

Agilent Sample Scheduler for OpenLab

Installation & Configuration Guide

Notices

Document Information

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This guide is valid for revision 2.8 of Sample Scheduler for OpenLab

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1 In This Book

This guide describes the requirements, installation, configuration and maintenance of the Sample Scheduler for OpenLab software, revision 2.8.

In addition, it contains information on LIMS commands, XML structures, and troubleshooting hints.

Revision 2.8 of Sample Scheduler for OpenLab is shipped and installed together with OpenLab CDS v2.8.

Table 1: Terms and abbreviations

Term	Description
CDS	Chromatography Data System
Secure Storage	Data storage component provided as part of the OpenLab system
Control Panel	Control Panel for Agilent OpenLab software
OLDR	Data Repository for OpenLab software
Microsoft Control Panel	Part of the Microsoft Windows operating system
AIC	Agilent's Analytical Instrument Controller
Sample Scheduler	Sample Scheduler for OpenLab
Feature	Part of the software that can be installed individually via the installer.

2 Overview

Sample Scheduler for OpenLab improves the productivity of chromatographic analysis in the laboratory by fully automating the analysis. It optimizes use of the laboratory instruments and sample throughput.

The Sample Scheduler serves as the interface between a front-end platform such as a Laboratory Information Management System (LIMS) that sends analysis orders, and the OpenLab Chromatography Data System (CDS) solution that performs and processes the analysis.

Sample Scheduler for OpenLab supports two types of LIMS:

- LIMS that are able to provide analysis orders via a structured XML file in a dedicated folder
- LIMS that can provide the information required to create an analysis order, by answering a structured SQL query sent by the Sample Scheduler

When Sample Scheduler receives a LIMS command in which the analysis status is set to **Scheduled**, it checks the command's validity and the availability of the required chromatographic instrument. A user can review and complete the analysis parameters in Sample Scheduler before the acquisition. If the parameters are specified by the LIMS, Sample Scheduler automatically schedules the order for acquisition. When Sample Scheduler submits the analysis to the instrument queue in the CDS, it is acquired as soon as the instrument is idle and an instrument connection license is available.

Sample Scheduler architecture on page 8 shows how the individual components work together.

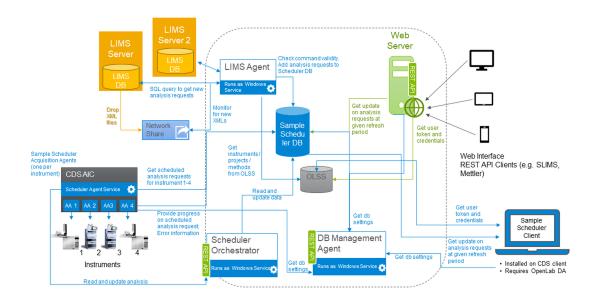


Figure 1: Sample Scheduler architecture

Component	Description
Acquisition agent	handles the acquisition via the CDS acquisition processupdates the analysis state
Scheduler agent	monitors instrument licence, activity and statussubmits acquisitions to the CDS via the acquisition agent
Database (SQL Server or OpenLab Data Repository)	stores the Sample Scheduler configuration parametersstores analyses with their parameters and states
Database Management agent	 root entry point for other services provides information about the Sample Scheduler database configuration
LIMS agent	 scans the LIMS_Commands folder (target folder for the LIMS-generated XML or SQL commands) transforms valid commands into analysis requests stores analysis requests in the database sends invalid commands into a trash folder located in the LIMS_Commands folder root

Component	Description	
OLSS (OpenLab Shared	• set of services and tools, that offer security and other capabilities:	
Services)	· central authentication, authorization, application configuration	
	 system configuration, application configuration, licensing, logging, and notification 	
Sample Scheduler Configuration user interface	 allows you to edit configuration parameters allows you to remotely start/stop Sample Scheduler services on the various CDS machines 	
Sample Scheduler client user interface	displays in real time the analysis statesallows you to display and edit all analyses	
Sample Scheduler webserver	service to provide the Sample Scheduler web interface	
Sample Scheduler web interface	 allows you to display, edit, and schedule all analyses provides an overview of total analyses, daily workload, and instrument status 	
Sample Scheduler Orchestrator service	 handles the communication between the Sample Scheduler database, the Sample Scheduler agent, and the Acquisition agent on the AIC 	

3 Requirements

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Software Requirements

General software requirements

The requirements for .NET, .NET Core, web browsers, and antivirus software are defined by OpenLab CDS. For details, refer to *OpenLab CDS Requirements and Supported Instruments (CDS_v2.8_Requirements_en.pdf, D0028027)*.

Sample Scheduler for OpenLab supports the following web browsers in addition:

- Safari iOS version 16
- Safari macOS version 16

Language compatibility

User interfaces are displayed in the language of the Windows operating system for the following languages:

- English
- Chinese
- Japanese

The English version of the Software can run also with Western European language operating systems, provided the OS Region settings are configured correctly

A localized Sample Scheduler web interface is displayed for the following browser languages:

- Chinese
- Japanese

For other browser languages the web interface will be in English.

Software Requirements

Supported operating systems

Table 2: Supported Operating Systems by components

Windows Product	Server ¹	AIC ²	Sample Scheduler Client ³
Win 10 64 bit, Professional or Enterprise	×		✓
Windows 11 64 bit, Professional or Enterprise	×	*	*
Windows Server 2016	√	√	✓
Windows Server 2019	√	✓	✓
Windows Server 2022	√	✓	✓

See respective OpenLab CDS requirements for details on supported Windows version

OpenLab CDS Supported Configurations

Sample Scheduler for OpenLab is supported on OpenLab CDS client/server topologies with a content management system.

Sample Scheduler for OpenLab revision 2.8 is compatible with:

- OpenLab CDS v2.7 client/server topologies
- OpenLab CDS v2.8 client/server topologies

Computer Date/Time

All Sample Scheduler computers must be synchronous: same date/time.

¹ LIMS agent, Database, Web interface

² Scheduler agent, (not recommended: Scheduler Client, LIMS agent)

³ Scheduler Client, (not recommended: Scheduler agent, LIMS agent)

Software Requirements

Supported Databases

Sample Scheduler for OpenLab can use one of the following databases:

Data Repository

The Data Repository is part of the OpenLab Framework. It is used to store diagnostic and topology related information. It may host a Sample Scheduler database. The Data Repository is supported on Postgres as well as on Microsoft SQL.

SOL Servers

If you use an SQL Server instance, a valid administrator name and password must be available prior to the Sample Scheduler installation. You will have to enter the name of the SQL Server computer, the name of the instance and the associated credentials during the Sample Scheduler installation.

For more information about configuring the SQL Server, refer to **Microsoft SQL Server Configuration** on page 56.

Supported SQL server versions

- SQL Server 2016 Express or Standard
- SQL Server 2017 Express or Standard
- SQL Server 2019 Express or Standard
- SQL Server 2022 Express or Standard

Installing SQL Server Management Studio can be useful if you need to set up database users.

SLIMS Compatibility

Sample Scheduler for OpenLab v2.8 is compatible with

- SLIMS 6.8
- SLIMS 6.9
- SLIMS 7.0

Licensing

Licensing

You need the following licenses to use the full functionality of Sample Scheduler for OpenLab:

- One Sample Scheduler for OpenLab license for each LIMS.
- One Sample Scheduler Expansion Pack license per 10 concurrent instruments

The LIMS agent consumes one license for each LIMS connection and uses it during its operation.

NOTE

If the number of LIMS connections exceeds the number of available licenses, the last connections in the list **Selected LIMS** (Sample Scheduler configuration > LIMS tab) are not established by Sample Scheduler. XML commands or actions addressed to a not established LIMS connection will not be executed and moved to the trash folder.

The users defined in the **Notification** tab will be informed about the trashing of the XML and the reason for it (in this case, the missing license). For more information, check the System Configuration chapter of the Sample Scheduler online help.

To add a license:

- 1 In the Control Panel under Administration, select Licenses and click Add. Enter the license number.
- 2 After adding a Sample Scheduler for OpenLab license: Start the LIMS agent service on the respective computer, and set its startup type to **Automatic**.

Network Requirements

Network Requirements

The network requirements of OpenLab CDS must be fulfilled. For details, refer to the following guides:

- OpenLab CDS Requirements and Supported Instruments (CDS_v2.8_Requirements_en.pdf, D0028027)
- OpenLab Server and OpenLab ECM XT Hardware and Software Requirements (ECM_XT_v2.8_HardwareSoftwareRequirements_en.pdf)

The following firewall ports are used by default for the Sample Scheduler; they will automatically be opened if you install the Sample Scheduler web interface.

- TCP port 443
- Data Repository: port 5432 (or adjusted port according to CDS installation)

In addition add any exceptions for the ports used by Microsoft SQL Server. For details, see **Configure Firewall for SQL Server** on page 70.

NOTE

With increasing latency, the general performance of the Sample Scheduler decreases.

Documents about this

<OpenLab CDS Requirements> (https://www.agilent.com/cs/library/usermanuals/public/CDS_v2.8_Requirements_en.pdf)

Hardware Requirements

Hardware Requirements

All OpenLab CDS client/server topologies are supported by Sample Scheduler. For the server hardware requirements, refer to *OpenLab Server and OpenLab ECM XT Hardware and Software Requirements*

(ECM_XT_v2.8_HardwareSoftwareRequirements_en.pdf). Additional requirements might apply depending on other software that is installed on the same machine, for example, SQL server.

Sample Scheduler for OpenLab adds the following requirements:

Table 3: Minimum additional hardware needs for Sample Scheduler

Item	HW requirement	
Physical memory (RAM) depends on the number of analyses stored in Sample Scheduler database.	LIMS agent	120 MB
	Sample Scheduler agent + Scheduler Acquisition agents	150 MB + 150 MB x per instrument
	Sample Scheduler client	5,000 analyses: 500 MB20,000 analyses: 900 MB
	SQL Server/OLDR	SQL Server manages the memory usage in a nonlinear manner (not proportional to the number of entries in the database). Refer to SQL Server specifications to properly set the SQL server sizing.
	Database Management agent	50 MB
	Web server	Approx. 150 MB depends on number of instruments and users in the system
Hard disk	dedicated to Sample Scheduler for OpenLab	220 MB
Screen Resolution	web interface Sequence View within the web interface	≥ 360 pixels ≥ 768 pixels

Requirements

3

Hardware Requirements

Table 4: Example RAM calculation for an OpenLab CDS client PC

Sample features, require	additional RAM
Sample Scheduler client, about 5000 analyses displayed in the Sample Scheduler user interface	500 MB
Sample Scheduler agent	150 MB
Acquisition agent managing five instruments	750 MB
Total additional required RAM	1.4 GB

Considerations in a Regulated Environment

In regulated environments, you must reduce user privileges to a minimum in order to protect the system. Therefore, a specific OpenLab CDS user account is required for a Service user: This is a user with the privileges required to run automated Sample Scheduler services in the background. For example, the service user schedules analyses that are provided by the LIMS. The service user must remain enabled if you use Sample Scheduler for OpenLab in your laboratory environment.

NOTE

The Sample Scheduler Audit Trail can track which processes were done automatically by the system, and which were done interactively by a user. If you want to use this function, you can assign OpenLab CDS privileges to the Service User, but no Sample Scheduler privileges.

For more information, see Create a Service User in OpenLab CDS on page 42.

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Control Panel Configuration

- Internal, Windows Domain, and ECM authentication modes are supported.
- Projects are defined with a valid project folder path (parallel to CDS file-path: methods, chromatograms, etc.).
- At least one user with the required privileges to activate Sample Scheduler for OpenLab must exist in the Control Panel.

This user's credentials will also be used by Sample Scheduler services (Sample Scheduler LIMS agent, and Sample Scheduler agent) to run automated Sample Scheduler services in the background. In regulated environments, you will create a service user for this purpose (see **Create a Service User in OpenLab CDS** on page 42).

Sample Scheduler Supported Deployments

Database Install only one Sample Scheduler database in the entire system.

By default, the Sample Scheduler database runs on the OpenLab Shared Services server and is installed within the Data Repository. Ensure that your server hardware meets the combined OpenLab system requirements plus the Sample Scheduler RAM requirements.

Alternatively, use an SQL Server instance. If your activity is intense, you might need to install it on an external database server. If you are using SQL Server on an external database server, configure the SQL protocol for remote access, to make Sample Scheduler database accessible from computers other than the one it is installed. For more information, refer to Configure SQL protocol for remote access on page 56.

The Sample Scheduler database management agent service is installed together with the Sample Scheduler database feature. This service must always run on the Shared Services server.

LIMS agent In a client/server system with one server, install only one Sample Scheduler LIMS agent. In an Enterprise topology with several servers, you may install a LIMS agent on each Shared Services server.

> Always install the Sample Scheduler LIMS agent on a server operating system. If you install it on an OpenLab CDS client computer, ensure that the client runs on a server operating system.

Sample Multiple Sample Scheduler agents are allowed per system, but you may only **Scheduler agent** install one agent per computer. Sample Scheduler agents shall be installed on an instrument controller (AIC). An OpenLab CDS client/server installation, will install a Sample Scheduler agent on the AIC automatically.

> Each Sample Scheduler agent can manage up to 20 instruments. However we strongly advice to distribute your instruments on several Sample Scheduler agents to ensure to not overload the AIC. Check the Configuration capacity section of the OpenLab CDS Requirement guide for more details.

Client The Sample Scheduler client can be installed on OpenLab CDS clients or AICs. It is pre-installed on OpenLab CDS clients.

Sample Scheduler Supported Deployments

Web interface In a client/server system with one server, install only one Sample Scheduler web interface in the system. In an Enterprise topology with several servers, you may install a web interface on each Shared Services server.

> The Scheduler web server may be installed on any server with the necessary CDS components.

Table 5: Summary: Features per Hardware PC

	Scheduler database	Scheduler LIMS agent	Scheduler Webserver	Scheduler agent	Scheduler Client
Shared Services Server	1	1 per OLSS server	1 per OLSS server	-	-
CDS AIC	-	-	-	1 per PC	Х
CDS client	-	-	-	-	Χ
CDS client on server OS	-	1 per OLSS server	X	1 per PC	Х

For a detailed list of components that are installed with each feature, see Appendix B: Components and Features on page 165.

Deployment examples

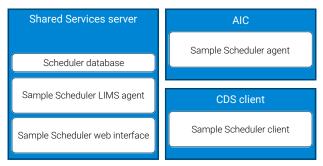


Figure 2: Default deployment

Sample Scheduler Supported Deployments

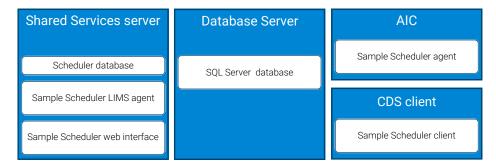


Figure 3: External database server

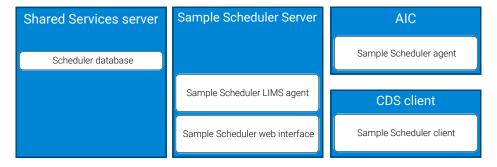


Figure 4: External Sample Scheduler server

Manually Install Sample Scheduler

Use the following instructions if you install or upgrade individual Sample Scheduler features on dedicated machines.

NOTE

If you have installed or upgraded OpenLab CDS, Sample Scheduler for OpenLab is installed automatically. In this case, skip the installation and proceed directly to Activation (see chapter **Activate Sample Scheduler** on page 40).

Start the Sample Scheduler Installation Wizard

Preparations

- The computer hardware meets the requirements specified in **Requirements** on page 10.
- The Control Panel configuration meets the requirements (see **Control Panel Configuration** on page 20).
- You use a supported Sample Scheduler configuration (see Sample Scheduler Supported Deployments on page 21)
- 1 Download the current Sample Scheduler for OpenLab zip package from SubscribeNet.
- 2 Unzip the package.
- 3 The first Sample Scheduler installation must be done on the Shared Services server. Execute the corresponding Agilent.Scheduler.Install_XX.msi(where XX stands for the language code).

