changes of the PC clock and so on. An unauthorized modification of the Windows system settings usually causes general problems of operating the PC, but some settings just modify your electronic records like changing the local PC clock time. Security Pack is designed to be fully secure even in a system that offers system setting access to standard users.

However, in order to minimize the operators access to the system control, we recommend to restrict access to certain important commands and programs from the Windows system control to users with administrative rights. The best way of implementing the restricted access in a Windows networked data system are Windows 2003 server *group policies*. Please refer to the Microsoft Operating System user documentation and online help for details.

Group policies can be used to further secure and simplify system usage. They allow a customizing of the desktop of each user and restrict access to important programs and commands for the system and control. Group policies operate in an entire domain and are setup by the domain controller. Contact your local IT organization for implementing these features, as they should fit in the overall security strategy of your laboratory.

For use with Security Pack, we recommend the following limitations for the operators:

Remove Run command from Start menu

- Disable Registry editing tools
- Disable Task Manager
- Disable Change Password (if generic logon for users is used)

Members of the local *Power Users* (XP only) and *Administrators* group should have the same restrictions, except the permission to change their own Window password.

The other system control functionality is not required for the administrative tasks of the Security Pack either.

User Profiles

To ensure that all users always have the same desktop and the same start menu on all computers, a mandatory user profile can be used. These profiles are stored on a central server and cannot be changed by the individual users. We recommend to remove all applications except the ChemStation Plus applications from the start menu as well as all icons from the desktop for the users that are operators.

Depending on the SOP used for back-up and archival the users that perform the administrative tasks need access to Windows Explorer and/or the Windows backup application. 2 Prerequisites, Configuration, and Installation Installation Procedure

Installation Procedure

To ensure a successful installation of the Security Pack, please follow this procedure step by step.

Preparation

- 1 Ensure that your PC meets the minimum requirements as outlined in the *Agilent ChemStore C/S Installation Guide*.
- 2 Ensure that your operating system is Windows XP with Service Pack 3, Windows 2003 R2 with Service Pack 2, or Windows Vista Business with Service Pack 1.
- **3** Ensure that the partition where Security Pack will be installed is in NTFS format.
- **4** If not already done, install the ChemStation software. Details on the ChemStation installation can be found in the respective ChemStation installation guide.
- **5** If not already done, install ChemStore C/S from the ChemStore/Security Pack CD-ROM. Details on the ChemStore C/S installation can be found in the respective ChemStore C/S installation guide.
- **6** Reboot your PC after ChemStore installation.

Security Pack Installation

- 1 Log on to the operating system as a user with administrative privileges
- 2 Browse the ChemStore/Security Pack CD-ROM for the G2183 folder.
- **3** Select to start G2183\setup.exe.
- 4 On Windows Vista: Confirm the User Account Control message with **Allow**.
- **5** Reboot the PC after the installation has finished.

Post Installation

 Turn on Windows Object Access Auditing to audit the access to the local *chem32\chemstor\database* directory. See also chapter "Security Settings" on page 90. On stand-alone systems, this can be done by Local Security Policies, located under Administrative Tools of the Control Panel. Navigate to the console tree Audit Policy. Change the settings according to Figure 1 and verify that the settings are effective after re-logging on to the operating system. In a networked environment, this should be done on a domain level.



Figure 1 Audit Policy Settings

2 Change the Security log settings to prevent deletion of events. Open Administrative Tools from Start > Programs (XP) or Start>Control Panel (Vista)

2 Prerequisites, Configuration, and Installation

Installation Procedure

3 Windows XP only: Open **Computer Management** and expand the Event Viewer, then right-click on **security > properties**. Select **Do Not Overwrite Events** (Clear Log Manually) as in Figure 2 on page 22.

Security Propertie	s	? X
General Filter		
Display name:	Security	
Log name:	C:\WINNT\System32\config\SecEvent.Evt	-
Size:	64.0 KB (65,536 bytes)	
Created:	Thursday, December 06, 2001 3:19:09 PM	
Modified:	Thursday, December 06, 2001 3:25:54 PM	
Accessed:	Thursday, December 06, 2001 3:25:54 PM	
Log size		
<u>M</u> aximum log si	ze: 512 🕌 KB	
When maximur	n log size is reached:	
O Overwrite e	events as needed	
O Overwrite e	events older than 7 🔄 days	
 Do not ove (clear log m 	rwrite events anually) <u>R</u> estore Defaults	
Using a lo <u>w</u> -sp	eed connection	2g
	OK Cancel <u>A</u> p	ply

Figure 2 Event Log Settings (Windows XP)

4 Windows Vista only: Open Control Panel > Administrative Tools and expand the Event Viewer, then right-click on Windows logs > Security > Properties. Select Do Not Overwrite Events (Clear Log Manually) as in Figure 3 on page 23.

neral				
Eull Name:	Security			
Log path:	%SystemRo	ot%\System32\Winevt\Logs	s\Security.evtx	
Log size:	1.07 MB(1,1	18,208 bytes)		
Created:	Friday, Nove	ember 10, 2006 2:29:41 AM		
Modified:	Tuesday, De	cember 16, 2008 2:46:16 PM		
Accessed:	Wednesday,	October 17, 2007 4:22:02 Al	vi	
Enable logging	g			
Ma <u>x</u> imum log siz	ze (KB):	20480 🚔		
When maximum	event log size is re	ached:		
Over <u>w</u> rite	events as needed (oldest events first)		
Archive the	ne log when full, do	not overwrite events		
O not ov	rerwri <mark>te ev</mark> ents (Cle	ar logs manually)		
				Classing
				Clea <u>r</u> Log
		OK	Canc	el Apply

Figure 3 Event Log Settings (Windows Vista)

- 5 If applicable create a new database as outlined in section "Creating New Databases in the Standalone Version" on page 82.
- 6 Configure a database connection for the users, as outlined in section "Assigning a Database Connection on Windows XP operating systems" on page 79 or "Assigning a Database Connection on Windows Vista operating systems" on page 80 respectively
- 7 The passwords for the default users should not be changed until the system is fully operational and productive. Agilent recommends to assign users with the tasks related to the default users. Once these users are established the default user accounts should be disabled.

2 Prerequisites, Configuration, and Installation

Installation Procedure

User Name Password Function		Function
Admin	admin	System administrator, has all permissions
Manager	manager	Lab supervisor, can not compact a DB and administer users
Chemist	chemist	Data reviewer, can not administer users and create studies
Operator	operator	Sample operator, can only create batches of assigned data
Support	support	Support logon, has all permissions

Table 1 Default Users and Functions

NOTE

Please ensure that always at least two users with the permission "Administer users" are configured in your database. Due to the strict account lockout policy it might happen that a single account might be locked out and the database can no longer be administered.

8 A successful installation of the Security Pack is documented in the ChemStation menu **Help** under **About ChemStore**. This screen will display both the ChemStore revision and the Security Pack revision number.





Adding a ChemStation Instrument

If you decide later to add another ChemStation instrument to your Security Pack installation, it is mandatory to run the Security Pack installation again after the installation of the ChemStation instrument. This will ensure that the data from the second instrument is also fully protected.

To do this, perform step 1 and step 3 from the "Installation Procedure" on page 20.

Now the directories of the new ChemStation instrument are protected as outlined in the section "Security Settings" on page 90.

Removing Security Pack

If you want to remove the Security Pack from your computer, you need to uninstall ChemStore from your computer. This will also remove the Security Pack. Removal of the software requires a user that is a member of the Windows user group *Administrators*. Only these users can completely remove all directories created by ChemStore and protected by the ChemStation Plus Security Pack. Refer to the *Agilent ChemStore C/S Installation Guide* for details on how to remove ChemStore from your computer.

2 Prerequisites, Configuration, and Installation **Installation Procedure**



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Mandatory Logon, User Management and Lock-out

Mandatory Logon, User Management and Lock-out

Security Pack allows only authorized users to start the application. The user management is a user privilege arranged in the ChemStore C/S database. It should be performed only by administration managers. To prevent unauthorized access to the database or unauthorized use of the database, each ChemStation Plus user is given an access password and a set of permissions, defining which facilities are available for that user (see *Agilent ChemStore C/S Concepts Guide*, "Setting Up and Managing Users", page 99).

To prevent unauthorized access of data within a different section of the same database, Security Pack allows to restrict data access of data subsets in one database. Access is restricted on a study level where the study is an organizational element in the database that can be set and managed by Security Pack administrators from within the database.

One of the most important requirements for limited system access is that only the individual users know their passwords and even the system administrator can only manage the users and the user IDs—but not the passwords. The implementation in the software therefore is a two-step approach. First, the database administrator sets up user identifications and appropriate permission rights for the individual users. Second, when the users first log on to the application, a log-on screen prompts for specification of the individual password.

This two step approach ensures that only the individual users knows their passwords. If the password is lost or forgotten, the database administrator can clear the user's password and make the user re-run password specification and log-on script.





Mandatory Logon, User Management and Lock-out

hemStore C/S: Chan	ge User Password	
User Name:	pjohanson	
Old <u>P</u> assword:		
New Password:		
Confirm Password:	Γ	
<u>0</u> K	Cancel <u>H</u>	elp

After clicking **OK**, the **Change User Password** dialog box is automatically opened.

Figure 6 Change User Password Dialog Box

To apply the company's individual password policy for minimum password length, expiry date, password uniqueness and account lock-out, set the appropriate parameters in the ChemStore C/S application.

Minimum password length	8	characters
Password <u>e</u> xpires in	120	_ days
Password <u>u</u> niqueness: Remember	3	passwords
Account lock out after	6	attempts

Figure 7 Password Settings Dialog Box

Following the FDA regulations, both the ChemStation and ChemStore C/S can be locked while they are running. The lock-out may be private, when either the current user's password or an administrator's password must be supplied to unlock the session, or non-private, when any valid user ID/password combination is sufficient to unlock the session.