Manually Install Sample Scheduler

4 Click Next on the Welcome page.

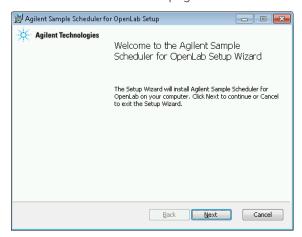


Figure 5: Welcome page

- **5** Read the License Agreement and accept it. Click **Next** to continue the installation.
- 6 On the Custom Setup page, select the features that you want to install.

Manually Install Sample Scheduler

To install a feature, select either **Will be installed on local hard drive** or **Entire feature will be installed on local hard drive**. Both lead to the same result. To not install it, select **Entire feature will be unavailable**.

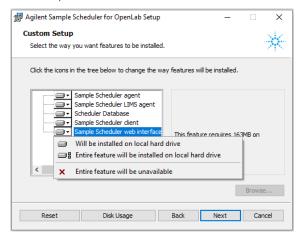


Figure 6: Install features

NOTE

Depending on the installation environment (server, AIC, client) different features are available.

For a detailed list of components that are installed with each feature, see **Appendix B: Components and Features** on page 165.

Install a Sample Scheduler Agent

To install Sample Scheduler agent, follow the wizard.

The Sample Scheduler agent service must be started via a user account with administrative privileges for actions related to machine configuration or certificate installation

NOTE

The Sample Scheduler agent service will not start automatically after the activation if there are no instruments in CDS system.

4

Manually Install Sample Scheduler

Install Sample Scheduler web interface

To install either the Sample Scheduler client or the web interface, follow the OpenLab installation wizard.

Installing the web interface will install the webserver as a service. Deploy Sample Scheduler web interface only on the Shared Services server.

The web interface will be available under the address https://<hostname>/openlab/samplescheduler, or via Agilent Technologies > Agilent Sample Scheduler from the Start menu.

Install Sample Scheduler database

NOTE

If a Sample Scheduler database already exists although Sample Scheduler is not installed (for example, as a relict from a previous Sample Scheduler uninstallation):

V2.7 databases and data are automatically upgraded to v2.8.

V2.6 or older databases will remain unchanged. They are not removed.

- **1** Follow the wizard.
- 2 Identify the database instance (SQL Server or OpenLab Data Repository) used by the Sample Scheduler.

The Sample Scheduler database access parameters have to meet the requirements for all Sample Scheduler components which need to access the database. It is not sufficient to meet the needs of the local services which are checked during the installation - services on other computers may not be able to start after installation.

You can adjust the database access parameters after installation with the Database Access Reconfiguration Tool

(Agilent.Scheduler.Database.Access.Reconfiguration.exe), available from the \bin folder of the Sample Scheduler installation directory on the Shared Services server (default path: C:\Program Files (x86)\Agilent Technologies\Sample Scheduler for OpenLab\Bin).

Manually Install Sample Scheduler

Create or connect to a Data Repository database

- 1 Run the installation wizard as described under **Start the Sample Scheduler Installation Wizard** on page 24.
- 2 As database type, select OLDR.

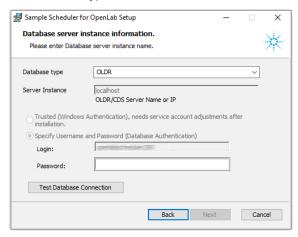


Figure 7: OLDR server instance information

If you use OLDR as a database, Windows authentication is not available and disabled. The instance name is the Shared Services server name. The login name is set to a default name that cannot be changed. You only need to enter the password for the OLDR database. There are no restrictions regarding the characters and length of the password. If you are re-installing Sample Scheduler and want to keep the existing database, you must provide the credentials used for the first installation when the database was created

Click Test Database Connection.

The setup will check if the database instance is reachable. If the connection is established, the setup checks if the Scheduler database already exists in the instance. If it exists, it proposes you either to keep the existing database or to create a new one (empty). Then click **Next**.

NOTE

Creating a new database will delete all stored analyses and reset the configuration parameters.

4 If the test succeeds, click **Next** and finish the installation.

Manually Install Sample Scheduler

Create or connect to an SQL Server database

- 1 Run the installation wizard as described under **Start the Sample Scheduler Installation Wizard** on page 24.
- 2 As database type, select SQLServer.

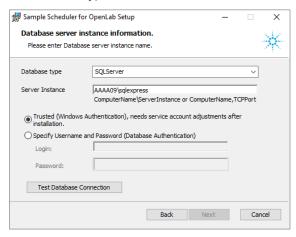


Figure 8: SQL server instance information

- **3** Enter the SQL Server instance name. Different ways of connecting to the SQL Server are possible. Check with your IT department which one to use:
 - Enter the name of the computer where the SQL Server is installed, and the name of the instance to be used with Sample Scheduler for OpenLab:
 Computer Name\Instance Name
 - Enter the IP address of the computer where the SQL Server is installed, and the name of the instance to be used with Sample Scheduler for OpenLab: IP address\Instance Name
 - Enter the name of the computer where the SQL Server is installed, and the associated port number: Computer Name, Port number

Manually Install Sample Scheduler

4 Select the authentication mode: Windows Authentication or Database Authentication (recommended). If you select Database Authentication, specify the database administrator.

CAUTION

If you select the Windows Authentication mode, the Sample Scheduler services will not be able to connect to the Sample Scheduler database with the default 'Local System account'.

Ask your system database administrator to assign a Windows account that has enough privileges to access the OpenLab Scheduler database (for example: sysadmin) to the following services: Agilent Sample Scheduler LIMS agent, and Agilent Sample Scheduler Orchestrator.

Ensure that all the Windows users that will log on to Sample Scheduler computers are also assigned the privileges to access the OpenLab Scheduler database.

To learn more about authentication mode and the OpenLab Scheduler database users privileges, refer to **Microsoft SQL Server Configuration** on page 56

5 Click Test Database Connection.

The setup will check if the SQL Server instance is reachable. If the connection is established, the setup checks if the Scheduler database already exists in the server instance. If it exists, it proposes you either to keep the existing database or to create a new one (empty).

NOTE

Creating a new database will delete all stored analyses and reset the configuration parameters.

6 If the test succeeds, click **Next** and finish the installation.

If you are experiencing troubles while connecting to the SQL Server instance (instance not reachable), do not hesitate to pause the installation and to check the SQL Server connectivity as described in **Microsoft SQL Server Configuration** on page 56. Check the following parameters:

- Credentials and connection mode,
- Replace the computer name by its IP address (in case of a DNS issue) in the SQL Server Instance section,
- Firewall for SQL Server (on the SQL Server computer),
- TCP/IP Protocol for SQL Server instance (on the SQL Server computer).

Once the connectivity is established, resume or re-launch the installation.

4

Manually Install Sample Scheduler

Install Sample Scheduler LIMS agent

Preparations

You have one or more LIMS and a sufficient number of connection licenses.
 The amount of LIMS connection licenses must be the same or more than the number of LIMS connections specified in the Sample Scheduler configuration.

CAUTION

Insufficient licenses

All attempts to import XML files will be trashed when the XML-based LIMS agent starts.

- Ensure you have sufficient connection licenses.
- **1** Follow the wizard
- 2 Provide the path where the LIMS will push the command files. Then click Next.

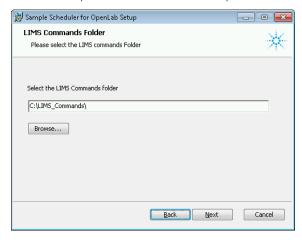


Figure 9: LIMS Commands folder

The LIMS_Commands folder is the target folder for the LIMS-generated XML commands. This folder can be defined on any computer, with or without OpenLab CDS or Sample Scheduler for OpenLab installed. In this example, the

Manually Install Sample Scheduler

'LIMS_Commands' folder is created by the setup. If it is not on the CDS machine, the LIMS_Commands folder must be shared over the network. It is possible to modify the LIMS commands folder afterwards.

NOTE

If the LIMS_Commands folder is a network share, enter:

\\ComputerName\SharedFolderName or

\\ComputerIPAddress\SharedFolderName.

The LIMS agent service must be started on a user account that has full access (write, read, delete, create permissions) to this share.

Silent Installation

Sample Scheduler supports a command-line mode for installation (silent installation). This mode supports installation, upgrade and uninstallation. You can execute silent installations either manually or as part of software management systems such as LANDesk or HP CM.

Run silent installation

Silent installation can be used by executing the Sample Scheduler .msi package with msiexec and providing the needed parameters for installation.

- 1 Copy the content of the installation media to a centralized folder.
- 2 Right-click the executable of the command prompt or Power shell prompt, and run it as administrator.
- 3 Navigate to the drive where you have saved the content of the installation media.
- **4** To start the installation, call msiexec with the required parameters (see tables below).
- **5** Wait for the installation to end (about 5 minutes). To check the process of installation, look at the log files. By default, the log files will be in the same folder as the installer.

If a required installable is missing, the installer will create an entry in a log file. Depending on the component type, it will continue or roll back the installation. An error code will be returned in such scenarios.

Silent Installation

6 After the installation has finished, reboot the PC.

NOTE

4

After the installation, the Scheduler agent and LIMS agent services are set to disabled. The services will be set to automatically start when the Sample Scheduler is successfully activated (see **Activate Sample Scheduler** on page 40).

7 To qualify the Sample Scheduler for OpenLab installation, launch the Agilent Software Verification Tool (from Agilent Technologies/Software Verification Tool).

Parameters

Table 6: Mandatory Parameters

Parameter name	Allowed values	Description
ADDLOCAL	SchedulerAgent SchedulerLimsAgent SchedulerClient SchedulerWebInterface SchedulerDatabaseAgent	Sample Scheduler component to be installed. To install multiple components at the same time, combine the values with a comma (","). For example: ADDLOCAL=SchedulerAgent,SchedulerClient
INSTALLDIR	Any valid Windows path	Directory where Sample Scheduler should be installed to.
DATABASE_LOGON_TYPE	For OLDR: "DatabaseAccount" For SQL Server: "DatabaseAccount" or empty	Database connection mode. If "DatabaseAccount" is specified for the SQL Server, you must provide DATABASE_USERNAME and DATABASE_PASSWORD as well. If nothing is specified for the SQL Server, the database connections will use the Windows Account under which the process runs that connects to the database. In this case you must set USEINTEGRATEDSECURITY to 1.
DATABASE_TYPE	SQLServer or OLDR	Database type to be used to create the Sample Scheduler database instance.
DATABASE_USERNAME	In the case of the SQL Server, any valid SQL Server Username	DB account used by Sample Scheduler to connect to its database. For OLDR, the username is set as default and cannot be modified.
DATABASE_PASSWORD	Password of DB user.	Password of DB user.
DATABASE_SERVER	Any string	The name of the computer on which the database is installed, and the name of the instance that should be used with the Sample Scheduler for OpenLab software.

Silent Installation

Parameter name	Allowed values	Description
USEINTEGRATEDSECURITY	For OLDR: 0 For SQL Server: 0 or 1	0: use - server with database credentials. 1: use - server with Windows credentials. If Windows authentication is used, you must provide SERVICE_LOGON_FULLY_QUALIFIED_NAME and SERVICE_LOGON_PASSWORD as well.
CREATE_DATABASE	0 or 1	Set to 1 to create a new database. Only do this if no database for this version of Sample Scheduler has been created yet on the DB instance. Otherwise the existing database will be overwritten.
SERVICE_LOGON_FULLY_QUAL IFIED_NAME	Windows NT User account	User account that should be used for the Sample Scheduler service. In a regulated environment, this is the Sample Scheduler Service user. Provide this parameter if Services should be started with a user that is not "Local System", for example, if the LIMS agent needs to access a network share.
SERVICE_LOGON_PASSWORD	Windows NT User password	Password for the SERVICE_LOGON_FULLY_QUALIFIED_NAME.

Example 1: Sample Scheduler database instance is managed by SQL Server

First Step: Installation of LIMS agent and Webserver with database creation:

Msiexec -I Agilent.Scheduler.Install_EN.msi

ADDLOCAL="SchedulerLimsAgent,SchedulerDatabaseAgent,SchedulerWebInterf
ace" INSTALLDIR="C:\Scheduler" DATABASE_LOGON_TYPE="DatabaseAccount"

DATABASE_TYPE="SQLServer" DATABASE_SERVER="servername\sqlexpress"

DATABASE_USERNAME="sa" DATABASE_PASSWORD="Password123"

USEINTEGRATEDSECURITY="0" CREATE_DATABASE="1" /q /lxv "log.txt"

Install Sample Scheduler agent on another machine:

Msiexec -I Agilent.Scheduler.Install_EN.msi ADDLOCAL="SchedulerAgent"
INSTALLDIR="C:\Scheduler" /q /lxv "log.txt"

Install Sample Scheduler Client on another machine:

Msiexec -I Agilent.Scheduler.Install_EN.msi ADDLOCAL="SchedulerClient" INSTALLDIR="C:\Scheduler" /q /lxv "log.txt"

Uninstallation:

Msiexec -X Agilent.Scheduler.Install_EN.msi -q

Silent Installation

Example 2: Sample Scheduler database instance is managed by OLDR

Installation of LIMS agent and Webserver with database creation:

Msiexec -I Agilent.Scheduler.Install_EN.msi

ADDLOCAL="SchedulerLimsAgent,SchedulerDatabaseAgent,SchedulerWebInterface
" INSTALLDIR="C:\Scheduler" DATABASE_LOGON_TYPE="DatabaseAccount"

DATABASE_TYPE="OLDR" DATABASE_SERVER="servername,port"

DATABASE_NAME="datarepo" DATABASE_USERNAME="openlabscheduler270"

DATABASE_PASSWORD="Password123" USEINTEGRATEDSECURITY="0"

CREATE_DATABASE="1" /q /lxv "log.txt"

NOTE

In the DATABASE_USERNAME, openlabscheduler270 is correct for both Sample Scheduler revision 2.7 and revision 2.8.

Automatic Generation of Installer Logs

An installation log file is created automatically during a new installation or upgrade. The log file is created both during installation by the set-up wizard and in silent mode. The installation log file remains on the system even after uninstallation.

The installation logs are located in the \ProgramData\Agilent\ Sample Scheduler for OpenLab\InstallLogs folder.

You can manually collect and export installation log files from the local computer in Sample Scheduler configuration (Maintenance ribbon tab > Save all Logs). For more information, refer to Sample Scheduler online help (search for "Save all log files").

Remove Registry Entry on Cloned VMs

Remove Registry Entry on Cloned VMs

Before you start any Sample Scheduler services and run Sample Scheduler on a cloned VM: Remove the following registry entry:

 $\label{local_machine} Computer\HKEY_LOCAL_MACHINE\SOFTWARE\WOW6432Node\Agilent\Scheduler\Computer\Identifier$

5 Activation

Documents about this

■ <OpenLab CDS: Configuring OpenLab CDS with OpenLab ECM> (https://www.agilent.com/cs/library/usermanuals/public/CDS_v2.8_configure-with-ECM_en.pdf)

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Activate Sample Scheduler

The Sample Scheduler instrument dashboard is included with your purchase of OpenLab CDS client/server configuration and installed by default. In order to work with the full edition of Sample Scheduler - e.g. to submit analysis requests to instruments - you need to activate Sample Scheduler.

Activation will cause the following changes:

- The functionality of the full edition is available
- The entered Sample Scheduler service credentials are applied
- The system creates Sample Scheduler roles and privileges
- The system automatically assigns your instruments
- Scheduler agent and LIMS agent services are started, and the startup type is set to automatic
- The number of concurrent user sessions is unlimited
- The start menu entry **Agilent Technologies** > **Agilent Sample Scheduler** proceeds directly to the login screen, skipping the information page.

NOTE

Ensure you have the 60 days trial license or Sample Scheduler Expansion pack license.

Preparations

- In a regulated environment: Ensure that you have created a service user for Sample Scheduler before activation. See Create a Service User in OpenLab CDS on page 42.
- Ensure that the service user has the privilege
 Manage Security (Shared Services). Privileges are configured in the Control Panel for OpenLab.





- 1 Ensure that all instrument controllers can be pinged.
 - **a** In the Control Panel, select **Administration** > **Instrument Controllers**.
 - **b** Select each instrument controller and click **Ping Instrument Controller**.
- 2 Open the Sample Scheduler web interface

Activate Sample Scheduler

The web interface is available at https://<hostname>/openlab/samplescheduler.

Alternatively, click **Agilent Sample Scheduler for OpenLab** in OpenLab Acquisition, and click **Access free dashboard** on the opened page.

- 3 Log in as a user that has the Manage Security (Shared Services) privilege.
- 4 In the menu, click Activation.
- **5** In a regulated environment: Enter username and password of the Sample Scheduler service user. Otherwise, use the built-in OpenLab CDS administrator. In a Windows domain environment, also provide the domain.
- 6 During activation all instruments are automatically assigned. To only assign a subset of instruments, clear the check box Instruments are assigned automatically and assign instruments during the configuration.

NOTE

Each assigned instrument will consume a license (see **Licensing** on page 14). This includes virtual instruments that may be created for OQ.

7 Click Activate.

A success message opens.

8 To apply the changes to your user session, log in again.

NOTE

The Scheduler agent, LIMS agent, and Sample Scheduler orchestrator services were disabled after the installation. They are set to automatically start when the Sample Scheduler is successfully activated.

In a Regulated Environment

Verify privileges in OpenLab ECM

If you use OpenLab ECM v3.x as a backend, make sure you have a Service User with the following View privileges in OpenLab ECM:

- CDSPRIV
- · Content: File
- Content: Folder

Create a Service User in OpenLab CDS

NOTE

The Service User is required to run Sample Scheduler for OpenLab. Do not disable this user as long as you use Sample Scheduler for OpenLab in your laboratory environment.

1 In the Control Panel (Administration > Roles and Users), create a new role Operator.

Enter Operator as role name and Laboratory Operator as description.

Assign the following project privileges to this role:

- View project or project group (Role type Project > Project Management), enabled by default, cannot be disabled
- Edit content of project (Role type Project > Project Management)
- Create and modify sequence (Role type Project > Sequence)
- 2 In the Control Panel (Administration > Users), create a new service account user.

Enter Sample Scheduler Service as a login name and Account used by the Sample Scheduler services as a description.

OR

In a Regulated Environment

Import the Service User from ECM (for details, refer to the guide *Configuring OpenLab CDS with OpenLab ECM (CDS_v2.8_configure-with-ECM_en.pdf, D0028024*)).

NOTE

The Sample Scheduler Audit Trail can track which processes are system-triggered, and which are initiated by a user. If you want to use this function, do not assign Sample Scheduler privileges to the Service User. OpenLab CDS privileges may be assigned.

- **3** Assign the following roles to this user:
 - Instrument User (built-in role)
 - Operator (created in step 1)

Restrict access to LIMS result folder

If you use a LIMS system, access to the LIMS **Result folder** must be restricted at operating system level. There will be reports created in this folder, and only the LIMS system should be allowed to access these reports.

To restrict access, ensure:

- A specific Log On user is specified in the properties of the Agilent Sample Scheduler LIMS Agent service.
- This user has Read and Write access to the LIMS Result folder.
- Access to the LIMS Result folder is restricted for other users.

6 Post Installation Tasks

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Run Software Verification

The Software Verification Tool (SVT) provides documentary evidence that your system has been built and installed correctly, and that all design specifications have been met. You do not need to run the software verification again if it has run successfully at the end of the installation.

- 1 Using your Windows operating system, go to Start > Agilent Technologies > Software Verification Tool.
- 2 Select the components to qualify.
- 3 Select Qualify.

The system will run the application and generate a Software Verification Report. Reports are automatically saved to **C:\SVReports**.

If the report indicates failure, verify the computer requirements and reinstall the data system. Do not use the system until the Software Verification Report gives a 'pass' result.

Configure Antivirus Program

If you use an antivirus program with behavior monitoring, add the files below to the list of approved programs:

- C:\Program Files (x86)\Agilent Technologies\Sample Scheduler for OpenLab\Bin\Agilent.OpenLab.Scheduler.Client.exe
- C:\Program Files (x86)\Agilent Technologies\Sample Scheduler for OpenLab\Bin\Agilent.OpenLab.Scheduler.Configuration.exe
- C:\Program Files (x86)\Agilent Technologies\Sample Scheduler for OpenLab\Bin\Agilent.Scheduler.Acquisition.Agent.exe
- C:\Program Files (x86)\Agilent Technologies\Sample Scheduler for OpenLab\Bin\Agilent.Scheduler.Agent.exe
- C:\Program Files (x86)\Agilent Technologies\Sample Scheduler for OpenLab\Bin\Agilent.Scheduler.Lims.Agent.exe
- C:\Program Files (x86)\Agilent Technologies\Sample Scheduler for OpenLab\Bin\Agilent.Scheduler.WebserverService.exe
- C:\Program Files (x86)\Agilent Technologies\Sample Scheduler for OpenLab\Bin\Agilent.Scheduler.Webstarter.exe
- C:\Program Files (x86)\Agilent Technologies\Sample Scheduler for OpenLab\Bin\Agilent.Scheduler.DBManagement.Agent.exe
- C:\Program Files (x86)\Agilent Technologies\Sample Scheduler for OpenLab\Bin\Agilent.Scheduler.Orchestrator.exe
- C:\Program Files (x86)\Agilent Technologies\Sample Scheduler for OpenLab\Bin\Agilent.ICDS.Remote.Satellite32.exe

Start Services

Start Services

Start LIMS agent service

If you installed the LIMS agent manually (that is, you do not use the LIMS agent that is automatically installed with OpenLab CDS):

- 1 Set the startup type of the LIMS agent service to Automatic.
- 2 Start the LIMS agent service.

Start Sample Scheduler agent

If you have an additional Instrument Controller (AIC) in your OpenLab CDS system:

- 1 Set the startup type of the Sample Scheduler agent service to **Automatic**.
- 2 Ensure that the Sample Scheduler Webserver is running. Then start the Sample Scheduler agent service.

When adding a new AIC to the system after the Sample Scheduler is activated:

- 1 Open the Sample Scheduler configuration.
- 2 Open the Maintenance tab.
- 3 Click Update OpenLab Service Credentials.
- **4** Enter valid credentials for the OpenLab Services user.
- 5 Click Save.

Configure LIMS Transfer

Configure LIMS Transfer

If you want to use the Sign-Off for LIMS feature, the following requirements must be met:

- A LIMS result folder must be available, to which the result reports are copied and then collected by the LIMS. The folder can be located on any computer, it does not need to be on the same device as the LIMS agent.
- A folder path is defined that allows the LIMS agent to access the LIMS result folder. This path must be available on the computer where the Sample Scheduler LIMS agent is installed.
- The LIMS agent collects all files with the specified extension (for example, csv, txt) regardless of the name. For dual injections assigned with front and back, the name of the report file is extended with 01 and 02, respectively.

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User Privileges

Configure the Sample Scheduler user privileges in the Control Panel.

The privileges described in **Table 7** on page 50 can be associated with roles in the Control Panel. The administrator of the OpenLab system may modify these roles or create new ones and assign them to Sample Scheduler users. The following default roles are available:

- Sample Scheduler Administrator: Ability to configure the Sample Scheduler. For
 example, you can define default settings and mandatory commands,
 establish the LIMS connection (LIMS Commands folder or SQL statements),
 monitor notifications, and create auto-fill templates.
- Sample Scheduler Analyst: Ability to manage the entire laboratory workload. You have insight into the workload of all instruments and their users. You can review the results in the CDS for reprocessing.
- Sample Scheduler Technician: Ability to manage the instruments and determine the analysis workflow. For example, you can create, change, delete, reset, or restart analyses and sequences, set their priority, merge single or split dual analyses, and correct instrument errors. You have access to the data in the CDS.
- Sample Scheduler Operator: Ability to prepare analyses/sequences, determine
 the vial position, select the instrument, and stop it in case of failure. This role
 restricts you to working in the web interface.

Table 7: (Sample Scheduler) related privileges

Privilege	Allows the user to
Add analysis	use the Add button
Change priority	use the Sooner or Later buttons
Create sequence	manually create a sequence from selected analyses
Delete notifications	delete all or selected notifications on trashed commands
Delete analysis	delete the selected analyses or sequences, and remove them from the Sample Scheduler database
Is an administrator	connect to Sample Scheduler configuration

Privilege	Allows the user to
Edit analysis	appear in the Assign User (client), Assign to (web interface), and OpenLab default user (configuration) drop-down lists schedule, pause, stop, and restart analyses or sequences stop instruments
Edit System Configuration (web interface)	access the configuration within the Sample Scheduler web interface
Merge / Split analysis	merge analyses into a dual analysis or split a dual analysis
Open data	open data acquired in the CDS from Sample Scheduler
Perform actions on sequence	use the actions buttons in the Sequence grid (add, delete, move, etc.)
Reset analysis	to release an analysis that is blocked in the Sample Scheduler database, and reset to original state
Restart analysis	restart the selected analyses or sequences
Review & submit results	submit results to LIMS
Schedule analysis	use the Schedule button
Set favorites for all users	assign your favorites list to all users of the lab group
Stop / Stop instrument	immediately stop all active analyses in the queue of an instrument
View activity log	(in the Activity Log Access node) view the activity log and error information for instruments in the dashboard.
Configure Analyses view and details (web interface)	view the tabs of the categories and their parameters in the Details pane of the Sample Scheduler web interface, use the column chooser The Favorites tab is visible for all users
View and edit other users' analyses	view and edit analyses that are assigned to other users; analyses with no user entry are visible for all users view and assign other users in the Assign User (client) and Assign to (web interface) drop-down list
View lab manager start page (web interface)	view the start page of the lab manager
View report	use the View PDF button in the Review ribbon tab of the Sample Scheduler client
Wait analysis	transfer an analysis or sequence back to waiting state

Audit Trail

Audit Trail

Enable audit trail

After installing or upgrading Sample Scheduler, the audit trail is disabled by default. Proceed as follows to enable the audit trail:

- 1 In Sample Scheduler configuration, go to the **System Configuration** tab.
- 2 For the parameter Enable Audit Logging, select True.

CAUTION

Once you have enabled the audit trail, you can no longer disable it.

Audit trail settings

If the **Write activity log** option is enabled for your CDS, every action in the Sample Scheduler will be recorded in the *System Activity Log* of the Control Panel. For the audit trail to function correctly, Sample Scheduler needs specific audit trail settings in the CDS project. Proceed as follows to ensure that the settings are correct:

- 1 In the Control Panel, click **Projects** and select the project to edit.
- 2 On the CDS settings tab, expand the Audit Trail Settings section.
- 3 Select the Sequence tab.

Only the Sequence Audit Trail settings are relevant for Sample Scheduler.

Audit Trail

If reasons are required, Sample Scheduler will automatically enter its own default reasons to the entries. These can not be edited, unless you enable Allow users to type their own reason when saving sequences.

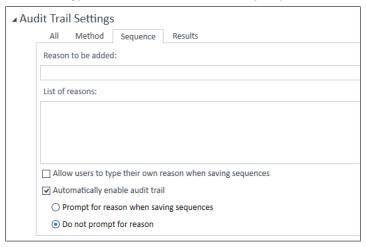


Figure 10: No reasons required



Figure 11: Allow Sample Scheduler to add reasons

NOTE

Only users with a role containing the **View activity log** permission are able to view the activity log and all its entries. By default, these roles are **Activity Log Access** and **Everything**.

Audit Trail

When an audit trail entry is generated, it automatically checks whether the current user has any Sample Scheduler privileges.

If the user has no Sample Scheduler privileges, the audit entry marks the actions as automatically executed by the user. This label helps distinguish between system-induced changes and changes done interactively by users.

Enable Single Sign-On

Enable Single Sign-On

If Single Sign-On is enabled, you do not need to provide credentials to start Sample Scheduler configuration or Sample Scheduler client. This feature is available if you use Windows Domain authentication.

To enable Single Sign-On:

1 In the Control Panel under Administration > System Configuration, set the authentication provider to Windows Domain.

For more information, refer to the Control Panel online help (search for "set the authentication provider").

- 2 In the Control Panel under Administration > Set Security Policy, enable Single-On for the system.
- 3 Import the domain users.

For more information, refer to the Control Panel online help (search for "import users").

Once you have enabled **Single Sign-On** for the system, you can enable and disable **Single Sign-On** for each local computer (in the Control Panel under **Administration** > **Local Configuration**). To learn more about how to enable **Single Sign-On**, refer to the Control Panel online help (search for "single sign on").

Microsoft SQL Server Configuration

Find below some information regarding the configuration of SQL Server. According to the version of SQL Server you are installing, the interfaces could be different, but you should access the same options.

Configure SQL protocol for remote access

1 Start the application *Microsoft SQL Server 20xx/Configuration Tools/SQL Server Configuration Manager*.



- 2 Select the SQL Server Instance in the left panel.
- 3 Edit the TCP/IP properties.

Microsoft SQL Server Configuration

4 Enable the protocol TCP/IP.

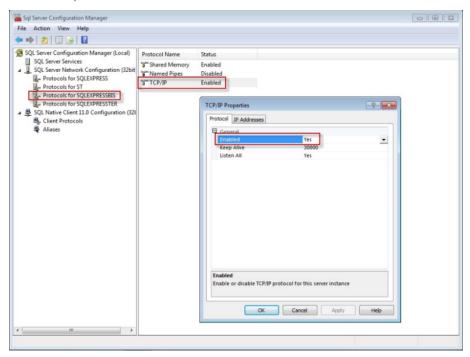
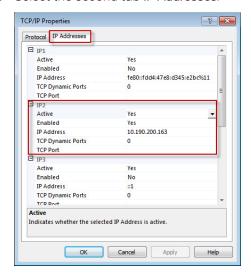


Figure 12: Enable TCP/IP

Microsoft SQL Server Configuration

5 Select the second tab IP Addresses.



- **6** Activate and enable the IP address allocated to the current machine over the network.
- **7** Close the dialog.

Configuration of the used SQL instance

Another option is to make the SQL Server instance listening to a static port. This TCP port must be defined with the help of your network IT people. Also, you may have to allow this static port in the Firewall's exclusions.

Setting a static port can be done by disabling all TCP dynamic Ports options in the scrolling list. Then you must define the static TCP Port in the IP All section.

7

Microsoft SQL Server Configuration

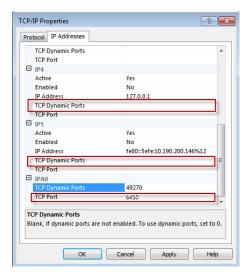


Figure 13: TCP Port

- 1 Select SQL Server Services in the left pane.
- 2 In the right pane, select the following services:
 - SQL Server (INSTANCE NAME),
 - SQL Server Browser (if fixed port is not set).