All manual session locks allow ongoing monitoring of the ChemStation Plus applications in case, for example, a sequence is running. The locking is also individual for each instrument session thus allowing to operate more than one instrument version from one PC.

Mandatory Logon, User Management and Lock-out

To lock a session privately, hit the lock button in ChemStation or ChemStore toolbar or select the ChemStation menu View > Lock ChemStation > privately or the ChemStore C/S menu Administration > Lock Session > privately. The 'Privately locked by user ...' dialog box can only be unlocked by entering a valid user name and password.

NOTE

Administrators have the permission to unlock a privately locked session in cases where a users leaves the lab without handing over a running session. A hand-over can be done by a non-private session lock.

	<u> </u>
Name:	11-1-
Password:	
)atabase	

Figure 8 Private ChemStore session lock

To lock a session non-privately, select the ChemStation menu View > Lock ChemStation > non-privately or the ChemStore C/S menu Administration > Lock Session > non-privately. The Locked by user '...' dialog box can be unlocked by entering any valid user name and password.

Each unsuccessful attempt to unlock (privately and non-privately) the session is noted in the ChemStore database logbook as "failed to logon" with the ChemStation client and the PC host name (e.g. instrument 1) as identifier.

Mandatory Logon, User Management and Lock-out

Name:	<u></u> K
	Help
Password:	
Database	
Demo	

Figure 9 Non-private ChemStore session lock

According to 21 CFR Part 11, an automatic inactivity lock-out is available as an additional security feature. It allows users with the appropriate privilege "Administer users" to set a time after which the session is locked, and can be unlocked only by supplying a valid password.

The inactivity time-out is controlled from the ChemStore database. If it is enabled in the ChemStore review client, all ChemStation sessions will be under control of this timeout setting. In case of a client/server installation of ChemStore, all connected ChemStation Plus clients in the network will have the same setting for the inactivity timeout. This inactivity setting can only be modified from the ChemStore review client from users with administrative privileges. It can not be modified by any system operator on a local data acquisition PC or data review PC without the appropriate ChemStore privileges.

The passwords that are valid depend on whether the session has been locked privately or non-privately.

In contrast to the manual locks, the automated lock minimizes the locked ChemStation session window to prevent undesired interruption of the work with the foreground application.

Mandatory Logon, User Management and Lock-out

∐ime-based se	ssion lock	
● privately ○ <u>n</u> on-privatel <u>W</u> ait: 10_ m	ly in.	
ОК	Cancel	Held

Figure 10 Time-based session lock settings



The default setting is Wait 10 min.

Storage of Data

The application is designed to store all data in the ChemStore C/S database. Within the database, runs can be logically grouped for any desired purpose. Such a group of runs is referred to as a *study*. A user with the requisite permissions may create as many studies as desired, but each study must be identified with a unique name. During study creation, study access is also configured. Only users who can access (they are "assigned to studies") a study can get access to the study data or transfer data into this study. The assignment of studies to users is an additional security measure to restrict data access within the database to those individuals that own the data.

Following the rule of part 11 on the requirements of closed systems the "assign studies to users" privilege is thus an additional tool to ensure closed subsystems within the closed system of global database.

This is particularly important in cases where different laboratories or even different departments store their data in one ChemStation Plus result database. By assigning parts of the database (studies!) to the different user groups the database administrator ensures that data is only accessible to the data owners and that is invisible to database users who do not own these data (i.e. from different departments who use the same database for their results as well).

NOTE

Assigning studies to users is not only a security tool but also helps increasing database performance on large systems. Studies containing unused or archived and deleted data should be de-assigned from all users. This change is reversible.

For more details on the assign studies to users functionality, please refer to ChemStore Concepts guide section "Setting up organizational information assigning studies to users".

When results are transferred from the ChemStation to ChemStore C/S, the individual runs (or group of runs) are assigned to a study; these runs, together with any previous runs assigned to the same study, are then available as a logical unit.

The Security Pack is designed to store all data that the FDA defines as mandatory for data integrity:

- the chromatographic *raw data*—the full content of the *d.files*
- the *meta data* containing the information and algorithm to turn the raw data into meaningful results—*methods* and *sequences*
- the *results* as calculated in the ChemStation registers and selected in the report type
- additional data acquisition parameters like method, sequence, instrument *logbooks*, instrument serial numbers, and column parameters

To create a study, select in ChemStore C/S Administration > Create Study > Store in Addition and follow the default setup to ensure that your study stores all data.

General	Store in Addition	Custom fields	Assign Study	Approva
	- Store in Addition to F I⊽ Chromatogra I⊽ Spectra for <u>C</u>	Result ams Quantified Peaks		
	⊽ Raw Data ⊽ S <u>e</u> quence ⊽ <u>M</u> ethod	Delete raw data after transferring	from file system to database	

Figure 11 Data storage configuration during study set-up

For further information on the study management, see *Agilent ChemStore C/S Concepts Guide*, "Setting Up Organizational Information."

The database also links raw data with the corresponding meta data. It documents the result version along with the individual method version that was used to calculate the specified result.

The meta data can be easily restored from one central **Run information** screen.

To display the Run information screen, select	Å	in ChemStore C/S.
--	---	-------------------

Injection				
Туре:	Normal	Operator:	agratz	
Time:	8/24/2000 00:17:33	Volume:	1.0	Unit: 📕
Processing	<u>.</u>		-	
Time:	12/7/2005 15:24:30	Operator:	oqadmin	
Raw data				
Original path:	C:\CHEM32\2\DATA\	NEWLIN\NEW	00045.D	
Time:	12/7/2005 15:24:30		Rela	oad raw data
Processing Metho	d			
Original path:	C:\CHEM32\2\METHO	IDS\LINICHE	I.M	
Comment:	Zorbax Eclipse XDB-C	B, 4.6 x 150mm	1, 5um	
Time:	12/7/2005 15:23:54	_		
Quantification type:	ESTD	_	Rel	oad method
Processing Seque	nce			
Original path:	C:\CHEM32\2\SEQUE	NCE\LINSEQ.	s	
Comment:				
Time	12/7/2005 15:23:46	_		
Repetition number:	1	_	Re	load all files
	' -	_	Belo	ad sequence
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Audit trail	Column i	dentification	Instrume	nt configuration.
	1720			

Figure 12 Run Information Screen

NOTE

The Run information screen is only available in the ChemStore sample tab view.

Data Transfer from ChemStation

Data Transfer from ChemStation

During Data Acquisition

Before starting a single run or a sequence for data acquisition, the user has to setup the ChemStore organizational information that defines the sample storage location in the database and, if configured, the values for the custom fields. For details on the setup of the ChemStore organizational information, please refer to the *Agilent ChemStore C/S Concepts Guide*, Chapter 2, "ChemStore Concepts", organizing results.

The data transfer settings are set to *transfer after each analysis*. This configuration of the data transfer is user-independent and can not be changed. As soon as the data analysis part of the method is finished and the results are calculated, the data is transferred to the database with the ChemStore C/S ODBC data spooler. In case of an "Acquisition-only" run, the data is transferred when the acquisition is completed.

During Data Reprocessing

A typical data analysis cycle consists of at least two steps:

- 1 Initial data analysis as part of the method execution right after data acquisition.
- 2 A review of the results that were created as part of the data acquisition.

For acquisition-only runs only: Separate result calculation is executed at a later point in time as a user-configured batch in the ChemStation batch review window.

The automated data transfer during data acquisition is described in the above section. The data transfer during the data review process is also managed by the application. As soon as one or more result values are changed or a new result is created, the Security Pack application transfers all runs with new results automatically to the ChemStore C/S database. The application automatically detects updated or new results by comparing the last actual value with the new value. Each result comparison is denoted in a text file
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named Sec_Trac.txt. This file is stored along with the raw data files in the raw data *.d subdirectory. The data comparison is initialized by any activity creating a new result like:

- first pass result calculation after initial acquisition
- printing a report
- · applying a data analysis method to a data file
- integrating a chromatogram with the integrate or auto-integrate commands
- modifying the calibration table

The application of manual integration events is different in the interactive data analysis view and in the batch review. The views are discussed separately in the next two sections:

- The interactive review in "ChemStation Data Analysis View" on page 37
- The batch review window for reprocessing of an entire batch of data in "ChemStation Batch Review" on page 39

ChemStation Data Analysis View

The ChemStation data analysis view is designed for advanced review of individual data files, as well as reprocessing of sequences.

Sequence reprocessing offers certain recalibration options, like floating re-calibration or bracketing calibration. Other tasks - like modifying integration events or applying manual baselines - can be processed more conveniently in the batch review. For ChemStation operators these tasks are accessible in the batch review only.

Therefore, the standard data analysis view is not designed being the default data review window with the ChemStation Plus Security Pack. In addition, if the data storage is configured as recommended in "Storage of Data" on page 33 no data will be available on the hard disk any longer for loading into the data review. The data files are deleted immediately after the transfer to the database.

3 A Brief Tour

Data Transfer from ChemStation



Figure 13 ChemStation Plus Interactive Data Analysis View with ChemStation Operator Access Level

In order to perform sequence reprocessing data has to be reloaded completely via the ChemStore Run Information panel. See also "Transferring Data to ChemStation from the Run Information Interface of ChemStore" on page 65. The sequence naming concept introduced with ChemStation B.02.01 helps avoiding interference with currently acquired data files.

NOTE

Sequence data acquired with ChemStation B.02.01 or higher can be reprocessed in Data Analysis view. This can be done in an idle on-line or off-line ChemStation instance.

Previously acquired sequence data needs to be reprocessed in ChemStation's Method and Run Control view, preferably loaded to an off-line ChemStation instance.

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Another option is preventing 'file deletion after transfer' in the ChemStore study setup dialog. In any case the workflow should be well-defined and protected by user permissions. E.g. by withdrawing "Batch reload" permissions, the data flow can be forced in one direction only.

Data Traceability and Versioning in the Interactive Data Analysis View

The data review functions of the data analysis view of the ChemStation Plus are restricted to the ChemStation manager user level because the data versioning in this view does not cover the manual integration of a chromatogram.

ChemStation operators in the data analysis view can only execute a pre-defined method, reprocess a sequence with a different method or print a report. ChemStation operators cannot change the integration events or report type in this view. The ChemStation operator must use the batch review interface for reintegration of chromatograms.

What is different in the data analysis view compared to the batch review for manual integration?

- The manual integration events are not automatically stored with the run
- The peak table is updated immediately after the manual event was finished
- The application does not detect changed peak parameter and therefore does not transfer data to the database even if new results were calculated.

If the user wants to store the latest results in the database, the manual integration events must be saved to the data file and a report must be generated to initialize the result transfer.

ChemStation Batch Review

Data Traceability and Versioning in Batch Review

Batch review is the default view for reanalyzing data. It can be used for reprocessing the latest ChemStation sequence and for all runs that are submitted from the ChemStore C/S database for reanalysis. In the batch review also the ChemStation operator can reintegrate and recalibrate runs. Batch review also allows the review of a list of runs in one window. Users can step through runs and calculate new results both automatically and interactively.

3 A Brief Tour

Data Transfer from ChemStation

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Figure 14 Batch Review Interface in ChemStation

Versioning in Batch Review

For a detailed overview of the modifications of the batch review compared to the standard ChemStation Plus batch review operation, see "Changes to Batch Mode" on page 56. This section focusses on the data transfer from the batch review to the Chemstore C/S database.

The batch review includes a fully automated data versioning covering also the manual integration events. In the batch review, the manual events that were applied to a chromatogram are stored along with the chromatogram.

In order to avoid the storage of preliminary results, the result creation is split in the graphical rework of a chromatographic data file and the result calculation. During the graphical rework of chromatograms and data files i.e. during drawing of a manual baseline, the peak table will not show the new results immediately like it does in the interactive data analysis. The peak table

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is locked until the calculation is actively performed and it includes a small info button that explains the different operation mode of the batch review in the ChemStation plus Security Pack batch review.

The result calculation is a separate step–graphical data review does not create a result.

File In Integration R	sult Information		Info #	Time	Area	Height	Width	Area%	Symmetry	
LC-File 005-01			1	0.747	300.1	106.9	0.0447	29.855	0.726	
File Path C:\CHE The Chem	Station is operating in Security Mo	ode	2	1.022	276.2	79.9	0.0523	27.475	0.712	
Date 4/19/9 The integr	tion results will not change if you		3	2.569	176.7	26.7	0.1011	17.581	0.632	
Sample Isocrati draw a new	baseline or change integration e	events	4	5.849	252.2	16.8	0.2228	25.089	0.669	
Sample Info	differences were being to templar th									
Barcode results to the	onerence you have to transfer tr	the								
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*s Isocratic Std Calibration	1 005-0101.D	0.747	0.08	15 1.021	0.08733			D	imethylphthalate	
->s Isocratic Std Calibration	2 005-0102.D	0.747	0.09	85 1.022	0.09267			D	iethylphthalate	
*s Isocratic Std Control	3 005-0103.D	0.748	0.08	84 1.023	0.08883			B	iphenyl	
*s Isocratic Std Sample	4 006-0201.D	0.747	0.13	72 1.024	0.13639			0	-Terphenyl	
"s Isocratic Std Sample	5 007-0301.D	0.748	0.19	21 1.025	0.19366					_



As soon as the user calculates the result by pressing the **Integrate** button, the new results are calculated and they are compared with the last results that were stored. If there is any deviation, the data are transferred to the database creating a new result version.

Manual integration events are typically not stored with the method. In order to track these changes along with the other modifications the ChemStation plus Security Pack writes all changes including manual integration events to a text file that is stored along with the raw data in the *.d subdirectory of the ChemStation. **Data Transfer from ChemStation**

The manual integration events are also transferred to the ChemStore run audit-trail. They can be reviewed with **manual integration details** button in the ChemStore audit-trail. This information can be re-used for a later recreation of the manual events i.e. in an audit situation.

	Reason for entry	Status	Modified by	Modified at	Processed
	New	Approval Pending	Administrator	12/29/2008 17:15:42	12/29/2008 17:15:42
	New	Approval Pending	Administrator	12/29/2008 17:15:42	12/29/2008 17:15:42
	New	Approval Pending	Administrator	12/29/2008 17:10:43	12/29/2008 17:10:43
	New	Approval Pending	Administrator	12/29/2008 17:10:43	12/29/2008 17:10:43
	Loaded as part of	Approval Pending	Administrator	12/29/2008 17:10:10	12/29/2008 16:36:01
	Added to Batch	Approval Pending	Administrator	12/29/2008 17:09:32	12/29/2008 16:36:01
	New	Approval Pending	Instrument Operator	12/29/2008 16:36:01	12/29/2008 16:36:01
mment	for selected entry:				
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Figure 16 Review of Manual Integration Events in the ChemStore Audit Trail

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In addition, the application prompts the user for a comment to document the reason for the last change. The comment is documented in the ChemStore audit trail comment field along with a pointer to the text file for the proper identification of the changed events.

Predefined comments	
Baseline settings changed	🔽 Baseline drawn <u>m</u> anually
Peakwidth parameter changed	🔲 Peak <u>d</u> eleted
Slope sensitivity changed	🕅 <u>R</u> ecalibrated
er comment:	Tangent skim set
Area reject changed	Iangent skim set
er comment:	Iangent skim set

Figure 17 Result Comment after Manual Reintegration in Batch Review

Data Transfer from ChemStation

Overview of Data Transfer from ChemStation to ChemStore C/S Database

Any data that has been selected to be saved along with the results (chromatograms, spectra or raw data, method and sequence files in the client/server version) is transferred along with the analysis results.

If configured in the study setups, the Security Pack deletes the raw data locally after the transfer to the database was performed successfully.

The local delete process is controlled by a separate application, the ChemStore C/S ODBC spooler.

ChemStore C/S: ODBC Spooler	
Show Error <u>R</u> esume	<u>H</u> elp

Figure 18 ODBC spooler (Windows users' interface)

The spooler application handles the transfer to the server and makes sure that all data is integrated and stored in the database tables. This check for complete data transfer to the server database is mandatory to enable the delete process of the raw data on the local drive. The entire data transfer is documented in the sequence log book and in the ChemStore C/S audit trail.

The spooler also controls and secures the data transfer from ChemStation to the ChemStation Plus database. In case of transfer problems or network trouble, the spooler pauses or stops the transfer after a certain time limit. After a spooler pause or spooler stop, the user can display the error and resume the data transfer in the spooler application after the error correction.

Members of the Windows user groups *Power Users* (XP only) and *Administrators* can delete spooler jobs in addition to the review and resume function of system users. In case a spooler job is deleted, an entry in the Windows operating system security log is generated.

NOTE

The spooler access for deleting spooler jobs is limited to members of the operating systems *Power Users* (XP only) and *Administrator* groups.

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This data transfer processing allows users to store all data in one central place while preventing any data loss and documenting each transfer step.

To process your data further, ChemStore C/S allows you to export information to MS Excel, or to print reports to a file in *.html, *.xml or *.csv format. The data export to file is checksum protected to ensure the identity of original data and exported copy. You can also export the data to the Windows Clipboard for use in other Windows applications.

3 A Brief Tour

Retrieval of Raw and Meta Data in ChemStation Batch Review

Retrieval of Raw and Meta Data in ChemStation Batch Review

The data storage application is the ChemStore C/S database. Following the default study setup, the ChemStore C/S ODBC spooler transfers all data to the central database and deletes the new data from the default **chem32\data** directories.

In order to re-analyze runs in the ChemStation, the user must transfer data from the Database Review Client back to the local hard disk drive. The raw data files will be removed from the client computer after retransfer. The data transfer from the result management is a four step process. The first step is querying the database.

A *query* is a request to retrieve a set of runs from the many thousands of runs your database comprises that matches certain criteria.

Start the ChemStation and select View > ChemStore Review Client.

Select from the ChemStore C/S Database Review Client and run a query. The query retrieves the results and data information in order to review and approve data. If you need to re-analyze or reprocess your raw and meta data, the data must be transferred back into the Data Analysis view of the ChemStation.

There are two ways to transfer data from ChemStore C/S to the ChemStation:

- 1 Transferring data from ChemStore C/S to the batch review of the ChemStation (default and recommended transfer), see "Transferring Data from ChemStore to Batch Review of ChemStation" on page 60.
- **2** Transferring data from the run information interface of ChemStore C/S to the ChemStation, see "Transferring Data to ChemStation from the Run Information Interface of ChemStore" on page 65.

Audit Trails

All activities associated with each sample are documented in audit trails which track all changes that are made to a run from data acquisition over re-analysis to long-term archiving.

Each sample has an *audit trail* which is maintained separately from the sample data. The audit trail is archived separately from the run, so that archiving and de-archiving activities can be added to the audit trail; the link to the audit trail is maintained, even when the run is archived.

The audit trail for any run can be displayed. It contains a table showing information about each change in the status or the value of a custom field for the run. For manual re-integration events check the details of the re-integration with the **Man. Integ. Details** button. It will open an additional window with all manual integration details for the selected run version if the database query was executed based on 'all versions'. (see Figure 16 on page 42)

The storage of modification time and processing time in local time (calculated and documented with the difference to GMT) also indicates when a change took place. The processing time documents the time of the data transfer from the application to the database, the modification time documents the time the audit trail generating activity was performed.