Microsoft SQL Server Configuration

3 Set Automatic start mode.

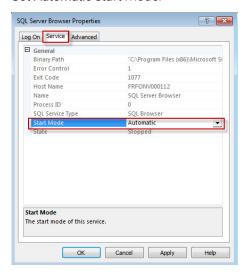


Figure 14: Automatic Start Mode

4 Restart both services.

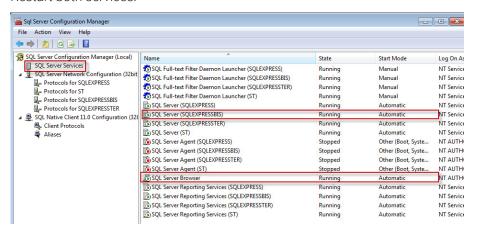


Figure 15: Configuration Manager

5 Close the application.

Switch SQL server authentication mode

1 Start SQL Server Management Studio.



Figure 16: SQL Server Management Studio

2 Connect to the SQL Server instance with valid authentication mode and credentials.



Figure 17: Connect to server

Microsoft SQL Server Configuration

3 Select the instance and click Properties.

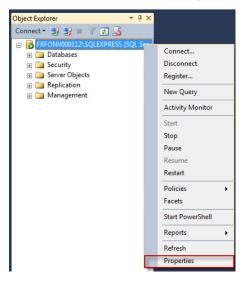


Figure 18: Properties

4 Select Security and change the Server Authentication mode.

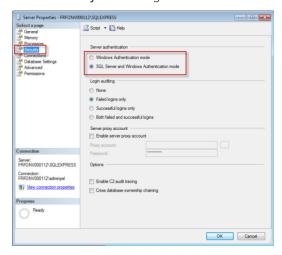


Figure 19: Security

5 Close the dialog.

Microsoft SQL Server Configuration

After switching to Server Authentication Mode, you must restart the SQL Server service SQL Server (INSTANCE NAME).

NOTE

7

If configuring the Windows Authentication mode, ensure that all the Windows users that will log on Sample Scheduler computers have the privilege to access the OpenLab Scheduler database (for example, sysadmin). Contact your database administrators to know which privilege you must set to be consistent with your company policy rules.

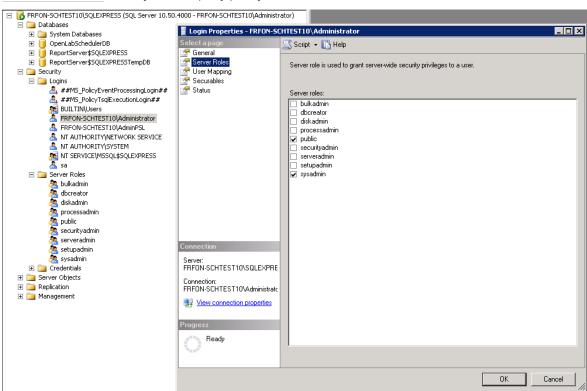


Figure 20: Mimimum Server roles for Windows users to access an existing database

Microsoft SQL Server Configuration

Edit or add system administrator

If you have selected SQL Server and Windows Authentication Mode, you can add a system administrator user or edit the default one (sa).

- 1 Start SQL Server Management Studio.
- 2 Edit the System Administrator password (sa):
 - a On the left pane, select Security/Logins/sa.
 - b Click Properties.

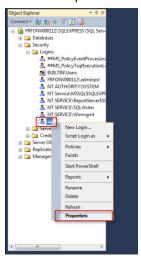


Figure 21: Properties

Microsoft SQL Server Configuration

c Change the password.



Figure 22: Change password

3 Ensure the user is Enabled.

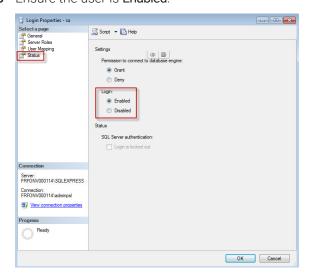


Figure 23: Enabled user

4 Close the dialog.

Configure Sample Scheduler Settings Microsoft SQL Server Configuration 7

The SQL Service (INSTANCE NAME) service does not need to be restarted.

Setting up SQL server accounts other than 'sa'

NOTE

If you want to use Windows Authentication Mode to let the Sample Scheduler components log in to the SQL Server database, you must change the user who runs the Sample Scheduler agent and Sample Scheduler LIMS agent. Change users via the Windows Services application. The services need to run with an account that has the required privileges on the database, as described below.

If the installation was done by an administrator using an SQL Server account with the privilege to create a database, it might be required to make Sample Scheduler use an SQL Server account with less privileges. This depends on your company policies.

The following instructions are guidelines on how to setup accounts that should be used by Sample Scheduler. There are other options for setting up and organizing the privileges on the SQL Server side, however this document is not the SQL Server documentation. This document lists which privileges are required to get Sample Scheduler working, and it shows how to achieve that goal in a simple way.

Create the user/group that should be used by Sample Scheduler

- 1 To add a new database user for use with Sample Scheduler, connect to the database instance with Microsoft SQL Management Studio. You need to do this with an account that has the privilege to create new users and assign permissions to them.
- 2 On the instance level, right-click **Security** > **Logins**, then select **New Login**.

7

Microsoft SQL Server Configuration

3 If the new user should be a Windows user or group, you can search for it. For finding groups, click Object Types... and select Groups to add Groups to the object types that should be searched for.

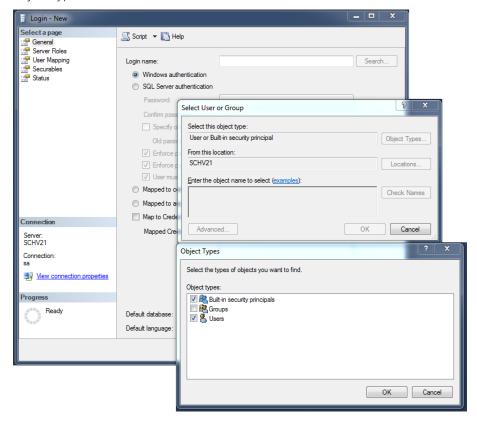


Figure 24: Object types

- 4 If you want to use SQL Server authentication with the new account, you need to specify passwords. Make sure that you either clear User must change password at next login, or that you change the password manually before using the account with Sample Scheduler.
- **5** After you are done specifying the login details, switch to the **Server Roles** tab.
- 6 Select Server Roles. Select public and dbcreator.

7

Microsoft SQL Server Configuration

7 Switch to the **User Mapping** tab. Select OpenLab Scheduler database (OpenLabSchedulerDB270).

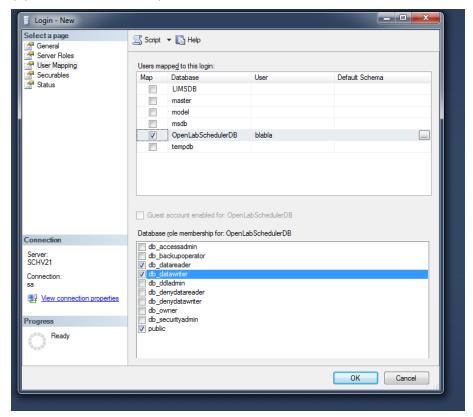


Figure 25: User mapping

- **8** The user column will be set to the new user you created. You can leave that as it is, no default Schema has to be selected.
- 9 In the list of database roles, select public, db_datareader and db_datawriter.

Give execute permission to the new user/group

- 1 Select the Sample Scheduler database (OpenLabSchedulerDB+ <version number>) in the Object Browser (InstanceName > Databases > OpenLabSchedulerDB270 > Properties).
- **2** Go to the **Permissions** tab and execute a search for the user/group that was just created. Then select that user/group under the **User or roles** section.
- 3 On the Explicit tab, select the Grant check box for Execute:

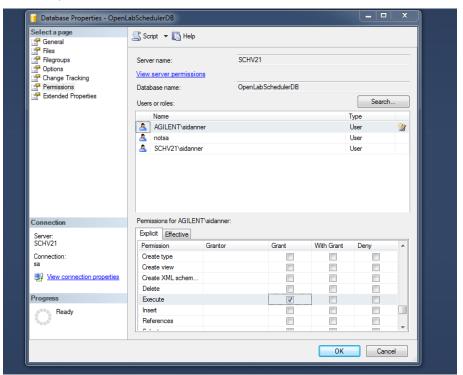


Figure 26: Grant execute permission

Configure Firewall for SQL Server

The Firewall can block the communication between the SQL Server and the client application.

Add the following exclusions:

Microsoft SQL Server Configuration

- Inbound rule, protocol TCP, port 1433
- Inbound rule, protocol UDP, port 1434
- Inbound rule, all ports for the application
 For SQL Server 2019, use %Program Files%\Microsoft SQL
 Server\MSSQL15.SQLEXPRESS\MSSQL\Binn\sqlservr.exe. The path can differ depending on the SQL Server version.

See Microsoft documentation:

https://learn.microsoft.com/en-us/sql/sql-server/install/configure-the-windows-firewall-to-allow-sql-server-access?view=sql-server-ver16

If you still have some issues, check the firewall on the client side.

Check Sample Scheduler database connectivity

Microsoft SQL Server has been installed successfully, providing an "instance" in which the Sample Scheduler database exists or is going to be created. Use the following steps to check that the instance (and the databases inside) can be accessed from any machine that has a role in the Sample Scheduler deployment or check that connectivity is easy, at any time, for example in case of network configuration changes.

The steps below provide a persistent way to check the implementation by defining an ODBC source.

- 1 Gather the following information, depending on your network architecture:
 - The name of the SQL Server machine.
 - The IP address of that machine if the name cannot be resolved automatically by the DNS (The SQL Server machine could be unknown to the DNS which manages the current machine).
 - The name of the SQL Server instance in which the Sample Scheduler database is created.
 - Check if the TCP/IP port is static or dynamically determined. (This refers to the section Configure SQL protocol for remote access on page 56, TCP/IP properties in the SQL Server installation above).
- 2 Launch Microsoft Control Panel from the start menu.
- 3 Select Administrative Tools, then launch Data Sources (ODBC).

7

Microsoft SQL Server Configuration

4 Select the **User DSN** tab and start creating a brand-new data source by clicking **Add**.

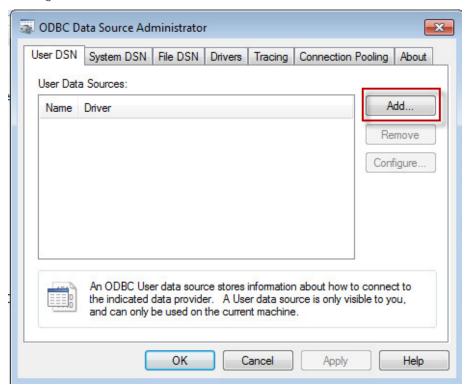


Figure 27: User DSN

Microsoft SQL Server Configuration

5 Select the SQL Server. If it is not in the list, check your SQL installation or manual.

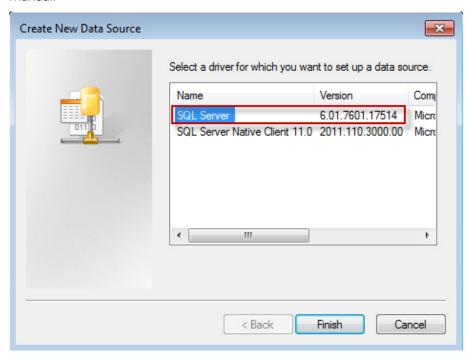


Figure 28: Create new data source

6 Click Finish.

Microsoft SQL Server Configuration

7 In the Create a New Data Source to the SQL Server window, provide a name and description, and select the SQL Server. You may select from the drop-down list, or manually enter the IP address of your SQL server. If you select an SQL Server name without SQL Server instance, add \<Server instance>.

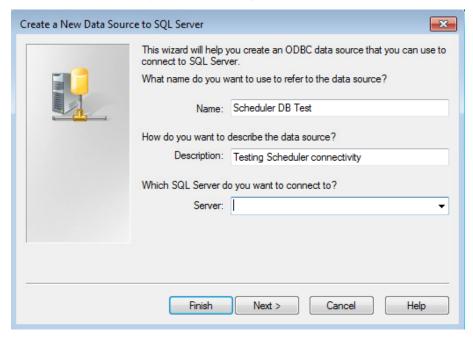


Figure 29: Choose a name

- **8** The **Server** field can be filled manually or with the help of the combo box. You have several options:
 - The combo box provides an option composed by the SQL Server machine and the SQL Server instance:

Go ahead; you probably do not have any problem of connectivity from that computer.

 The combo box provides an option only composed by the SQL Server machine:

7

Microsoft SQL Server Configuration

Select that option and append it with "\" and the name of the instance.

• Enter the IP address of the SQL Server machine by yourself, forget the instance.

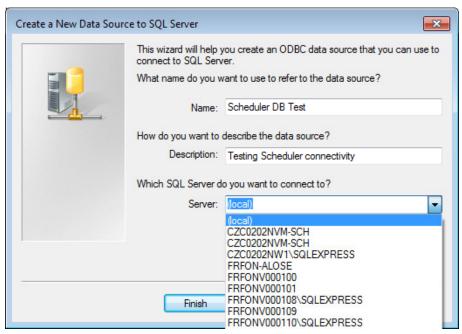


Figure 30: Identify SQL server

9 Click Next.

Microsoft SQL Server Configuration

- 10 Select the authentication method and provide the login credentials. If you defined a static TCP/IP port, click Client Configuration (see Configure SQL protocol for remote access on page 56), and perform the following actions:
 - a Set Network libraries to TCP/IP.
 - **b** Provide Server name (SQL Server machine name only).
 - **c** Deselect **Dynamically determine port** and enter the port number that the SQL Server instance is expected to listen to.
 - **d** Click **OK** to go back on the authentication panel and click **Next** from there.

Otherwise click **Next**

7

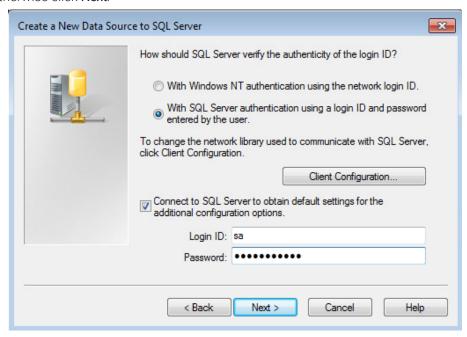


Figure 31: Select authentication parameters

Microsoft SQL Server Configuration

7

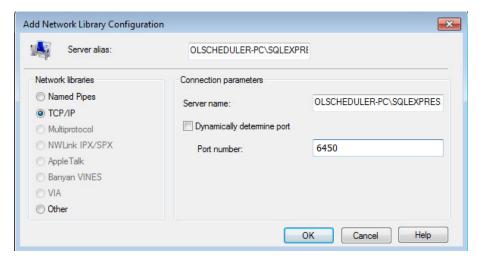


Figure 32: Client configuration

- 11 At this stage, the process tries to connect to the SQL Server instance with all parameters you gave. In case of failure a popup message appears. The connection could not be established, and you may consider the following actions:
 - Check SQL Server installation (machine and instance name, authentication mode, credential and TCP/IP properties).
 - Check firewall settings on the SQL Server machine.
 - Replace the name of the SQL Server machine by its IP address (DNS issue).
 - Check that the SQL Server machine is really reachable over the network from where you are.

Microsoft SQL Server Configuration

It might be useful to report to the network IT people you usually contact in case of trouble.

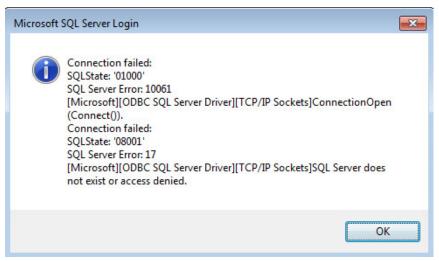


Figure 33: Error message

12 If the connection succeeded, click **Next** on the following panels until you can click **Finish**.

This creates the ODBC source. Then the last panel opens and summarizes the settings of the ODBC source. You can now use **Test Data Source**. From now you are able to test your data source at any time without having to define again all parameters (except possible passwords).

Microsoft SQL Server Configuration

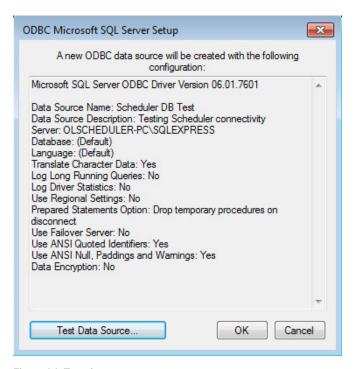


Figure 34: Test data source

8 Upgrade and Migration

Overview

Upgrading Sample Scheduler for OpenLab to revision 2.8 includes the following sections:

- 1. Upgrade OpenLab CDS on page 82.
- 2. Upgrade Sample Scheduler features on page 84.
- 3. Transfer the Sample Scheduler data on page 85.