In addition the two time stamps immediately reveal a deviation of data modification and data transfer showing a review activity of the individual run version.

The audit trail information can be printed directly from the table or individually configured in complete reports for a set of runs. Some questions, particularly those at the administrative level of the application, cannot be answered by the run-related audit-trail.

All interactions that affect the security of the database and the application are tracked and documented in the *database logbook*. ChemStore can also be configured to send a notification by e-mail in case of potential security violations. See chapter "E-Mail notification" in the ChemStore Concepts Guide for details of how to set up this service.

The log book entries can be displayed in a table.

Δ	11	d	it.	т	11	9	ï	lc
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#	User	Created at	Reason for entry	Affected user	Client	PC name	
			Successfully logged on		Review Client		
34	admin	12/29/2008 5:35:32	Logged off		Review Client	DATASYSTEM01	
33	admin	12/29/2008 5:35:10	Logged off		Instrument 2	DATASYSTEM01	
32	admin	12/29/2008 5:09:35	Created batch		Review Client	DATASYSTEM01	
31	admin	12/29/2008 4:53:24	Session unlocked		Instrument 2	DATASYSTEM01	
30	operator	12/29/2008 4:53:24	Logged off		Instrument 2	DATASYSTEM01	
29	operator	12/29/2008 4:53:17	Session locked		Instrument 2	DATASYSTEM01	
28	operator	12/29/2008 4:44:41	Successfully logged on as Operator		Instrument 2	DATASYSTEM01	
27	operator	12/29/2008 4:36:22	Session unlocked		Instrument 2	DATASYSTEM01	
26	admin	12/29/2008 4:36:22	Logged off		Instrument 2	DATASYSTEM01	
25	admin	12/29/2008 4:36:15	Session locked		Instrument 2	DATASYSTEM01	
24	admin	12/29/2008 4:34:53	Successfully logged on as Manager		Instrument 2	DATASYSTEM01	
23	admin	12/29/2008 4:20:17	Assign Study to User	operator	ReviewClient	DATASYSTEM01	
22	operator	12/29/2008 4:19:52	Session unlocked		Instrument 2	DATASYSTEM01	
21	admin	12/29/2008 4:19:52	Logged off		Instrument 2	DATASYSTEM01	
20	admin	12/29/2008 4:19:41	Session locked		Instrument 2	DATASYSTEM01	
19	admin	12/29/2008 4:18:45	Successfully logged on as Manager		Instrument 2	DATASYSTEM01	
8	admin	12/29/2008 4:10:41	Successfully logged on		Review Client	DATASYSTEM01	
17	admin	12/29/2008 4:10:34	Failed to log on		Review Client	DATASYSTEM01	
16	admin	12/17/2008 11:21:59	Successfully logged on		Utility	DATASYSTEM01	
15	admin	12/17/2008 11:21:59	Changed password		Utility	DATASYSTEM01	
4	(built-in)	12/17/2008 11:21:46	Updated database schema		Review Client	DATASYSTEM01	
13	(built-in)	12/17/2008 11:21:46	Updated database schema		Review Client	DATASYSTEM01	
12	(built-in)	12/17/2008 11:21:45	Updated database schema		Review Client	DATASYSTEM01	

Figure 20 Database log book

With this database log book and the current list of authorized users and their permissions, the application can be checked for its security status for the full record retention time.

In an audit situation, a user is now able to proof the ongoing secure status of the data plus the short periods of insecurity when a user with administrative capabilities was logged on to the system. As an example, one user had logged on to the system and had access to sensitive activities like archiving/deleting data. In a review situation, the responsible operator could prove that, except from this time line, the full application was secure by:

- showing the list of current permission rights in the user administration screen of ChemStore C/S.
- querying the database log book session **Reason for entry** for **Permission right** changed.

This combination of current status documentation and a query for backwards changes reveal all user rights and changes for the entire database lifetime.

The documentation of the data acquisition is stored in the instrument and sequence log book as well as in the run-specific run log books.

💷 Opened Logbook	File SIMTEST.log		
Sequence	SIMTEST.S completed	10:47:18 01/02/09	*
ChemStore	Data spooled to 'OQtrace'	10:47:17 01/02/09	
Method	Method completed	10:47:17 01/02/09	
Method	Saving Method DADSIM.M	10:47:12 01/02/09	
ChemStore	No error	10:47:12 01/02/09	
ChemStore	Changing permissions of 'C:\Chem32\Chemstor\	10:47:12 01/02/09	
CP Macro	Analyzing rawdata NV0501.D	10:47:09 01/02/09	
Method	Saving Method DADSIM.M	10:47:06 01/02/09	
Method	Method started: line# 5 blank run inj# 1	10:47:06 01/02/09	
ChemStore	Data spooled to 'OQtrace'	10:47:05 01/02/09	
Method	Method completed	10:47:05 01/02/09	
Method	Saving Method DADSIM.M	10:47:01 01/02/09	
ChemStore	No error	10:47:00 01/02/09	
ChemStore	Changing permissions of 'C:\Chem32\Chemstor\	10:47:00 01/02/09	
CP Macro	Analyzing rawdata NV0401.D	10:46:57 01/02/09	
Method	Saving Method DADSIM.M	10:46:55 01/02/09	
Method	Method started: line# 4 blank run inj# 1	10:46:54 01/02/09	
•			ان ۱

Figure 21 Instrument and Sequence Log book

Automated Data Versioning

Daily work quite often requires more than one analysis copy of results. The FDA rules require storing all reanalysis data as versions together with the original raw data and results. The implementation in Security Pack first needs to uniquely identify the initial run version in the database. To define the initial run version, it uses a combination of injection time in local time using the local time zone settings of the computer operation system and the unique injection ID. Following this definition, all reprocessing copies or reanalyzed versions of the initial run are linked together, offering a complete history of final results with all intermediate steps and results. This versioning is user independent, computer generated and documented in the audit trail.

To ensure the full versioning, the ChemStation also must

- identify each new result
- automatically send the new result data to the database whenever a new result is created

Organize 🔻 🏢 Views 🔻 📥 Print 🔞 B	um	_	_	_	_
vorite Links		Name	Date modified	Туре	Size
P		ACQ.M	1/2/2009 10:58 AM	File Folder	
Documents		DA.M	1/2/2009 10:58 AM	File Folder	
Pictures		ACQRES.REG	1/2/2009 10:58 AM	Registration Entries	2 KB
Music		CHROM.REG	1/2/2009 10:58 AM	Registration Entries	6 KB
More »		CHROMREG.REG	1/2/2009 10:58 AM	Registration Entries	6 KB
ders	×	dad1A.ch	1/2/2009 10:58 AM	CH File	7 KB
Chamatas		LCDIAG.REG	1/2/2009 10:58 AM	Registration Entries	2 KB
Chemistor	_	RUN.LOG	1/2/2009 10:58 AM	Text Document	3 KB
5300		SAMPLE.MAC	1/2/2009 10:58 AM	MAC File	1 KB
M4420J9		SAMPLE.MAC.bak	1/2/2009 10:58 AM	BAK File	1 KB
100-0201.D		SEC_SAVE.REG	1/2/2009 10:58 AM	Registration Entries	3 KB
DAM		sec_Trac.txt	1/2/2009 10:58 AM	Text Document	1 KB
DEFAILT D					

Figure 22 New files for Full Audit trail in the Raw Data Subdirectory

Security Pack therefore stores the numeric results in a registry file sec_Save.reg. The registry file is stored with the data. Each new result version has a different registry file. Prior to creating a new result version, the system compares the current results with the data stored in the registry file. As soon as it detects a deviation, a new result version is stored in the database. For a full traceability of the modified results, the difference between the result versions are documented in a text file sec_Trac.txt stored in the *.d subdirectory of the raw data. The storage management of the database minimizes the file size by limiting the result storage to the delta values.

Documentation of Versioning

In addition, the FDA regulations require a documentation of the person performing the changes as well as a time-stamp of the reprocessing. This information is automatically transferred with the new entry in the database; the change person ID is obtained from the log-in and is documented with the person's display name. The time stamp is automatically generated from the time setting of the PC (for the standalone version) or the server (for the client/server version).

Retrieval of Result Versions in ChemStore C/S Database

When you set up a query for data retrieval in the ChemStore C/S database, you can choose to retrieve either all versions of the run or only the latest version. When all versions of the run are displayed, the **Audit** column of the **Run** List shows the version number of the run: **1** is the oldest version, **2** the next oldest; the run marked with + is the latest version. If only the latest version of the run is displayed, a star "*" in the **Audit** column of the run list denotes that multiple versions of the run exist in the database.

Run	Mark run for	Sample name	Audit	Status
				1st level approved
2		calib1	1 <a>	Approval Pending
3		calib2	+ <a>	1st level approved
4		calib2	2	Approval Pending
5		calib2	1 <a>	Approval Pending
6		calib3	+	Approval Pending
7		calib3	2 <a>	1st level approved
8		calib3	1 <a>	Approval Pending



Automated Data Versioning

Security Pack does not allow to delete non-archived data. To delete data, the user must first be granted the privilege to archive and delete data. In case of a standalone system, the user can archive and delete data by copying and archiving the complete *.mdb file and creating a new *.mdb copy through the ChemStore utility.

For more details on managing standalone MS Access databases, please refer to the "ChemStore C/S concepts guide", Section "Backing up your local access database".

Data can only be deleted in the Client/Server Oracle based ChemStore C/S product and must have been archived prior to deleting from the database.