Upgrade OpenLab CDS

Sample Scheduler for OpenLab is supported on OpenLab CDS client/server topologies with a content management system.

Sample Scheduler for OpenLab revision 2.8 is compatible with:

- OpenLab CDS v2.7 client/server topologies
- OpenLab CDS v2.8 client/server topologies

If you use an older revision of OpenLab CDS, upgrade OpenLab CDS first:

- If you use OpenLab CDS v2.6 or lower: Upgrade OpenLab CDS to v2.7 or v2.8.
 Upgrading OpenLab CDS will automatically upgrade the Sample Scheduler features that are installed on your OpenLab CDS systems (server, AIC, client).
 Sample Scheduler v2.6 and v2.5 databases are not touched by the installer.
 Transfer your Sample Scheduler data in a separate step. See Transfer the Sample Scheduler data on page 85.
- If you use OpenLab CDS v2.7 and want to upgrade:
 - Upgrading OpenLab CDS to v2.8. will automatically upgrade the Sample Scheduler features (independent of the previously used version). In several scenarios, it will also upgrade the Sample Scheduler data. See ${\bf Table~8}$ on page 85.

If a Sample Scheduler v2.7 database is present on the system without a Sample Scheduler installation, the database will be overwritten and the data is removed during the installation of Sample Scheduler v2.8

The upgrade does not change the database type specified in an existing Sample Scheduler installation.

For details on upgrading OpenLab CDS, see the instructions in the following guides:

- Agilent OpenLab Server and OpenLab ECM XT Installation (openlab-server-ecmxt-v2.8-installation-guide-en.pdf)
- OpenLab CDS Clients and Instrument Controllers Installation and Configuration (CDS_v2.8_ClientAICGuide_en.pdf)

Documents about this

8 Upgrade and Migration

Upgrade OpenLab CDS

Upgrade Sample Scheduler features

Follow this procedure to upgrade Sample Scheduler features to v2.8 on an existing OpenLab CDS v2.7 system. Upgrade Sample Scheduler on each relevant system (server, AIC, client).

- 1 Shut down all components of the Sample Scheduler system.
- **2** Stop all the services.
- **3** Run the Sample Scheduler installation wizard.

After the upgrade:

- All previously installed components are upgraded.
- The web server is always installed on the Shared Services server.
- The upgrade keeps using the database type specified in the existing Sample Scheduler installation.
- Sample Scheduler data may be already migrated in-place (see Table 8 on page 85).

Transfer the Sample Scheduler data

When upgrading Sample Scheduler to the latest revision, Sample Scheduler data such as configurations and analyses must be transferred to the new Sample Scheduler database. In some scenarios, this is done by an automated in-place upgrade. In other scenarios you transfer the data manually with the help of the Database Migration Tool.

Table 8: Migration scenarios by database type

Source database	Source revision	Destination database in Sample Scheduler v2.8	Description
Data Repository on PostgreSQL	2.7	Data Repository on PostgreSQL	Automated in-place upgrade when upgrading OpenLab CDS or Sample Scheduler database feature
Data Repository on PostgreSQL	2.7	Data Repository on SQL Server ⁴	Manually, use the Database Migration Tool
SQL Server	2.7	Data Repository on PostgreSQL	Manually, use the Database Migration Tool
SQL Server	2.7	Data Repository on SQL Server ⁴	Automated in-place upgrade when upgrading OpenLab CDS or Sample Scheduler database feature
SQL Server	2.7	SQL Server installed on the Shared Services server	Automated in-place upgrade when upgrading OpenLab CDS or Sample Scheduler database feature
SQL Server	2.7	SQL Server installed on a separate database server	Manually, use the Database Migration Tool
Any	2.6 or lower Any version with EZChrom	Any	Manually, use the Database Migration Tool. The old database remains unchanged.

⁴ Data Repository on SQL Server is available starting with OpenLab CDS v2.8.

Database Migration tool

The Database Migration tool supports you in transferring the Sample Scheduler data to a new database version or system. The tool is provided in the installation package from SubscribeNet.

It helps with the migration of the following:

- Analyses and sequences in Waiting, Stopped, and Incomplete state in your Sample Scheduler client
- Auto-Fill templates
- Sample Scheduler configuration settings for
 - the System Configuration module
 - the Commands module
 - the LIMS module
 - the Instrument Groups module
- Settings of the Projects module including the association to project groups
- Notifications about invalid commands generated by the LIMS

Set Sample Scheduler password for Data Repository

Follow this procedure if Sample Scheduler has been installed automatically together with OpenLab CDS 2.6 or higher.

During OpenLab CDS installation, a random Sample Scheduler password is generated for the Data Repository storage. When you transfer the data to a new Sample Scheduler version, you will need this password. Use the Data Repository Registration Tool to replace this randomly generated password.

- 1 Navigate to the subfolder **RegistrationTool** in the installation path.
- 2 Execute Agilent.OpenLab.DataRepository.RegistrationTool.exe.
- **3** To replace the password, use the following command (replace NewPassword with the password of your choice):
 - Agilent.OpenLab.DataRepository.RegistrationTool.exe DbRegister --

AppName "openlabschedulerxxx" --AppPassword "NewPassword" --Overwrite --AppKey "HKEY_LOCAL_MACHINE\SOFTWARE\Agilent\Schedulerxxx" where xxx is the revision of Sample Scheduler that you are upgrading from.

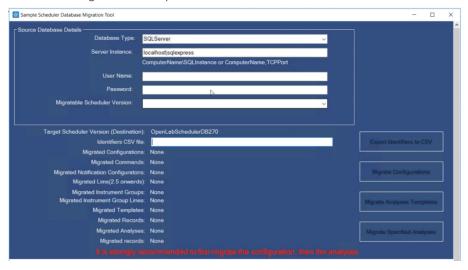
- 4 Note down the new password in a secure location.
- 5 Use the new password when you run the Database Migration Tool.

Run the Database Migration Tool

Follow this procedure on the OpenLab Server.

- 1 Navigate to the files downloaded from SubscribeNet, and execute DBMigration.exe.
- **2** Provide the credentials of a CDS user who has access to all projects.

The Database Migration tool opens.



- 3 Enter the Server Instance on which the Sample Scheduler database is located (the database server and instance name is displayed in Sample Scheduler configuration in the Deployment tab). Different ways of connecting to the SQL Server are possible. Check with your IT department which one you should use.
 - **a** Enter the name of the computer where the SQL Server is installed, and the name of the instance that should be used with Sample Scheduler for OpenLab: Computer Name\Instance Name
 - **b** Enter the IP address of the computer where the SQL Server is installed, and the name of the instance that should be used with Sample Scheduler for OpenLab: IP address\Instance Name
 - **c** Enter the name of the computer where the SQL Server is installed, and the associated port number: **Computer Name, Port number**.
- 4 Specify the SQL authentication account and enter the corresponding credentials (user name and password) of the database administrator. The data migration utility searches for the database. It only reads from the source database. It does not delete any records, database tables or databases.
 - If the connections were specified correctly and the databases are accessible, the detected version appears under **Migratable Scheduler Version**.
- 5 If multiple database versions are available, select the Migratable Scheduler Version from the drop-down list.
- **6** To import configuration settings, select **Migrate Configurations**.

If you have any configuration settings (for example, commands, LIMS configurations, LIMS database queries, Instrument groups, notifications) to migrate, do this first before importing analyses, sequences, or templates.

The migration tool checks the existing settings of the target system. The number of migrated configurations, commands, and notifications is displayed after migration.

If instrument groups are also migrated, both the number of existing groups and the number of instruments (instrument group lines) are displayed.

Upgrade and Migration

8

Transfer the Sample Scheduler data

- 7 To migrate analyses or sequences:
 - **a** Specify a path under which a csv file with their identifiers is to be exported.
 - **b** Click Export identifiers to CSV. The identifiers as well as given mandatory parameter values (for example, project, instrument, injection source) of the analyses and sequences will be exported to the csv file.
 - **c** If necessary, make changes to the file, for example, by limiting only the analyses and sequences of a specific instrument in the file. Save your changes and keep the file in the above specified path.
 - **d** Select **Migrate Specified Analyses** to start the import of the identifiers.

The migration tool checks the existing analyses of the target system. The number of migrated analyses is displayed after migration.

- **8** To migrate templates, select **Migrate Analyses Templates**. The migration tool checks the existing templates of the target system. The number of migrated templates is displayed after migration.
- **9** To monitor the migrated elements, you can compare the number of migrated items with the number of actual records available for migration in the old database.
- **10** After the migration is finished, open Sample Scheduler configuration on the target system to confirm the successful migration.
- **11** Open the Sample Scheduler client on the target system to verify that all desired analyses and sequences have been migrated.

New or upgraded items

New or upgraded items

Starting with Sample Scheduler for OpenLab revision 2.8, project groups are included in the migrated data. Therefore, you may find more projects than expected after an upgrade from a previous version. The additional projects have been present in the previous version, but they had ambiguous project names, and were part of different project groups. Ambiguous projects are hidden in previous Sample Scheduler versions.

9 Uninstallation

To uninstall the application, you can either launch the setup and select the **Remove** option, or uninstall it from the Microsoft Control Panel.

All the files installed by the setup will be deleted, and the registry keys are removed. The Sample Scheduler database stays intact.

If your topology includes multiple OpenLab servers, uninstall Sample Scheduler from those servers that do not host Shared Services. Alternatively, disable the Sample Scheduler Webserver service on those servers.

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Uninstall Sample Scheduler for OpenLab

If your topology includes multiple OpenLab servers, uninstall Sample Scheduler from those servers that do not host Shared Services. Alternatively, disable the Sample Scheduler Webserver service on those servers.

- 1 Close the Sample Scheduler client and Sample Scheduler configuration user interfaces.
- 2 Launch the setup and select the **Remove** option. Alternatively, uninstall from the Microsoft Control Panel

NOTE

Sample Scheduler automatically stops the Sample Scheduler Agent and Sample Scheduler LIMS agent services. If this fails, you are prompted to stop these services manually.

All the files installed by the setup will be deleted, and the registry key is removed. The Sample Scheduler database stays intact.

Remove Sample Scheduler Button from OpenLab CDS Acquisition

- 1 Run PowerShell as Administrator.
- 2 To check your execution policy, run: get-executionpolicy

The execution policy must allow scripts to run. This is given, for example, with the execution policy remotesigned or unrestricted.

NOTE

If the PowerShell execution policy does not allow scripts to run, contact your IT administrator

3 Copy the following script, paste it into a text editor, and remove superfluous line breaks.

```
[xml]$xml = Get-Content "C:\ProgramData\Agilent Technologies
, Inc\OpenLAB CDS - Acquisition\CustomToolsConfiguration.xml"

$nodes = $xml.SelectNodes("//CustomToolsGroup") | Where
{ $_.CaptionForCustomToolsGroup -match 'Sample Scheduler' }

foreach($node in $nodes){$node.ParentNode.RemoveChild($node)}

[xml]$xml.Save('C:\ProgramData\Agilent Technologies
, Inc\OpenLAB CDS - Acquisition\CustomToolsConfiguration.xml')
```

4 Copy the corrected script, paste it into PowerShell, and execute it.

10 LIMS Commands

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Analysis Order Generated by the LIMS

A command is an analysis order generated by the LIMS, leading to the analysis of a sample by OpenLab CDS via the Sample Scheduler.

Two types of commands are handled:

- XML commands generated by the LIMS and respecting the Scheduler XML command structure.
- Commands collected from the LIMS database by a periodically executed SQL query as defined in the Sample Scheduler configuration.

Both command types are handled by the Sample Scheduler (Scheduler LIMS agent) in the same consistent way.

- Collection of the command
- Checking the command validity
- Creation of an analysis in the Sample Scheduler database

NOTE

If you used to work with Sample Scheduler for OpenLab CDS A.02.x:

XML commands and SQL queries can remain unchanged. The existing structures can be used as is, the current version of Sample Scheduler for OpenLab is backwards compatible. A new parameter **Identifier** will be added that contains the sample name.

This chapter describes the XML scheme the LIMS must respect when it generates XML commands.

The structure of an XML file is defined to fit the CDS instrument/method architecture.

An XML template is provided with the user documentation to help you build your own command: It is installed with the Sample Scheduler software under <Scheduler Install path>/Documentation/xml/Advanced_Command.xml.

Sample Scheduler for OpenLab manages two types of XML files:

- XML commands, that handle:
 - The analysis of a sample with OpenLab CDS
 - The population of the Auto-Fills table with Auto-fill templates (to be used to automatically fill incomplete commands).
- XML actions that initiate an action, for example:
 - Deleting an analysis, an entire sequence, or an analysis with a matching identifier from a sequence
 - Creating a sequence from a group of analyses
 - Creating an instrument group

For more information on the XML scheme, see the Sample Scheduler for OpenLab Command Guide (in the installation folder under Documentation\xml\Sample_Scheduler_for_OpenLab_Command_Guide.chm).

Encoding

Always declare the correct encoding in the XML file. To see how to declare the encoding, refer to the **Advanced_Command.xml** example in the **Documentation/xml** folder.

NOTE

If you do not specify the encoding, the file is treated as UTF-8. This may lead to issues if the XML file was not saved as UTF-8.

High level XML command structure

The structure of an XML command corresponds to the analysis of one sample on one instrument configured with one Injection source. It must conform with the following high-level structure:

- The General parameters are the parameters defined for the entire sample.
- The Task parameters are related to one instrument. In most cases only one
 task is defined by an XML command as the sample acquisition is performed
 on one instrument. For some applications (for example, online gas analysis),
 the sample can be analyzed by two coupled instruments simultaneously. In
 this case, two tasks are defined in the XML command. A maximum of two
 tasks can be handled by the XML command.
- The Tower parameters are related to one injection source of the instrument. Acquisition parameters, sample information, calibration parameters and internal standards are defined in this section.

If the instrument is configured with two Injection sources, two Tower sections must be defined in the XML command.

Restart an analysis from the LIMS

If the LIMS offers this function, you can restart analyses or sequences that are in **Ended**, **Error**, or **Stopped** state. Configure the LIMS to supply the same information in the XML as on the first submission to the Scheduler. Only the **Identifier** needs to be changed, since it must be unique.

Basic XML command

The basic command lists the minimum set of parameters that need to be defined in an XML command to allow the CDS to perform the analysis.

The prerequisite to use such a command is to define a value for all the following default parameters in Sample Scheduler configuration/System configuration:

OpenLab default user, OpenLab default project, Default Sample name,

Default data file, Default result path, and Default result name parameters.

```
<SchedulerCommand>
<Identifier>LIMS_ID</Identifier>
                                              Sample Identifier generated by
                                              the LIMS
 <Tasks>
  <Task>
   <InstrumentMethods>
    <InstrumentMethod>
     <InstrumentName>
                                              The instrument name is case.
                                              sensitive. If the case is
      OpenLabValidInstrument
                                              different from the one defined
     </InstrumentName>
                                              in the Control Panel, the XML
                                              command will be considered
                                              as not valid, and sent to the
                                              <LIMS_Commands>/trash
                                              folder.
     <AcquisitionMethodName>
      OpenLabValidMethod.amx
     </AcquisitionMethodName>
    </InstrumentMethod>
   </InstrumentMethods>
  <Towers>
   <Tower>
    <InjectionSource>
     InjectionSourceName
    </InjectionSource>
    <SampleInfo>
     <UseMethodInjectionVolume>
                                              Use the injection volume
                                              defined in CDS Acquisition
      true
     </useMethodInjectionVolume>
                                              method
     <Vial>1</Vial>
                                              Autosampler position
    </SampleInfo>
   </Tower>
  </Towers>
 </Task>
</Tasks>
</SchedulerCommand>
```

Advanced XML command

The XML command allows you to define many parameters used to perform the acquisition (vial, injection volume...) and the processing (multiplier, sample amount, ...). In the XML command, you can set up an analysis with the instrument groups configured in the Sample Scheduler configuration. Later, when the analysis is edited in the analysis table, you can switch between the instruments (and their associated parameters) of this group. The XML command also allows you to define an instrument group that consists of specific instruments for a particular analysis.

NOTE

Ensure the instrument name, injection source and project are defined using the same spelling (including capitalization) as used in the Control Panel, otherwise the XML command will be considered as not valid, and sent to the <LIMS Commands>/Trash folder.

The list of available parameters and their position in the XML is described below.

For more information on instrument groups, refer to **Instrument groups with XML** commands on page 106.

Elements in <SchedulerCommand> ...

<template>false</template>	'true' to create a template command in the Auto- Fills tab, 'false' to create an analysis
<identifier> LIMS_ID </identifier>	Sample Identifier generated by the LIMS
<limsconnection> ValidLIMSConnectionName </limsconnection>	The LIMS connection configured in the LIMS tab of Sample Scheduler configuration. If the command does not contain a LIMS connection, the default LIMS connection is used. If the tag is blank or has an invalid LIMS connection specified, it will be not accepted and sent to the trash folder.
<state>Waiting</state>	Waiting or Scheduled
<project> OpenLabValidProject </project>	Project defined in OpenLab, defines the path where CDS files will be stored. If an instrument group is defined (see <instrumentmethods>), this project is assigned to the first instrument group.</instrumentmethods>
<instrumentgroupname> ValidInstrumentGroup </instrumentgroupname>	The instrument group name refers to the name of the instrument group that is defined in Sample Scheduler configuration. See example XML file InstrumentGroup_Command.xml.
<pre><user>OpenLabValidUser</user></pre>	User defined in OpenLab CDS
<pre><alternativeprojects> <project>OpenLabValidProject2 </project> <project>OpenLabValidProject3 </project> </alternativeprojects></pre>	If an instrument group is defined (see <instrumentmethods>), the alternative projects are assigned to the instruments at the corresponding positions. For example, the first alternative project will be assigned to the second instrument in the group.</instrumentmethods>
<replicates>3</replicates>	Number of injections
<pre><analysisvariable1>value 1value 2value 3value 4value 5</analysisvariable1></pre>	sVariable2> sVariable3> sVariable4>
<tasks> </tasks>	

Elements in <Tasks><Task> ...

<pre><instrumentmethod> Ad <instrumentname> gr OpenLabValidInstrument1 fir</instrumentname></instrumentmethod></pre>	you define several InstrumentName/
OpenLabValidInstrument2 <acquisitionmethodname> OpenLabValidMethod2.amx </acquisitionmethodname>	oup Defined by LIMS is created for this analysis, id the user can choose the instrument. The st Instrument/method couple defined in this ction will be applied to the analysis by default.

Elements in <Towers><Tower>...

<pre><limsid1>LIMSID1</limsid1></pre> <pre><limsid2>LIMSID2</limsid2></pre> <pre><limsid3>LIMSID3</limsid3></pre>	Parameters supplied by the LIMS
<pre><processingmethodname> OpenLabValidMethod1.pmx </processingmethodname></pre>	
<pre><alternativeprocessingmethodname> <processingmethodname> OpenLabValidMethod2.pmx </processingmethodname> <processingmethodname> OpenLabValidMethod3.pmx </processingmethodname> </alternativeprocessingmethodname></pre>	If an instrument group is defined (see <instrumentmethods>), the alternative processing methods are assigned to the instruments at the corresponding positions. For example, the first alternative processing method will be assigned to the second instrument in the group</instrumentmethods>

<pre><samplename>Sample1</samplename></pre>	CDS Sample name, stored with the raw data
<injectionsource> InjectionSourceName </injectionsource>	
<pre><alternativeinjectionsource> <injectionsource>Dual </injectionsource> <injectionsource>Dual2 </injectionsource> <injectionsource>Dual3 </injectionsource> </alternativeinjectionsource></pre>	If an instrument group is defined (see <instrumentmethods>), the alternative injection sources are assigned to the instruments at the corresponding positions. For example, the first alternative injection source will be assigned to the second instrument in the group</instrumentmethods>
<pre><sampleprepmethodname> OpenLabValidSamplePrepMethod1.smx </sampleprepmethodname></pre>	
<sampleinfo> </sampleinfo>	
<calibration> </calibration>	
<internalstandard> </internalstandard>	
<sampleinfo></sampleinfo>	
<pre><description> <line>long description in</line> <line>several lines</line> </description></pre>	
<vial>1</vial>	Autosampler location
<pre><usemethodinjectionvolume> False </usemethodinjectionvolume></pre>	'false' if the injection volume defined in the CDS Acquisition method is not used to perform the analysis 'true' if the injection volume defined in the CDS Acquisition method is used to perform the analysis

```
<Multiplier1>2.369</Multiplier1>
 <Multiplier5>2.369</Multiplier5>
 <Dilutor1>3.124</Dilutor1>
 <Dilutor5>3.124</Dilutor5>
 <Target1>3.124</Target1>
 <Target5>3.124</Target5>
 <CustomParameters>
  <SampleCustomParameter1>
  <Name>CDSSampleCustomParameter</Name>
  <Value>limsvalue3</Value>
  </SampleCustomParameter1>
  <SampleCustomParameter20>
  <Name>20thCDSSampleCustomParameter</Name>
  <Value>limsvalue20</Value>
  </sampleCustomParameter20>
 </CustomParameters>
</SampleInfo>
<Calibration>
 <SampleType>Sample
                                        Sample type: Sample, Cal. Std., Blank, Double
                                        blank, QC check, Spike, Sys. Suit
 </SampleType>
                                        Mandatory if SampleType = Cal. Std.
 <Level>1</Level>
 <CalibrationRuntype>
                                        Calibration run type: ClearAllCalibration,
                                        ClearCalibrationAtLevel
ClearAllCalibration
 </CalibrationRuntype>
</calibration>
```

<InternalStandard>
 <InternalStandardAmount1>5
 </InternalStandardAmount1>

 <InternalStandardAmount5>5
 </InternalStandardAmount5>

 <InternalStandardAmountUnit>mg
 </InternalStandardAmountUnit>
 </InternalStandardAmountUnit>

Multiple LIMS connections

Sample Scheduler provides the ability to connect to more than one LIMS with a single instance of the Sample Scheduler database. For backwards compatibility, Sample Scheduler is pre-configured with a default LIMS connection that allows existing installations to continue using Sample Scheduler, just as before, with a single LIMS connection after an upgrade. The default LIMS connection contains a minimum set of configuration parameters that you can change, if necessary.

You can add multiple LIMS connections, specifying the associated parameters for each LIMS connection. To address an XML command to a specific LIMS connection, you must specify the name of the LIMS connection in the XML command. Analyses and sequences will be processed by the Sample Scheduler with the corresponding parameters configured for the LIMS connection.

If an SQL query is specified for a LIMS database, the SQL command query is preferred for that LIMS connection. If XML commands are defined for the same LIMS connection, they are neglected and trashed. LIMS connections are set up in the **LIMS** tab of Sample Scheduler configuration.

Dual simultaneous injection with XML commands

For dual simultaneous injections the LIMS needs to write an XML file that has two Tower sections in a Task. The Injection Source must be the same for both towers and needs to support dual simultaneous injection. The string must match exactly the one provided by the acquisition client. Dual simultaneous injection is possible only if supported by the injection source.

NOTE

If dual simultaneous injection is not available in the acquisition client for the selected injection source, the device does not support dual simultaneous injections.

The acquisition method must be the same for both towers. The processing methods can be different.

The samples will be assigned to the injection source (front or back injector) in the same way as in the acquisition client. The first line will be assigned to the front injector, the second line to the back injector and so on, in alternating order.

An XML template is provided with the user documentation to help you build your own dual simultaneous injection command: It is installed with the Sample Scheduler software under

<Scheduler Install path>\Documentation\xml\DualInjection_Command.xml.

Using parameter 'Use Method Injection Volume' in XML command

If a default injection volume is defined in the acquisition method (only for instruments configured with an autosampler), it can be explicitly used to perform the acquisition when submitted by the Sample Scheduler.

To use this option, you must define a 'true' value for the parameter <useMethodInjectionVolume> in the XML command:

<UseMethodInjectionVolume>true</UseMethodInjectionVolume>

The <Injectionvolume> </Injectionvolume> section is then optional in the XML as it is not used to perform the acquisition.

Note that even if an injection volume is defined in the Acquisition method, another value can be defined in the XML. In this case, <useMethodInjectionvolume> must be false in the XML. In addition, it is mandatory that you set a value for the Injection volume in the XML (strictly positive value).

Instrument groups with XML commands

Instrument groups logically combine a set of alternative instruments that can do the same type of analysis. If instrument groups are configured, users can easily switch to another instrument for a specific analysis. The project, injection source, acquisition method, processing method can be defined for each instrument in the group and are automatically filled when the instrument is selected.

One XML file can contain only one instrument group.

The XML command can have the following functions:

Create an analysis using existing instrument groups.

The instrument groups are set up in Sample Scheduler configuration. The XML specifies the instrument group by its instrument group name, which is set in Sample Scheduler configuration.

See example XML file under <Scheduler Install path>/Documentation/xml/InstrumentGroup_Command.xml.

Define a temporary instrument group for a given analysis.

This instrument group is not visible in Sample Scheduler configuration. In the analysis table, the instrument group is referred to as **Defined by LIMS**. You can use the instrument group to switch to a different instrument as defined in the XML, but the group is not permanently stored in the Sample Scheduler database. Therefore, it cannot be used for another analysis, unless it is again completely defined in the respective XML.

See example XML file under <Scheduler Install path>/Documentation/xml/InstrumentGroupSpecifiedByLims_Command.xml.

Add multiple instrument lines to a group

For each parameter you can provide multiple entries. The structure depends on the parameter:

Instrument names and acquisition methods:
 They are always provided as a pair within an <instrumentMethod> tag.

NOTE

For backwards compatibility, the <InstrumentMethod> tag structure is the same as in previous releases.

Projects:

The second and all further tags are added within the <alternativeProjects> tag.

· Processing methods:

The second and all further tags are added within the <alternativeProcessingMethodName> tag.

· Injection sources:

The second and all further tags are added within the <alternativeInjectionSource> tag.

Always define the same number of alternative parameters. The first instrument line will contain the first project/instrument name/acquisition method/processing method/etc., the second line will contain the second parameter of each type, and so on. To use empty values, add empty tags.

Analysis variables in the XML command

Analysis variables (Analysis variable i) are variables created by the user in the Sample Scheduler configuration. They allow the user to display information in the Sample Scheduler client that is not provided by default by the Sample Scheduler: For example, the laboratory name where the instrument is located.

The user can assign a value to these variables either in the XML command or in the Sample Scheduler client.

These variables can also be part of the result name or sample name.

Up to five analysis variables can be defined per analysis. Analysis variable values are displayed in the Sample Scheduler client in the analysis table, in **Analysis variable i** columns.

NOTE

The values of these variables are not transferred to the CDS and cannot be displayed or reported in the CDS. They only exist in the Sample Scheduler database.

Sample custom parameters in the XML command

Sample custom parameters (Sample custom parameter i) are variables created by the user in OpenLab CDS on project level, or alternatively just in the Sample Scheduler. They allow the user to display and enter information in the Sample Scheduler client that may be transferred to and used by the CDS, but only if they were previously defined in the CDS settings for a given project.

The user can assign a value to these variables either in the XML command or in the Sample Scheduler client.

These variables can be part of the result name for single runs, and of the sample name.

Up to 20 sample custom parameters can be defined per analysis. Sample custom parameter values are displayed in the Sample Scheduler client in the analysis table, in **Sample custom parameter i** columns.

Use tokens in the XML command

It is possible to use the same predefined identifiers (tokens) as the ones proposed by the Single Sample or Sequence in the CDS Acquisition to define the result name and the sample name in the XML command.

It is also possible to use Scheduler-specific tokens.

NOTE

Only Sample Scheduler tokens are applied, not CDS tokens.

Table 9: Tokens

Parameter	Token
SampleName	Acq. Method <amx> Instrument name <i> Local date & time <d> Custom local date & time <cd> Proc Method <pmx> Short local date & time <ds> Username <u> Vial <v> Identifier <id> Analysis variable i [i=1 to 5] <a1> to <a5> LIMS IDi [i=1 to 3] <lid1> to <lid3> Sequence name <seq> (Sequence only)</seq></lid3></lid1></a5></a1></id></v></u></ds></pmx></cd></d></i></amx>
Result Name (single run)	Acq. Method <amx> Instrument name <i> Local date & time <d> Custom local date & time <cd> Proc. Method <pmx> Sample name <s> Short local date & time <ds> Username <u> Vial <v> Identifier <id> Analysis variable i [i=1 to 5] <a1> to <a5> LIMS ID I [i = 1 to 3] <lid1> to <lid3></lid3></lid1></a5></a1></id></v></u></ds></s></pmx></cd></d></i></amx>

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Parameter	Token		
Result Name (sequences and dual simultaneous injections)	Instrument name <i> Local date & time <d> Custom local date & time <cd> Short local date & time <ds> Username <u> Sequence name <seq></seq></u></ds></cd></d></i>		
Result Path	Instrument name <i> Local date & time <d> Custom local date & time <cd> Short local date & time <ds> Username <u> Analysis variable i [i=1 to 5] <a1> to <a5> Sequence name <seq> Invalid characters that are not allowed in data backends are removed from the resolved path</seq></a5></a1></u></ds></cd></d></i>		
DataFile	Sample name <s> Acq. Method <amx> Instrument name <i> Local date & time <d> Proc Method <pmx> Short local date & time <ds> Username <u> Vial <v></v></u></ds></pmx></d></i></amx></s>		

If using Sample Name or Sequence Name as tokens, ensure that these names do not contain invalid characters, such as ?/|<>*:". OpenLab CDS predefined name types contain <> symbols. Those symbols have a meaning in XML language and therefore cannot be expressed in this way in the Scheduler XML command.

Table 10: Syntax for < and > with examples

Correct syntax	Wrong syntax	Comment	
<	<		
>	>		
<samplename> <amx> </amx></samplename>	<samplename> <amx> </amx></samplename>	Generates the sample name based on the acquisition method name.	
<pre><resultname> <ID>_<E1> </resultname></pre>	<pre><resultname></resultname></pre>	Generates the sample name based on ID, date and time, and analysis variable 1.	

Priority rules

The parameter values used by the CDS to perform an analysis (project, instrument, user, vial, etc.) can be defined in three ways in the Sample Scheduler:

- XML command: all parameters,
- Sample Scheduler configuration: user, project, result name, sample name, initial state (default values used to perform the analysis when no value is defined in the command),
- Sample Scheduler client: all parameters can be edited.

To manage possible priority conflicts, the following priority rules have been set:

Table 11: Priority rules

Parameter	Priority rules
Sample name, Result name, User, Project	XML commands Sample Scheduler configuration default values
All parameters that are editable in Sample Scheduler client	Values as edited in the Sample Scheduler client XML commands

XML command creation

Some example XML commands are available in the *SampleScheduler>/ Documentation* folder. They help with generating the XML commands properly in your LIMS.

Minimal_Command.xml:	Minimal structure of the XML in the case no mandatory parameter has been added in the Sample Scheduler configuration System Configuration tab (only Identifier and Sample name are checked).
Basic_command.xml:	Minimal required information to perform an acquisition. The OpenLab default user, OpenLab default project, Default sample name and Default result name must be assigned a value in the Sample Scheduler configuration to use such a command.