The entire data transfer is documented in the database log book and the audit trail. The database log book denotes the transfer initialization, the audit trail documents the completion of the transfer, including the processing time-stamp.



4

Agilent ChemStation Security Pack for AD, GC, LC, CE, LC-MSD, and CE-MSD User's Guide

Access Level and Batch Review Interface Changes

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Changes to ChemStation Operator Level

In order to limit operators' data access and to track modifications, the Security Pack modifies the ChemStation operator mode significantly for the data review privileges. The standalone ChemStation mode does not allow the operator to perform any interactive reanalysis activities because these activities can't be traced. The Security Pack modifies the data analysis tasks to

- store all individual run modifications with the run.
- store all method versions with their current settings in the database.

NOTE

To access these features, the batch mode of the Data Analysis view must be used.

In the batch mode, the ChemStation operator is allowed to apply manual integration events. He is also allowed to open the integration user interface to change and save the global integration settings of the method.

Table 2 Shows the modifications to ChemStation operator level compared with the user rights of a standard ChemStation operator.

User Task	ChemStation Security Pack Operator	Standard ChemStation Operator
Save acquisition method	No	No
Save data analysis method	Yes	No
Load/Save sequence	Yes	Yes
Modify acquisition parameter	Yes	Yes
Reintegrate automatically	Yes	No
Reintegrate manually	Yes, only in batch review	No
Change integration events	Yes, only in batch review	No
Recalibrate overview and peak summing	Yes	No

 Table 2
 Modifications to ChemStation operator level

User Task	ChemStation Security Pack Operator	Standard ChemStation Operator
Recalibrate other	No	No
Apply method to data and print report	Yes	Yes
User-independent automated result versioning	Yes	n/a
Access to tasks with manual result versioning	No	No

Table 2 Modifications to ChemStation operator level (continued)

NOTE

Due to the extended method modification permissions for ChemStation Security Pack operators it is recommended to store validated master methods along with an example chromatogram in a specific study in the ChemStore database.

Protection of validated master methods on the file system can be achieved by setting the read-only flag on the chem32\x\methods folder and all subfolders.

Changes to Batch Mode

When re-integrating a chromatogram in the standard ChemStation, the peak results table is updated at the same time as the display of the baseline, retention time and compound name in the chromatogram. The ChemStation Plus Security Pack operates differently.

The Security Pack splits the re-analysis task in two steps. The first one allows to perform a graphical review of a set of runs (step through runs) and to work with manual integration events for each compound in a run without generating new results.

The second step is the result calculation including an automated data versioning. The result calculation can either be initialized with a separate

button in or by clicking run by run or automatically stepping through the full list of runs.

The \fbox button is added to the batch toolbar. Calculating a new result will start the comparison with the last results in the sec_save.reg file and in case of a difference, transfer the data to the database. This mechanism allows constructing the baseline for multiple peaks without transferring data with every change.

In batch processing the new baseline is stored with the signal and hence individual to the signal, while in the interactive data analysis it is stored with the method. The signal is added to the raw data file and it might be stored in ChemStore C/S as part of the raw data file. In the case of manual integration in the interactive data analysis, the manual integration events are stored in an extended method file.

In the security mode of the ChemStation plus, all changes are saved automatically with the chromatogram. In case a user wants to disregard the manual integration events prior to calculating the new result, he has to reapply the "last-saved settings" by executing the integrate command from the integration menu.

The transfer of the results to the database is performed after a valid comment is given by selecting one of the predefined comments with a check mark or by typing an individual comment in the text field. The free comment must have at least 5 characters, if no predefined comment has been check marked. If the batch was loaded from a disk, all runs are calculated and transferred when leaving the batch processing mode. Also, in case the user prints a report of a selected run or creates integration results, the data will be transferred immediately.

The data files and the method used by the batch review are loaded into a write-only directory, preventing operators to make unauthorized copies of those files. This directory stores under the "data" directory of the ChemStation session and is named *Chemstor*. Example for this directory: C:\ chem32\1\data\Chemstor

If configured to delete raw data, the files are deleted as soon as the user leaves the batch processing mode or loads a new batch.

For reasons of security, it isn't possible to load a signal as long as the batch mode is active. Therefore the **Load Signal** option in the **File** menu and the ChemStation explorer are disabled. However, the ChemStation software allows overlaying multiple chromatograms of selected runs within the loaded batch. Re-integration and result generation are not possible, as standard reports cannot be generated across multiple runs.

4 Access Level and Batch Review Interface Changes

Changes to ChemStation Operator Level



Agilent ChemStation Security Pack for AD, GC, LC, CE, LC-MSD, and CE-MSD User's Guide

Data Reanalysis

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5 Data Reanalysis

Transferring Data from ChemStore to Batch Review of ChemStation

Transferring Data from ChemStore to Batch Review of ChemStation

The default setup of Security Pack deletes the raw data from the local PCs after the transfer to the database. In order to re-analyze this data, raw data must be transferred back to the local ChemStation PC. The application transfers the data from the database to the ChemStation batch review. Batch review is a mode of data analysis that allows you to do a first-pass review of a batch of samples quickly and easily. You can manually modify the chromatograms and save the modifications for later use. You can also print reports of the batch results.

NOTE The setup of runs for reprocessing is a ChemStore C/S user privilege that must be granted.

Transfer of data from ChemStore C/S to the ChemStation takes place in two stages. First you set up a batch in ChemStore C/S, and then you load the batch in the ChemStation.

NOTE During data transfer from the database to the local hard disk, the application performs a checksum re-calculation. It checks if the hash values are identical. Any mismatch is reported as an error with the message: "Hash values are different."

Setting up a Batch

You can review data and mark it for transfer to the ChemStation in any of the **Sample** layouts or in **Compound** graphics layout. For more details on the batch transfer, see *Agilent ChemStore C/S Concepts Guide*.

- 1 In the ChemStore C/S review client, select a run from the **Run List (Sample** layouts) or the **Summary Results Table (Compound** graphics layout).
- 2 Check the Batch box at the bottom of the table. You can also select Review > Mark Run For > Batch Processing or Batch Processing from the Run List popup menu (right mouse button) to mark a run. To mark all runs for batch processing, select Review > Mark Run For > All For Batch Processing, or All For

Transferring Data from ChemStore to Batch Review of ChemStation

Batch Processing from the Run List popup menu (right mouse button). To remove the batch processing marks from all runs, select Review > Mark Run For > None For Batch Processing or None For Batch Processing from the Run List popup menu.

3 After marking the run(s), select or **Review > Create Batch**. The **Create new batch** dialog box appears.

24/2000 5:43:57 AM	LINDELIENAN	Lange and the second se					
	LINILREM M	12/7/2005 3:25:25	Rev. B.01.03 [204]		calib1	8/24/2000 12:17:33 AM	
24/2000 5:53:12 AM	LINICHEM.M	12/7/2005 3:25:25	Rev. B.01.03 [204]		calib2	8/24/2000 1:47:50 AM	
24/2000 6:02:28 AM	LINICHEM.M	12/7/2005 3:25:25	Rev. B.01.03 [204]	-	calib3	8/24/2000 3:18:21 AM	
24/2000 6:11:44 AM	LINICHEM.M	12/7/2005 3:25:25	Rev. B.01.03 [204]	>			
				>>			
				<<			
				_			
					•	•	
				r	Used method		
					C None		
					• Method		
			•		LINICHEM.M 1/	/2/2009 11:06:32 AM	•
				L	- User / Operator -		
- Phase Constant of Constant o			100		All upper a		
alloration runs			^		C Hoor		
							_
			-		Administrator		w
	24/2000 6:11:44 AM 24/2000 6:11:44 AM	24/2000 6:11:44 AM LINICHEM.M 24/2000 6:11:44 AM LINICHEM.M	44/2000 6:02:28 AM UNICHEM.M 12/7/2005 3:25:25 44/2000 6:11:44 AM UNICHEM.M 12/7/2005 3:25:25	44/2000 5:02:28 AM LINICHEM.M 12/7/2005 3:25:29 Hev. B.01.03 [204] 44/2000 6:11:44 AM LINICHEM.M 12/7/2005 3:25:25 Rev. B.01.03 [204]	44/2000 6:02:22 AM UNICHEMM 12/77/2005 3:25:25 Rev. B:01.03 [204]	44/2000 6:01:28 AM UNICHEM.M 12/7/2005 3:25:25 [Hev. B.01.03 [204] 24/2000 6:11:44 AM UINICHEM.M 12/7/2005 3:25:25 [Rev. B.01.03 [204] <	44/2000 6:02:28 AM UNICHEM.M 12/7/2005 3:25:25 Rev. B.01.03 [204] 24/2000 6:11:44 AM UINICHEM.M 12/7/2005 3:25:25 Rev. B.01.03 [204] ≤ S Calib3 B224/2000 3:18:21 AM Calib3 B22

Figure 24 Create new batch Dialog Box

- 4 Select the name of the run you wish to be included in the batch in the left panel and choose the forward arrow. To remove a run from the batch, select its name in the right panel and choose the back arrow.
- 5 Choose the Method option in the Used method group and select a method from the list to be saved with the batch. To specify that no method is saved, choose the None option in the Used method group; the ChemStation operator must then use a suitable method for processing.
- 6 Choose the **All users** option to ensure that all users of ChemStore get notification of a pending batch. To ensure that a single user gets

5 Data Reanalysis

Transferring Data from ChemStore to Batch Review of ChemStation

notification of a pending batch, choose the **User** option and choose the down arrow to select the user's name from the list.

7 Type a comment in the **Comment** field to add information about the batch. Choose the **Submit batch** button to prepare the batch for access by the ChemStation.

Loading a Batch

Batches created in ChemStore C/S can be loaded into the ChemStation for reprocessing or other handling.