Advanced_command.xml:	Structure containing all the possible parameters
SampleCustomParameters_command.xml:	Structure showing how to use Sample Custom Parameters with Sample Scheduler.
DualInjection_ command.xml:	Structure showing how to create dual injection commands.
Holding_Command.xml:	Structure to use in case of commands to merge (refer to the Sample Scheduler online help to learn more on the merge option).
Additional templates:	Structure of the XML to set single injection source and dual injection source instruments with or without calibration. These commands contain all the parameters required by the CDS to perform an acquisition.
UnknownSample_Single_InjectionSource_Command.xml:	Acquisition of an Unknown sample in External standard calibration runtype, on a single injection source instrument.
CalibrationSample_Single_InjectionSource_Command.xml:	Acquisition of a Standard sample in internal standard calibration runtype, on a single injection source instrument.
InstrumentGroup_Command.xml:	Acquisition of an analysis using the instrument group defined in Sample Scheduler configuration.
InstrumentGroupSpecifiedByLims_Command:	Structure of the XML to define an instrument group for a given analysis.

XML action

The Scheduler can manage XML files that are not intended to create an analysis, but to perform an action.

Those action commands do not match the classical XML command scheme, but a simplified scheme.

Examples provided by Agilent include cancel and create sequence commands.

Cancel command

Use the *cancel* command to delete an analysis or sequence that is stored in the Sample Scheduler database and that has not yet been started (i.e., in **Waiting** or **Scheduled** state only). The analysis or sequence to delete is identified by its Identifier.

<SchedulerAction>
 <Identifier>Analysis_Or_Sequence_To_Delete</Identifier>
 <Type>Delete</Type>
 <LimsConnection>ValidLIMSConnectionName<LimsConnection>
 </SchedulerAction>

The cancel command is sent into the <LIMS_Commands> folder. The Scheduler handles it and deletes the corresponding analysis or sequence from the Sample Scheduler database. The analysis or sequence is removed from the Scheduler interface. The cancel command does not generate an analysis or sequence and is never displayed in the Scheduler client.

The LIMS connection is used to identify the corresponding Processed command folder where the XML file will be moved to after successful execution. If no LIMS connection is specified in the XML file, the Processed command folder of the default LIMS connection is used. Commands that have an invalid LIMS connection specified are not accepted and sent to the trash folder.

You can use the Cancel_Analysis_Command.xml template located in the <SampleScheduler for OpenLab>/Documentation folder to build your own command. The XML scheme SchedulerAction.xsd, which is provided by the setup in the same folder, is used by the Sample Scheduler LIMS agent to check the command validity before its entry in the database.

Create sequence

Use the *create sequence* command to group a selection of analyses, stored in the Sample Scheduler database, into a sequence.

<SchedulerCreateSequenceAction>
 <LimsConnection>ValidLIMSConnectionName</LimsConnection>
 <SequenceName>MySequence</SequenceName>
 <SequenceState>Scheduled</SequenceState>
 <User>Analyst</User>
 <Identifiers>
 <Identifier>MySequenceLine-123</Identifier>
 <Identifier>MySequenceLine-456</Identifier>

```
<Identifier>MySequenceLine-789</Identifier>
  <Identifier>MySequenceLine-555</Identifier>
  <Identifier>MySequenceLine-999</Identifier>
  </Identifiers>
  <BarcodeReader>
  <UseBarcodeReader>false</UseBarcodeReader>
  <OnBarcodeMismatchAction>InjectAnyway</OnBarcodeMismatchAction>
  </BarcodeReader>
</SchedulerCreateSequenceAction>
```

You must define:

- A LIMS connection (not mandatory). If the XML command does not contain the tag, the default LIMS connection is used. If the tag is blank, the command is sent to the trash folder.
- A sequence name (not mandatory).
- The initial sequence state. If not defined, the default state defined in the Sample Scheduler configuration is used.
- The user who is assigned to the sequence. If not defined, the acquisition user defined in the Sample Scheduler configuration is used.
- The list of analyses to group, identified by their identifier. The sequence is created only if:
 - All analyses exist in the Sample Scheduler database.
 - All analyses are assigned to the same instrument, project, injection source, and LIMS connection.
 - All analyses are in Waiting, Incomplete, or Waiting on error state.

Otherwise the sequence is not created, and the XML file is sent to the trash folder.

 Instructions on using a barcode reader. The value of <usebarcodeReader> is boolean. Possible values if expected and real barcodes do not match are InjectAnyway and AbortCurrentInjection.

If the barcode reader section is missing, <useBarcodeReader> is set to false, and <onBarcodeMismatchAction> to InjectAnyway.

You can use the **Create_Sequence_Command.xml** template located in the <SampleScheduler for OpenLab>/Documentation folder to build your own command. The XML scheme **SchedulerCreateSequenceAction.xsd**, which is provided by the setup in the same folder, is used by the Sample Scheduler LIMS agent to check the command validity before its entry in the database.

Sample Scheduler XML file generator

The XML file generator enables the administrator to generate test XML commands for setting up the Sample Scheduler system. This tool makes it easy to create valid XML commands with the desired parameters that can be processed by LIMS.

The XML tool is located on the installation media in the folder Support>Xml_tool.

Working with the XML file generator

With the XML file generator, you can create single or multiple analyses. You can also create a sequence from the analyses.

Mandatory parameters are marked with an asterisk and require entry of a value:

Table 12: Mandatory parameters

Parameter	Comment
Scheduler Identifier	For multiple analyses the entered value is the start value. The ID of the following analysis is incremented by one.
LIMS identifier1	For multiple analyses the entered value is the start value. The ID of the following analysis is incremented by one.
Project	
Instrument	
Acquisition method	An extension is not required. If no extension is given, the extension .amx is automatically appended in the XML. Entries for the extensions .amx or .met are accepted for XML command creation.
Injection source	
Vial position	

Table 13: Optional parameters

Parameter	Comment	
Sequence name	The default name is sequence.	
Sample Name	For multiple analyses, select Use sample name start counter. The entered value is the start value. The value of the following analysis is incremented by one.	

Parameter	Comment
State	The state can be set to Holding, Scheduled , or Waiting .
Processing method	An extension is not required. If no extension is given, the extension .pmx is automatically appended in the XML. Entries for the extension .pmx are accepted for XML creation.
Sample Type	
Set injection volume	If selected, use MethodInjVol=false.
User	
Injection per sample	

The XML files are stored in a separate folder. This folder is created when generating the XML file. Sequence XML files are stored in a subfolder that is automatically created by the XML tool. The name of the subfolder corresponds to the name of the sequence. If a folder with this name already exists, an increment is automatically appended.

This section describes how Sample Scheduler must be configured to allow the collection of analysis orders directly in the LIMS database.

The Sample Scheduler provides a generic tool to gather analysis orders from the LIMS database (that handles SQL queries). As all LIMS databases are different, it is up to your database system administrator to configure the parameters detailed below to fit your LIMS database structure.

The configuration is done in the **LIMS** tab of the Sample Scheduler configuration (see also the **LIMS** section in the Sample Scheduler online help).

Both analyses and sequences can be submitted to the Sample Scheduler via SQL query. They are automatically assigned the LIMS connection from the configured LIMS database.

Configure the connection string

The connection string is a chain of characters containing the required information to establish a connection between the Sample Scheduler and your LIMS database, such as: the provider, the user/password, etc.

Examples for an MS SQL Server:

SQL Server and Windows authentication mode:

```
Server=ComputerName\DB_Instance Name;
Database=DatabaseName;
Password=XXX; User ID=Database_User;
```

Windows authentication mode:

```
Server= ComputerName\DB_Instance Name\SQLEXPRESS;
Database= DatabaseName;trusted_connection=yes;
```

Example for an Oracle Server:

```
Data Source= (DESCRIPTION =
  (ADDRESS = (PROTOCOL = TCP)(HOST = XXXXXX)(PORT = XXXXX))
  (ADDRESS = (PROTOCOL = TCP)(HOST = XXXXXX)(PORT = XXXXX))
  (CONNECT_DATA =
  (SDU = 8192)
  (TDU = 8192)
  (SERVER = DEDICATED)
  (SERVICE_NAME = XXXXX)
)
);user id=XXXXXX;password=XXXXX;
```

The database user must have 'Select' and 'Update' rights on the LIMS database.

To know which connection string is required according to your database, refer to http://www.connectionstrings.com/.

To test your connection string, click **Test connection**.

Write an SQL query

The LIMS query must be based on the structure of data expected by the Sample Scheduler.

- For an analysis on a single injection source instrument, the LIMS query returns a single entry to the Sample Scheduler, allowing the creation of the single injection source analysis.
- For an analysis on a dual injection source instrument, the LIMS query returns two entries to the Sample Scheduler, allowing the creation of the dual injection source analysis.
- For a sequence, the LIMS query returns the <number of sequence lines> entries for the specified sequence to the Sample Scheduler, allowing the creation of the sequence.

The LIMS query result must match the following structure and syntax:

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Table 14: SQL query

Sample Scheduler parameter	Value	Туре	Description
Identifier	n/a	Varchar (not null, unique)	The sample identifier. Must be unique. It is used to notify the LIMS that a command has been handled, to avoid it to be considered a second time.
Barcode	n/a	Varchar (null accepted)	Gives the option to identify a sample by scanning a barcode. Specific to individual analyses and analyses within a sequence, but not available for an entire sequence.
UseBarcodeReader	n/a	Boolean (null accepted)	Instruction for a barcode reader to read barcodes from your vials. If no value, set to false.
OnBarcodeMismatch	n/a	Varchar (null accepted)	Possible values if expected and real barcodes do not match are InjectAnyway and AbortCurrentInjection . If no value , InjectAnyway is used.
Template	n/a	Boolean (null accepted)	Specifies if this experiment should be used as a template for the auto-fill feature. Make sure that the template identifiers do not collide with analysis identifiers that will be handled by the system.
LimsIDi, [i=1 to 3]	n/a	Varchar (null accepted)	Values supplied by the LIMS for usage in the CDS.
SampleName	n/a	Varchar (not null)	The sample name
State	1= Scheduled 3=Waiting 10=Holding	Integer (null accepted)	The initial state assigned to the analysis. If no value, the default state defined in the Sample Scheduler configuration is used.
InstrumentGroupName	n/a	Varchar	Name of instrument group
Sequenceld	n/a	Integer (null accepted)	The sequence id assigned to the analysis. Analyses with the same sequence id belong to the same sequence. If no value is assigned, the analysis does not belong to a sequence.
SequenceName	n/a	Varchar (null accepted)	The sequence name
SequencePosition	n/a	Integer (null accepted)	The sequence position of the analysis in the sequence. The first sequence position of a sequence begins with 1.
ProjectName	n/a	Varchar (null accepted)	CDS project name
UserName	n/a	Varchar (null accepted)	CDS user name

Sample Scheduler parameter	Value	Туре	Description
Replicates	n/a	Integer (null accepted, default value 1)	Sample Scheduler parameter. If greater than one, the analysis will be replicated n times with the same parameters as specified in the XML/SQL result.
AnalysisVariableN, [N=1 to 5]	n/a	Varchar (null accepted)	Custom parameters
ResultName	n/a	Varchar (null accepted)	The name of the result files to be generated by the CDS. If no value is specified, the default result name defined in the Sample Scheduler configuration is used.
ResultPath	n/a	Varchar (null accepted)	Path where the CDS results are stored, including subfolders separated by slashes. If no value is specified, the default result path defined in the Sample Scheduler configuration is used.
InstrumentName	n/a	Varchar (null accepted)	CDS instrument name
AcquisitionMethodName	n/a	Varchar (null accepted)	Method used to perform the analysis in the CDS
ProcessingMethodName	n/a	Varchar (null accepted)	Method used to process the analysis in the CDS
AlternativeInstrumentsMethods	pattern like "inst1/meth1 inst2/meth2 inst3/meth3"	Varchar (null accepted)	Combination of instrument and acquisition method that can be used to perform the analysis instead of the nominal InstrumentName / AcquisitionMethodName couple. No limit in the number of alternative instrument/ method couples.
InjectionSource ⁵	n/a	Varchar (null accepted)	Injection source of the autosampler used to perform the analysis.
InjectionLocation ⁵	0=Front injection 1=Back injection	Integer (null accepted)	Location of the injector, for dual simultaneous injections. The two values need to be different. Is one set to a valid value and the other an incorrect value, the valid value is used to set the order. Are both set to null or another not valid value then the order will not be changed.
SampleDescription ⁵	n/a	Varchar (null accepted)	Description of the sample
Vial	n/a	Varchar (null accepted)	The vial position where the sample is taken.

⁵ Parameters to be defined by Injection source.

Sample Scheduler parameter	Value	Туре	Description
UseMethodInjection Volume ⁵	n/a	Boolean (null accepted)	The injection volume defined in the acquisition method that is used to perform the analysis.
InjectionVolume ⁵	n/a	Float (null accepted)	Volume of the sample injected
SampleAmount ⁵	n/a	Float (null accepted)	Amount of sample. Used to perform quantitation in the CDS.
SampleAmountUnit ⁵	n/a	Varchar (null accepted)	Unit of the sample amount
SamplePrepMethod ⁵	n/a	Varchar (null accepted)	Sample prep method used by the CDS
TargetN, [N=1 to 5] ⁵	n/a	Varchar (null accepted)	The target fields can be used to specify the target masses or formulas for compounds that are analyzed using an MS or LC/MS sample purity method.
MultiplierN, [N=1 to 5] ⁵	n/a	Float (null accepted)	Used to perform quantitation in the CDS
SampleCustomParameterNName [N=1 to 20] ⁵	n/a	Varchar (null accepted)	Used to submit custom parameters of the sample to the CDS.
SampleCustomParameterNValue [N=1 to 20] ⁵	n/a	Varchar (null accepted)	This value needs to be valid according to the type that was specified for the Sample Custom Parameter in OpenLab CDS. (E.g.: a value for a Custom Parameter with type Date has to be convertible to a date)
DilutorN, [N=1 to 5]	n/a	Float (null accepted)	Used to perform quantitation in the CDS.
SampleType ⁵	0=Sample 1=Cal. Std. 2=Blank 3=Double blank 4=QC check 5=Spike 6=Sys. Suit	Integer (null accepted)	Define if the sample is analyzed as a Sample or another type. Default is Sample
InjectionsPerSample ⁵	n/a	Integer (null accepted)	Define how often the sample should be injected by the CDS.
Level ⁵	n/a	Integer (null accepted)	Calibration level defined in the processing method.
CalibrationRuntype ⁵	0=ClearAllCalibr ation 1=ClearCalibrati onAtLevel	Integer (null accepted)	Define the way previous calibration points are considered when a new standard point is added to the calibration curve

Sample Scheduler parameter	Value	Туре	Description
InternalStandardAmountN, [N=1 to 5] ⁵	n/a	Float (null accepted)	Amount of internal standard in the sample. Used to perform quantitation in the CDS.
InternalStandardUnit ⁵	n/a	Varchar (null accepted)	Unit of the internal standard amount.

All the commands defined in the LIMS database must contain at least the following parameters to be considered valid by the Sample Scheduler:

- Identifier
- Sample name
- The list of mandatory parameters defined in the Mandatory column of the of the Commands tab.

SQL query examples

The SQL connection example provided with the Sample Scheduler software helps to understand how to setup a LIMS connection via SQL. The queries and the database show how to get the available parameters from a simulated LIMS into Sample Scheduler. The example scripts are written for a Microsoft SQL database and are installed at: <Scheduler Install path>/Documentation/sql.

dbo.command		
Lists all parameters to be defined by analysis		
dbo.tower_parameters		
Lists all parameters to be defined by Injection source.		

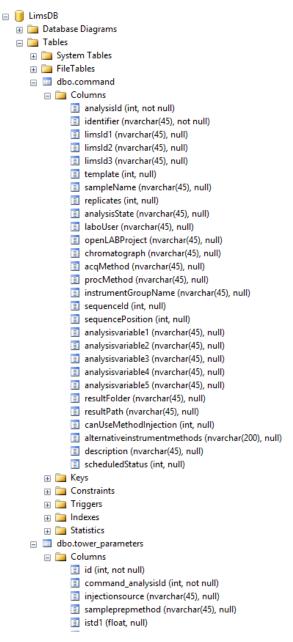


Figure 35: Example of a LIMS database (LIMS_DB) consisting of two tables

LIMS Commands

Command Collected via SQL Query

Find below simple examples of queries built for an MS SQL Server LIMS database that could be handled by the Sample Scheduler.