Loading a Batch from ChemStore C/S

1 Select Batch > Load Batch > ChemStore. The 'Load Batch from ChemStore database' dialog box appears where you can select a batch submitted from ChemStore by clicking to the left of the line, where the cursor changes to a black arrow.

creation rime	Creator	Comment
1/2/2009 12:00:04	P Administrator	1st review of calibration runs
1/2/2009 12:00:23	P Administrator	1st review of sample runs

Figure 25 Load Batch Dialog Box

2 Choose the **Load Batch** button to start loading the runs from ChemStore C/S into the **Batch Review** of the ChemStation.

If the **Files for batch missing** dialog box is displayed, listing the files that can not be found in their original locations, copy or move the files back to their original locations, then choose **Continue** to load the complete batch, or choose **Continue to load only those files that have been found in their original locations**, or choose **Abort** to abort the loading of all files.

NOTE

All raw data files that have been analyzed will be deleted from the local disk after closing the batch window. In order to reprocess data that is transferred to the database, these data has to be sent from ChemStore C/S to the ChemStation.

Loading a Batch from Disk

Batches can also be loaded from the local hard disk in case the user decided to disable the **delete raw data after transfer** button in the ChemStore study set-up (intending to keep the raw data on the local hard disk until first pass review has been completed).

NOTE

Agilent recommends to keep the ChemStore study functionality **delete raw data after transfer** enabled. Otherwise data management and data integrity gets more complicated by having identical analytical data in two locations.

5

5 Data Reanalysis

Transferring Data from ChemStore to Batch Review of ChemStation

1 Select Batch > Load Batch > Disk. The Load Batch dialog box appears.

File <u>n</u> ame:		<u>F</u> olders:	ОК
.в		c:\\2\data\demo	
BATCH.B	A	🗁 DATA	Cancel
		🗁 Demo	
		C 005-0101.D	
		C 005-0102.D	
		C 005-0103.D	
	~	C 005-0104.D	*
ist files of type:		Dri <u>v</u> es:	
Batch(* B)		C: Programs	- Network

Figure 26 Load batch from disk Dialog Box

- 2 Select the batch you want to load from the list by clicking on the name in the **File name** list box.
- 3 Click OK.

Transferring Data to ChemStation from the Run Information Interface of ChemStore

You can also choose to reload any or all files saved with a run or a complete sequence interactively from the **Run information** dialog box.

Reloading a run

- 1 Select a run from the **Run List**.
- 2 Select **I**. The **Run information** dialog box appears.

mjoodon			2244	
Туре:	Normal	Operator:	Instrument	Operator
Time:	12/29/2008 16:34:43	Volume:	0.0	Unit: 📕
Processing				
Time:	12/29/2008 16:36:01	Operator:	operator	
Raw data	54.0			
Original path:	C:\CHEM32\2\DATA\SI	4TEST 2008	3-12-29 16-34	-29\NV0101.E
Time:	12/29/2008 16:36:01		Rel	oad raw data
Processing Metho	J			
Original path:	C:\CHEM32\2\DATA\SI	4TEST 2008	3-12-29 16-34	-29\DADSIM.M
Comment:				
Time:	12/16/2008 13:29:04	-		
Quantification type:	Area Pct	1	Re	load method
D	Test for			
 Processing Seque 	nce			
 Processing Seque Original path: 	nce C:\Chem32\2\DATA\SIM	TEST 2008	-12-29 16-34	29\SIMTEST.S
- Processing Seque Original path: Comment:	nce C:\Chem32\2\DATA\SIM	TEST 2008	-12-29 16-34	29\SIMTEST.S
Processing Seque Original path: Comment: Time:	nce C:\Chem32\2\DATA\SIM 12/29/2008 16:34:30	TEST 2008	-12-29 16-34	29\SIMTEST.S
- Processing Seque Original path: Comment: Time: Repetition number:	IC:\Chem32\2\DATA\SIM	TEST 2008	- 12-29 16-34 Re	29\SIMTEST.S
Processing Seque Original path: Comment: Time: Repetition number:	Ince C:\Chem32\2\DATA\SIM 12/29/2008 16:34:30 1 1	TEST 2008	- 12-29 16-34 Βε	29\SIMTEST.S
Processing Seque Original path: Comment: Time: Repetition number: Line:	Ince C:\Chem32\2\DATA\SIM 12/29/2008 16:34:30 1 1	TEST 2008	- 12-29 16-34 Re	29\SIMTEST.S
Processing Seque Original path: Comment: Time: Repetition number: Line: Audit trail	Ince Ince Ince Ince Ince Ince Ince Ince	ITEST 2008	-12-29 16-34 Re	29\SIMTEST.S

Figure 27 Run information Dialog Box

5 Data Reanalysis

Transferring Data from ChemStore to Batch Review of ChemStation

3 Click the **Reload raw data** button. A dialog box appears.

Destination path:		
C:\CHEM32\2\DATA\SIMTE	ST 2008-12-29 16-	34-29\
		Browse
	1	

Figure 28 Reload Raw Data file Dialog Box

- 4 Enter a path.
- 5 Click **OK**.

Reloading a Sequence

- Execute a query based on all versions and select a version 1 run from the Run List. (Higher result versions may not have the sequence context any longer due to batch or single run reprocessing of some sequence runs).
- 2 Select **1** . The **Run information** dialog box appears.
- **3** Choose the **Reload all files...** button. Dependant on the age of the acquired sequence, the look of the reload dialog differs. Figure 29 shows the data reload dialog for sequences acquired with ChemStation B.02.01 SR1 or higher. For sequences acquired with earlier versions of ChemStation the raw data and method path are not fixed and need to be adjusted manually.

NOTE

For ChemStation B.02.01 SR1 and higher: The sequence reload destination should be part of the ChemStation data path preferences. If not, the reloaded data is not visible in the ChemStation explorer. Adding the path to the ChemStation path preferences needs to be considered, then.

Raw data			
Original full path:	C:\CHEM32\2\DATA\SIM	TEST 2008-12-29 16-34-29\	
<u>D</u> ata path:	as sequence path		
Method			
Original full path:	C:\CHEM32\2\DATA\SIM	TEST 2008-12-29 16-34-29\	
<u>M</u> ethod path:	as sequence path		
Sequence			
Original full path:	C:\Chem32\2\DATA\SIM1	FEST 2008-12-29 16-34-29\	
Container path:	C:\Chem32\2\DATA\	▼ SIMTEST 2008-12-29 16-34-29	

Figure 29 Sequence reload destination selection

5

Transferring Data from ChemStore to Batch Review of ChemStation

Step 4 to 7 apply to pre-B.02.01 ChemStation data only:

- 4 If the sequence file exists at the destination path you can choose to overwrite the existing sequence or not. It is recommended to overwrite the existing sequence, thus ensuring the same sequence parameters.
- 5 The destination path for the raw data should be empty, since the reload function does not allow to overwrite existing data. The original full path can be copied by using the Ctrl+C and Ctrl+V short keys.
- 6 Click **OK**.
- 7 If the **Overwrite existing method files** dialog box appears, check the **Overwrite** boxes for the you wish to overwrite with method from the database and click **OK**.
- 8 When the task is complete, a **Summary** appears.

Туре	Path	File name	Status
Sequence	C:\Chem32\2\DATA\SIMTEST 2008-12-29 16-34-28	SIMTEST.S	reloaded
Raw data	C:\Chem32\2\DATA\SIMTEST 2008-12-29 16-34-28	NV0101.D	reloaded
Raw data	C:\Chem32\2\DATA\SIMTEST 2008-12-29 16-34-28	NV0201.D	reloaded
Raw data	C:\Chem32\2\DATA\SIMTEST 2008-12-29 16-34-28	NV0301.D	reloaded
Raw data	C:\Chem32\2\DATA\SIMTEST 2008-12-29 16-34-28	NV0401.D	reloaded
Raw data	C:\Chem32\2\DATA\SIMTEST 2008-12-29 16-34-28	NV0501.D	reloaded
Method	C:\Chem32\2\DATA\SIMTEST 2008-12-29 16-34-28	DADSIM.M	reloaded
		Print	Close Help



Integration

This section will focus on the integration using the batch review. For integration using the interactive **Data Analysis** view of the ChemStation, please refer to the *Understanding the ChemStation* manual.

Integrating a Signal Automatically

- 1 Select Batch > Load Batch > ChemStore. The Load Batch from ChemStore database dialog box appears. (See Figure 25 on page 62)
- 2 Select the button Load Batch... mind the comment.
- **3** The batch review task starts with the application of a method to a run. The method usually is transferred along with the batch from the ChemStore C/S database. If the batch was submitted without a method, the application will ask you to load a local method.
- 4 Click either the manual integration events 🛛 🗟 🖾 🖄 🖄

or	P	
Select	M	

5 Select Integration > Integration Events or



1ch

Figure 31 Integration Events

- **6** Enter the integration events to be used by the integrator.
- 7 If you wish to apply the events to re-integrate a list of samples from the batch, click Start? . The software will step through the runs and re-integrate file after file until the batch is done or the operator stops the automated review.

Integrating a Signal Manually

- **1** Select **Batch > Load Batch > ChemStore**.
- 2 Select the batch to be loaded.
- 3 Select **Integration > Integrate** to integrate the signal using the initial values specified in the integration events table of the current method.
- **4** Select a sub-menu from the **Integration** menu to specify a manual integration action. All functions described below are also accessible from the **Status** toolbar.
 - a Select Draw Baseline to define a baseline.

Click and hold down your mouse button at one end of the baseline. Then, drag your mouse to the other end and release the button.

b Select **Negative Peak(s)** to define a baseline for negative peaks.

Click and hold down your mouse button at one end of the baseline. Then, drag your mouse to the other end and release the button.

c Select Tangent Skim to define a tangent.

Click and hold down your mouse button at one end of the tangent. Then, drag your mouse to the other end and release the button.

d Select **Split Peaks** to specify a drop line.

Point to the place along the x-axis where you want the drop line and click your mouse button to integrate the signal.

e Select Delete Peak(s) to draw a box around the peak you want to delete.

Click and hold down your mouse button at one corner of the box. Then, drag your mouse to the opposite corner and release the button.

5 If you are satisfied with the baseline position, continue with the next run or display the integration results. Both actions will trigger spooling of the new results to the database. If you are not satisfied with the baseline position reintegrate the signal. No run version will be spooled until as long as no new results are displayed.

Recalibration

For a recalibration using the **bracketed calculation mode**, you have to reload the sequence and reprocess it in ChemStation's data analysis view. For pre-B.02.01 ChemStation data you need to reprocess the sequence in the ChemStation's method and run control view of an off-line copy.

As an alternative, all brackets can be re-calibrate in batch mode if they are set-up as individual batches. If you do not want to use a **bracketing mode** for calibration, the recalibration can be performed through the batch review.

The batch review allows to recalibrate using an averaged result of all calibration runs or using individual run-based changes.

- 1 Load a batch in the ChemStation.
- 2 If you want to update the calibration table, use the standard calibration tools of the ChemStation.
- 3 After finishing the modifications on the run and/or in the calibration table, click



This will update the calibration table using the calibration samples in the batch.

4 To reprocess the data and to get new results with the up-dated calibration table, start the automated step through runs with **Start**.

The square brackets [] around compound results indicate results not generated by the current calibration. The brackets will be removed automatically when a new and different result using the current calibration is generated.


Agilent ChemStation Security Pack for AD, GC, LC, CE, LC-MSD, and CE-MSD User's Guide

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6 Administrator Tasks and Reference Introduction

Introduction

To keep track of actions that might affect data integrity in a ChemStore C/S system, certain tasks require to be logged on to the computer as a member of the Windows user *Power Users* (Windows XP only) or *Administrators*. Permissions to Chromatographic tasks like data acquisition and data review are administered within ChemStore C/S. Agilent does not recommend to perform routine work like review chromatographic data or acquiring data when logged on as a member of the Windows user *Power Users* (Windows XP only) or *Administrators*. All users that use the ChemStation Plus system must be members of the local Windows user group *users*. Otherwise the global group, they belong to, must be a member of the local group *users*. Within a Windows multi domain environment a trust relationship is not sufficient. Each global domain user group has to be explicitly included in the local Windows group *users*. Table 3 lists common administrative tasks and their respective ChemStation, ChemStore and Windows settings required.

Administrative task	Membership in WIndows group <i>Administrators</i> required	ChemStore C/S permission required	ChemStation manager access level required
Running instruments	No	No	No
Reanalysis of data	No	No	No
Modifying ChemStation sequences (Study, custom field values, samples)	No	No	No
Save acquisition method to disk	No	No	Yes
Save data analysis method to disk	No	No	No
Resume database spooler	No	No	No
Deleting spooler jobs	Yes	No	No
Creating a new ChemStore C/S users	No	Administer users	No
Assign user settings to users	No	Administer user settings	No

Table 3 Administrative Tasks

Administrative task	Membership in WIndows group <i>Administrators</i> required	ChemStore C/S permission required	ChemStation manager access level required
Select database connection	Yes	No	No
Data archiving (MS Access DB)	Yes	No	No
Data archiving (Oracle DB)	No	Archive / Dearchive runs	No
Creating new database (MS Access only)	Yes	No	No
Creating new database from template (MS Access only)	Yes	Create database	No

Table 3 Administrative Tasks (continued)

Tasks requiring a ChemStore C/S permission

Tasks requiring a ChemStore C/S permission

The *Administer users* permission in the ChemStore C/S user administration is the key privilege in managing user rights and user roles in Security Pack. It allows creating a new user with specific permissions, change the permissions or reset the password for an existing user.

Creating a new user

- **1** Select Administration / Administer Users...
- 2 The Administer Users dialog box appears.

Jser: admin	Create new user	
Deactivate User 🔽	Change display name	
🛛 ear password 🛛	<u>P</u> rint user profile	
User permissions:		
ndividual permissions:	Permissions granted:	
	Administer custom fields	
Operator Permissions ->	Create / Edit advanced filters Create / Edit advanced filters Create / Edit queries Create / Edit queries Create / Edit report templates	
Chemist Permissions ->	Create batch Data reload configuration	
Lab Manager Permissions ->	Define columns / Expression Edit / Save settings	
Administrator Permissions ->	Edit custom field values First level approval	
ChemStation access level:		
C Chem <u>S</u> tation Operator	ChemStation Manager	

Figure 32 Administer Users Dialog Box

3 Choose the **Create new user** button. The **Create user** dialog box appears.

gogin name.	lamilier	
Display name:	Anthony Miller	



- 4 Enter a Login name and a Display name.
- 5 Click **OK**.
- 6 Select permissions for this user from the **Individual permissions panel** and transfer them to the **Permissions granted panel** by using the forward arrow or grant standard sets of permissions by using the buttons below the **Individual permissions panel**.
- 7 Choose to set this user as a ChemStation Operator or as a ChemStation Manager.
- 8 Click **OK**.

Modifying an Existing User Profile

- Select Administration > Administer Users. The Administer Users dialog box appears.
- 2 Select the user you want to modify from the **User** list.
- **3** Add or remove permissions.
 - To add permissions, select them from the **Individual permissions panel** and transfer them to the **Permissions granted panel** using the forward arrow.
 - To remove permissions, select them from the **Permissions granted panel** and transfer them back to the **Individual permissions panel** by using the back arrow.
- 4 Choose to set this user as a ChemStation Operator or as a ChemStation.
- 5 Click **OK**.

Tasks for operating systems administrators

These tasks can only be performed when you log on to Windows as a member of the Windows Operating system user Administrators or if the corresponding application is started in *run as administrator* mode. On Windows XP systems the membership to the *Power Users* group is sufficient. Some tasks additionally require a ChemStore C/S permission.

NOTE

When running an application as administrator it is important to close this application when the work is finished.

Configuration of the DB Size Security Service

The size limit for a Microsoft Access database is 1 GByte. Therefore it is highly recommended not to exceed a size of 850 MBytes for the database. This ensures that sufficient space is left in the database to allow further reprocessing of the data already contained in the database.

When a size of 750 Mbytes is reached the software will display a warning message during log-on to notify user, that it is approaching the size limit. As this message is displayed a new Access database should be created using the ChemStore utility. Only a member of the Windows user *Administrators* able to configure the warning limits of the service and create a new Access database and assign the new database connection. For details on how to configure the size security service please refer to the 'ChemStore Concepts Guide'. For details on how to create a new Access database please refer to "Creating New Databases in the Standalone Version" on page 82.

Assigning a Database Connection on Windows XP operating systems

Only members of the Windows user *Power Users* or *Administrators* can change the database connection. All other users can only log on to the database currently selected. To change the database connection do the following:

- 1 Log-on to Windows as a user that is a member of the Windows user *Power* Users or Administrators
- 2 Select Programs > Agilent ChemStation > ChemStore Review Client from the Windows Start menu.
- 3 At the ChemStore Log On screen press the **Select** button (see Figure 35 on page 81)
- 4 Either select the appropriate database alias from the list or, in the case of a new database, select Browse and point to the new *.mdb file to create a new database alias in the list. (see Figure 36 on page 81)
- 5 In the 'Set as default' group,
 - a Mark the 'for this session' check box to specify that the selected database is the default for this instrument or application only. Windows users logging on to this instrument or application without *Power User* or *Administ*rator permissions must use the specified database.
 - **b** Mark the '**for all sessions'** check box to specify that the selected database is the default for all instruments and applications on this work station. Windows users logging on to any instrument or application without *Power User* or *Administrator* permissions must use the specified database.
- **6** click **OK** to make the selection active.
- 7 Start up the Review Client and log on with any valid user account
- 8 **Important:** Close down the Review Client and log on as a member of the Windows user group *users*.

Assigning a Database Connection on Windows Vista operating systems

Only members of the Windows user *Administrators* can change the database connection. All other users can only log on to the database currently selected. To change the database connection do the following:

- 1 Log-on to Windows as a user of any user group
- 2 Browse to All Programs > Agilent ChemStation > ChemStore Review Client from the Windows Start menu.
- 3 Right mouse click the ChemStore Review Client icon and select **Run as** administrator



Figure 34 Start ChemStore Review Client as adminstrator

4 At the Windows Vista **User Account Control** panel enter the password of an active Windows administrator account and allow the program **HPCsCl00.exe** to access your computer

5 At the ChemStore Log On screen press the **Select** button

ChemStore C/S: Lo	g On	
User <u>N</u> ame:	admin	Log on Cancel
Password:	*****	Help
Database hpcs	<u>S</u> elect	Change Pwd



6 Either select the appropriate database alias from the list or, in the case of a new database, select **Browse** and point to the new ***.mdb** file to create a new database alias in the list.

ChemStore C/S: Se	elect Database	×
Alias: Quality Lab	Comment: C:\Chem32\Chemstor\Database\Qualitytab.mdb	QK Cancel <u>H</u> elp
		Delete Browse Set as default □ for this session ✓ for all sessions

Figure 36 Selecting a new database

- 7 In the 'Set as default' group,
 - **a** Mark the **'for this session'** check box to specify that the selected database is the default for this instrument or application only. Windows users logging on to this instrument or application without *Administ* rator permissions must use the specified database.

Tasks for operating systems administrators

- Mark the 'for all sessions' check box to specify that the selected database is the default for all instruments and applications on this work station. Windows users logging on to any instrument or application without *Administrator* permissions must use the specified database.
- 8 click **OK** to make the selection active.
- 9 Start up the Review Client and log on with any valid user account
- **10 Important:** Close down the Review Client to end the program running in administrative mode

Creating New Databases in the Standalone Version

The ChemStore C/S Utility is used to create a new MS Access database in case the previous database has reached its size limit and/or has been archived onto a storage media. On Windows Vista operating systems the ChemStore C/S Utility application needs to be *run as administrator* (see also Figure 34 on page 80). On Windows XP operating systems it can only be used by members of the Windows user *Power Users* or *Administrators*.

To retain user settings, report templates, filters, queries, user interface settings, and customized settings, the last used database can be used as a template for the new database. To import settings from another database, you must log-on the template database as a user with the ChemStore C/S Permission Administer users in the template database.

NOTE

Password settings like minimum password length and account lock out will not be transferred to the new database.

- 1 Log-on to Windows as a user that is a member of the Windows user *Power Users* (XP only) or *Administrators*.
- 2 Select **Programs > Agilent ChemStation > ChemStore Utility** from the Windows Start menu.
- **3** Windows Vista only: Run the **ChemStore Utility** as administrator

4 Select File > Create Access Database. The 'Create a new ChemStore B.04' database dialog box appears.

Lieate a new Chemotore D.04 database	
Enter a filename for the ne w ChemStore B.04 database	.
C:\Chem32\Chemstor\Database\Qualitylab.mdb	Browse
In order to import all user settings and report templates from an existing database, logon to that database.	:
	Logon
	Logon

Figure 37 Create new MS Access database

- 5 Choose the **Browse** button
- 6 The **Save As** dialog box appears.
- 7 Enter a database name in the File name text box.
- 8 Choose the **Save** button.
- 9 Choose the **Logon** button if you want to import settings from a template database.
- **10** Select the database alias that should be used as a template.
- **11** Type in name and password of a user with administrative privileges.
- 12 Choose the **Create** button.
- 13 You should close the ChemStore C/S Utility once the database creation is successfully finished. If users should use this database now, you need to connect to the new database as outlined in "Assigning a Database Connection on Windows XP operating systems" on page 79 or "Assigning a Database Connection on Windows Vista operating systems" on page 80 respectively.

Database Backup in the Standalone Version

To protect the database from unauthorized manipulation, Windows users that are members of the group *users* only have special write access to the database directory. Therefore they can not copy the database onto a backup or archive media. To backup or archive the standalone database perform the following steps:

- If your operating system is Windows XP, log-on as a user that is a member of the Windows user groups *Power Users* or *Administrators*. On Windows Vista the following operations can be performed while beeing logged on as a Windows *user*. However, an administrator's password is required.
- 2 If the database is to be archived, create a new database as described in the section "Creating New Databases in the Standalone Version" on page 82. To allow a consitent data management the new database name should be unique.
- 3 Copy the database file (*.mdb) from chem32\chemstor\database to the backup or archive media.
- 4 If the database was archived additionally perform the following steps:
 - a Delete the original database from the hard drive.
 - b Select Programs > Agilent ChemStation > ChemStore Review Client from the Windows Start menu.
 - **c** Windows Vista only: Start the Review Client as administrator (see Figure 34 on page 80)
 - d Select to open the **ChemStore C/S: Select Database** dialog box.
 - e Select the database alias that was archived and click on **Delete** to delete this alias.
 - **f** Choose **Browse** and select the database created in step 2.
 - g Click on **Open**.
 - **h** Enter a database alias and select **OK**.
 - i Select the new database alias and click on **OK**.
 - j Start up the ChemStore C/S review client and close it again.
 - k Log-on as a member of the Windows user group *users*.

Further details about recommended back up procedures can be found in the *Agilent ChemStore C/S Concepts Guide*.

Event Log File Backup on Windows XP operating systems

If you are using Security Pack together with a standalone ChemStore C/S installation, it is mandatory not only to perform a regular back up on the database files containing the analysis data, but also the Windows Event log files, showing that no data was deleted or altered. To store the Windows security log on a backup or archive media do the following:

- 1 Log-on to Windows as a user that is a member of the Windows user group *Administrators*.
- 2 Select Settings > Control Panel > Administrative Tools > Event Viewer from the Windows Start menu.
- **3** Right-click the **Security Log**.
- 4 Select the **Save As** function and type in a file name. Agilent recommends to include the **Event log** as EVT files in the back up to allow for easy usage later on.
- 5 Copy the event log file on the backup or archive media.
- **6** To prevent excessive growth of the event log file, you have the option to clear it. Use this option only after you copied the current event log to an archive media. Select **Log > Clear All Events** to clear the security event log.

Further details about recommended back up procedures can be found in the *Agilent ChemStore C/S Concepts Guide*.

Event Log File Backup on Windows Vista operating systems

If you are using Security Pack together with a standalone ChemStore C/S installation, it is mandatory not only to perform a regular back up on the database files containing the analysis data, but also the Windows Event log files, showing that no data was deleted or altered. To store the Windows security log on a backup or archive media do the following:

Tasks for operating systems administrators

- 1 Log-on to Windows as a user of any user group
- 2 Select Control Panel > Administrative Tools > Event Viewer from the Windows Start menu.
- 3 Right-click on the **Event Viewer** icon and run it as administrator
- 4 Browse to Event Viewer(local) > Windows logs > Security and right-click the Security Log.
- **5** Select the **Save As** function and type in a file name. Agilent recommends to include the **Event log** as EVTX files in the back up to allow for easy usage later on.
- **6** Copy the event log file on the backup or archive media.
- 7 To prevent excessive growth of the event log file, you have the option to clear it. Use this option only after you copied the current event log to an archive media. Right-click the **Security Log** and select **Clear Log**.

Further details about recommended back up procedures can be found in the *Agilent ChemStore C/S Concepts Guide*.

Setting Up E-Mail Notification

The following facility is available on Client/Server systems only. It sends an automatic e-mail notification on specific events and needs to be set up by the administrator (or other user with administrator permissions). The events to trigger an automated e-mail notification are:

- locking of an user account due to exceeded number of unsuccessful log-on attempts.
- submitting a batch for review
- clearing a password
- creation of a new user
- permission modification

With the exception of 'notification of batch submission', the e-mail notifications should only be sent to administrators to warn about security violations.

For details about the set-up, please refer to the ChemStore Concepts Guide.

Troubleshooting Spooler Problems

Troubleshooting spooler problems splits into two sections: spooler resume after error correction and troubleshooting of persistent problems. The two associated workflows are illustrated in Figure 39 on page 88 and Figure 40 on page 89, respectively.

For resuming the spooler after error correction (e.g. a lost network connection or server downtime) members of the user groups *Users* can resume the spooler and display the error message. These users have a modified spooler window for resuming the transfer as shown in Figure 18 on page 44. This menu does not offer the option to delete spooler jobs or to pause the spooler.

Only members of the Windows user *Power Users* (XP only) or *Administrators* have full access to the database spooler. The database spooler transfers the data to the database and temporarily stores the data. In case of a server or database problem the spooler pauses and needs to be resumed. To resume the spooler or to evaluate error messages from the database spooler do the following:

- Double-click with the left mouse button on the database spooler icon in the lower right hand corner of the Windows task bar .
- 2 Check the error message by selecting **Show Error** and resolve the problem.



Figure 38 Database spooler window for members of the user groups administrators

3 Click on **resume** to continue the data transfer to the database after the error was corrected.

If the spooler data is corrupt and refuses to transfer to the database you should follow the workflow illustrated in Figure 40 on page 89.



Figure 39 Corrective action workflow in case of a spooler error

Tasks for operating systems administrators





Tasks for operating systems administrators

Security Settings

To prevent deletion or alteration of data by standard users, the access to crucial directories of ChemStation PlusSecurity Pack is imited to members of the Windows user groups *Power Users* (XP only) and *Administrators*. Agilent does not recommend to change the location, permissions or auditing of these directories. **Table 4** shows the required permission settings and **Table 5** shows the required auditing settings for Security Pack. Upon installation these settings will be set correctly.

In addition it is recommended to activate the auditing function on each local database after creation (For details refer to the Windows help). This triggers more specific information to be entered to the security log file.

Directory	Permissions	Comment
\chem32\chemstor\ database	Administrators (modify) (full control), Power Users (modify) (full control) Users (write+read permissions)(modify)	Used to store the local databases. Not required if used with a ChemStore C/S Oracle server database.
\chem32\chemstor\spool	Administrators (modify) (full control)(), Power Users (modify) (full control) Users (write+read permissions)(modify)()()	Used to store temporary data when transferring data between ChemStation and ChemStore
\chem32\1\data\chemstor	Administrators (modify) (full control), Power Users (modify) (full control) Users (full control)(modify)	Used to store temporary data when transferring data for a batch re-analysis from ChemStore ChemStation
\chem32\chemstor\ hputil00.exe	Administrators (full control) Power Users (full control)	ChemStore C/S Utility for creation of new databases

Table 4Directory and file permissions

Directory	Events to Audit	Comment
\chem32\chemstor\database	Administrators and Power Users: success + failure	Logs if database files were deleted by a member of the <i>Administrators</i> or <i>Power Users</i> group.

Table 5 Directory and file auditing

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In This Book

This book describes the Agilent ChemStationSecurity Pack for AD, GC, LC, CE, LC-MSD and CE-MSD techniques. The Security Pack is an add-on module for the Agilent ChemStation and helps you meet the requirements of the U.S. Food and Drug Administration's (FDA) ruling on electronic records and signatures, CFR 21 Part 11.

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Printed in Germany 02/09