The **scheduledStatus** parameter has been added to assign a flag to the command:

0: already handled by the Sample Scheduler,

1: properly handled, 2: handled but invalid.

Analysis to be performed on a single Injection source instrument:

One entry in the dbo.commands table

One entry in the dbo.tower_parameters table.

Analysis to be performed on a dual injection source instrument:

One entry in the dbo.commands table

Two entries in the **dbo.tower_parameters** table.

Sequence with analyses to be performed on a single injection source instrument:

- <Number of sequence lines> entries in the dbo.commands table
- <Number of sequence lines> entries in the dbo.tower_parameters table.

Sequence with analyses to be performed on a dual injection source instrument:

<Number of sequence lines> entries in the dbo.commands table

Twice the <Number of sequence lines> entries in the dbo.tower_parameters table.

NOTE

Only some of the parameters that can be defined in an analysis are proposed in this example, but you can define all the parameters listed in the table **Table 14** on page 119.

The following example handles the case where the LIMS database (LIMS_DB) provides parameters with names different than the ones expected by the Sample Scheduler (for example, 'chromatograph' in the LIMS database corresponds to 'InstrumentName' in the Sample Scheduler database). It is up to the LIMS query to link the LIMS parameters and the corresponding Sample Scheduler parameters: **chromatograph** as **InstrumentName**.

In this example, we also manage the notification back to the LIMS database, to inform that a defined command has been handled (with success or not), to avoid handling the same command several times. It is the role of the LIMS notification: Valid command and LIMS notification: invalid command queries.

SQL Query

```
SELECT
c.sampleName as SampleName,
c.analysisId as Identifier,
c.sequenceId as SequenceId,
c.sequencePosition as SequencePosition,
CASE
WHEN analysisState='Scheduled' THEN 1
WHEN analysisState='Waiting' THEN 3
WHEN analysisState='Holding' THEN 10
ELSE NULL
END as [State].
c.labouser as [UserName],
c.openLabProject as ProjectName,
c.chromatograph as InstrumentName,
c.CDSMethod as AcquisitionMethodName,
c.resultFolder as ResultName,
t.analysis_tower as InjectionSource,
t.analysis_sample_mass as SampleAmount,
t.analysis_dilutor as Dilutor1,
c. Variable as Analysis Variable 1,
CAST(t.analysis_multiplier as float) as Multiplier1,
t.analysis_level as Level,
t.analysis_vial as Vial,
t.analysis_injection_volume as InjectionVolume,
t.analysis_tower as InjectionSource,
'Plantidentifier' as SampleCustomParameter1Name,
t.customer_custom_field1 as SampleCustomParameter1Value
CASE
WHEN c.UseBarcodeReader='true' THEN 1
WHEN c.UseBarcodeReader='false' THEN 0
ELSE NULL
END as [UseBarcodeReader],
CASE
WHEN c.OnBarcodeMismatch='InjectAnyway' THEN 0
```

```
WHEN c.OnBarcodeMismatch='AbortCurrentInjection' THEN 1
ELSE NULL
END as [OnBarcodeMismatch],
CASE
WHEN t.analysis_sample_type='Sample' THEN 0
WHEN t.analysis_sample_type='Calib' THEN 1
ELSE NULL
END as SampleType,
c.alternative as AlternativeInstrumentsMethods
FROM [LIMS_DB].[dbo].[command] c LEFT JOIN
[LIMS_DB].[dbo].[tower_parameters] t ON (c.analysisId = t.command_analysisId)
WHERE scheduledStatus = 0;
```

The Sample Scheduler manages only commands with scheduledStatus = 0.

Once the Sample Scheduler has handled a command, it sends a value back to the LIMS database/scheduledStatus parameter. In this example:

- scheduledStatus=1 if the command has been properly handled (valid command),
- scheduledStatus=2 if the command was invalid (not transformed into an analysis in the Sample Scheduler database).

LIMS notification

LIMS notification: valid command (example for SQL server)

UPDATE LIMS_DB.[dbo].[command] SET **scheduledStatus = 1** WHERE analysisId = @Identifier;

LIMS notification: invalid command (example for SQL server)

UPDATE LIMS_DB.[dbo].[command] SET scheduledStatus = 2 WHERE analysisId = @Identifier;

Only the parameter **Identifier** can be provided by the Sample Scheduler for both the valid and the invalid command.

10 LIMS Commands

Command Collected via SQL Query

In the notification query, the variable name depends on the used database connection provider. For example, as variable name Microsoft SQL-Client expects **@Identifier** and Oracle-Client expects **:Identifier**. For an exact definition of the notation, see the documentation of the database connection provider that you use to access the LIMS database.

Dual Simultaneous Injection via SQL Query

The same identifier must be used for both lines of the dual injection command. This will instruct Sample Scheduler to create a dual injection sample analysis. For the parameters that are common to both injectors, it will use the values specified for the front injector (first line).

To ensure that the correct parameters are assigned to the front and back injector, the command creation query needs to consider the order of the analyses submitted by the LIMS. This can be achieved by adding a "sort by clause" statement. For example, if the LIMS always sends a higher value for the vial location of the back injection the analyses could be sorted by vial location. Alternatively, you may use an analysis or instrument custom parameter to sort by. Another way to determine the order of the analyses is to define the Injection Location field for each of the towers. Lines set to 0 refer to the front position, lines set to 1 refer to the back position. The injection source must be the same for both front and back injector, and it needs to support dual simultaneous injection.

Sequence Creation via SQL Query

To create a sequence via SQL query, the results from the command creation guery need to fulfill the following requirements:

- For all the analyses belonging to the same sequence, the sequence id must be the same.
- The first analysis of the sequence gets the first sequence position (sequence position = 1).
- For the other sequence lines, the sequence position must be incremented consecutively by one.
- Parameters that are common to a sequence must be the same for all sequence lines.
- The complete sequence must be present in the source/LIMS database at the time Sample Scheduler reads the corresponding lines.

It is not possible to append sequence lines via SQL query to an already existing sequence in the Sample Scheduler database.

Transaction To ensure that the complete sequence is present, perform the write and read **isolation** operation on the LIMS database in a transactional manner, and make sure the transaction isolation level of the database is high enough.

> Agilent recommends to set the isolation level to snapshot. For some database systems (like MS SQL) this level is not allowed by default and needs to be enabled first on database level.

Example to allow snapshot isolation level on MS SQL:

ALTER DATABASE LIMSDB SET ALLOW_SNAPSHOT_ISOLATION ON ALTER DATABASE LIMSDB SET READ_COMMITTED_SNAPSHOT ON GO

Usage:

SET TRANSACTION ISOLATION LEVEL SNAPSHOT BEGIN TRANSACTION <... SQL command...> COMMIT TRANSACTION

11 Command Validity Process

When a command is generated by the LIMS, it is handled by the Sample Scheduler (Sample Scheduler LIMS agent). The following validity control process is applied:

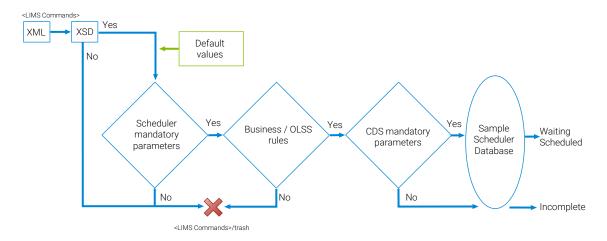


Figure 36: Validity control process

- 1. The command matches the expected syntax format.
 - The XML command must match the XML scheme (XSD). This scheme checks the XML syntax, the XML structure, the type (integer, boolean, etc.) and the properties of each parameter (For example, the sample type can only be Sample, Cal. Std., etc; the injection volume must be a number; etc.). The SchedulerXmlCommand.xsd file is provided in the installation folder under Documentation\xml.
 - The commands collected via SQL query must also respect the expected structure, and contain parameters respecting the rules defined in the query (valid parameter name, type, properties, etc).

11 Command Validity Process

- The command contains the mandatory parameters defined in the Command/Mandatory tab. If Project, User, Sample Name, Result Name or State parameters have no value, they are assigned the default values defined in the Sample Scheduler configuration, System Configuration tab.
- 3. The command satisfies the business rules (if **Dilutor** or **Multiplier** equal 0, they are assigned the value 1). The server in the OpenLab system checks if the **Project**, **User**, **Instrument**, and **Acquisition methods** exist.
- 4. If the command does not satisfy at least one of the steps 1 to 3, it is sent to the <LIMS Commands>/trash folder. No analysis is generated.
- 5. If steps 1 to 3 are satisfied, an analysis is generated in the Scheduler database.
- 6. Steps 1 to 3 are satisfied if:
 - all parameters needed by the CDS are defined,
 - the analysis is set to either the Waiting or the Scheduled state.
- 7. If at least one of these parameters is missing, the analysis is assigned the **Incomplete** state.
- 8. *Mandatory parameters in the CDS*: Instrument, Injection source, Project, Acquisition method, Result file name, Vial, Injection volume.

Auto-fill If the Auto-fill command option is used, the validity process is modified as follows:

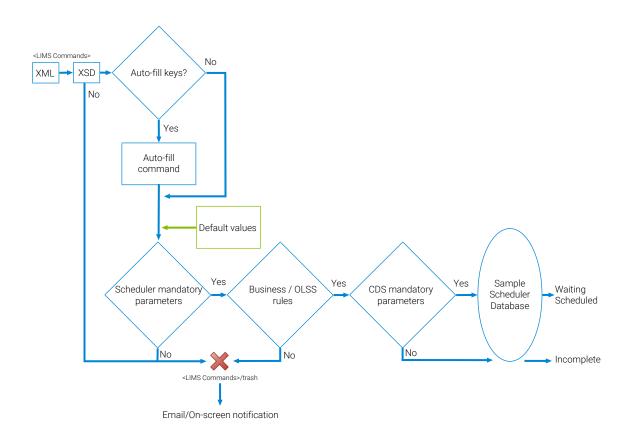


Figure 37: Auto-fill command validity process

- 1. The command matches the expected syntax, format.
 - The XML command must match the XML scheme (XSD). This scheme checks the XML syntax, the XML structure, the type (integer, boolean, etc.) and the properties of each parameter (for example, the sample type can only be Sample, Cal. Std., etc; the injection volume must a number, and so on). The SchedulerXmlCommand.xsd file is provided in the installation folder under Documentation\xml.
 - The commands collected via SQL query must also respect the expected structure, and contain parameters respecting the rules defined in the query (valid parameter name, type, properties, etc).
- 2. A value is assigned to all the *Auto-fill trigger* parameters, and a template analysis exists in the *Auto-fill command* table: the command is completed according to the template analysis.

11 Command Validity Process

- The command contains the mandatory parameters defined in the Command/Mandatory tab. If Project, User, Sample name, Result file name, and/ or State parameters have no value after completion with template analysis, they are assigned the default values defined in the Sample Scheduler configuration, System Configuration tab.
- 4. The command satisfies the business rules (if Dilutor, Multiplier, or Internal standard amount equal 0, they are assigned the value 1). The server in the OpenLab system checks if the Project, User, Instrument, and Acquisition methods exist
- 5. If the command does not satisfy at least one of the steps 1, 3 or 4, it is sent to the <LIMS Commands>/trash folder. No analysis is generated.
- 6. If steps 1, 3 and 4 are satisfied, an analysis is generated in the Sample Scheduler database.
- 7. Steps 1, 3 and 4 are satisfied: If all parameters needed by the CDS to perform an acquisition are defined, the analysis is assigned either the **Waiting** or the **Scheduled** state. If at least one of these parameters is missing, the analysis is assigned the **Incomplete** state.

If a wrong ticket is defined, for example the credentials correspond to an OpenLab user that cannot use the instrument, the Sample Scheduler will not be able to perform an analysis, as the Agilent Sample Scheduler agent service will not start.

12 Activity Logs

Sample Scheduler offers the possibility to log your activities in the software. Once the audit trail is enabled (Sample Scheduler configuration, System Configuration), all the actions performed by Sample Scheduler for OpenLab are traced in the System Activity Log of the Control Panel (under Administration). Those logs can be useful to understand the reason and to perform the appropriate action to correct a potential problem. For more information on how to search, filter, export, print or refresh the activity log, refer to the Control Panel online help (search for "System Activity Logs").

NOTE

Once the audit trail has been enabled, you can no longer disable it

If an error occurs, refer to **Troubleshooting** on page 146, to see if it deals with the issue you encountered. If not, send the above log files to your Technical Support. Some problems may be induced by a database connection issue, so be sure to check the database connectivity in case of doubt.

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General and Project Operations

Reconfigure Sample Scheduler database

If the Sample Scheduler database access has been modified (after the Sample Scheduler has been installed and configured), you must reconfigure the Sample Scheduler database access parameters.

This can happen in the following situations:

- Change of database computer/Instance
- Change of the authentication mode (Windows authentication or SQL authentication)
- · Change of user credentials (login and/or password).
- 1 To reconfigure the database access, ensure that no analysis is running.
- 2 Start the <Sample Scheduler for OpenLab>\bin\Agilent.Scheduler.Database.Access.reconfiguration.exe installed together with the Sample Scheduler database.

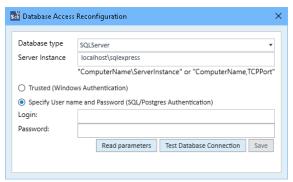


Figure 38: Database access reconfiguration

- 3 Update the values of the parameters:
 - Define the Database type (SQL server or OLDR)
 - Provide the Server Instance name

13 Maintenance Operations

General and Project Operations

- Authentication mode (in case of SQL Server instance) with credential (in case of SQL authentication)
- Password to access the OLDR (created during the installation of Sample Scheduler on the server)
- **4** Then click **Test Database Connection**. If the parameters are valid, you can save the new parameters. The connection parameters are updated in the registry.
- **5** Restart the Agilent Sample Scheduler LIMS agent service and all Agilent Sample Scheduler agent services (Sample Scheduler onfiguration: Deployment tab).

Change the Sample Scheduler agent assigned to an instrument

- 1 In the **Instrument management** tab of Sample Scheduler configuration:
 - **a** Assign the new Sample Scheduler agent computer name to the instrument, click **OK**.
 - **b** Save.
- 2 In the **Deployment** tab:
 - a Restart the two Sample Scheduler agent services: the old one and the new one (ensure no analysis is currently running on the instruments managed by the Sample Scheduler agents).
 - **b** Restart the Sample Scheduler LIMS agent.
 - c Click Refresh.

Rename a computer that is the host of a Sample Scheduler agent

- 1 Rename the computer.
- 2 If this computer is an OpenLab AIC, register the AIC.

13 Maintenance Operations

General and Project Operations

For details, see OpenLab CDS Clients and Instrument Controllers Installation and Configuration (CDS_v2.8_ClientAICGuide_en.pdf).

No action is needed in Sample Scheduler; the new computer name is automatically updated in both the **Instrument management** and **Deployment** tabs.

Documents about this

<OpenLab CDS Client and AIC Installation> (https://www.agilent.com/cs/library/usermanuals/public/CDS_v2.8_ClientAICGuide_en.pdf)

Change project settings in the Control Panel

If you change the project settings in the Control Panel (for example, enabling the audit trail, allowing to prompt for a reason), you must restart the Sample Scheduler agent in Sample Scheduler configuration (**Deployment** tab) for the changes to be applied.

Instrument Operations

Rename the instrument in the Control Panel

- 1 In the **Instrument Management** tab:
 - **a** Assign the Sample Scheduler agent computer name to the instrument and click **OK**.
 - **b** Save.
- 2 In the **Deployment** tab:
 - **a** Restart the Sample Scheduler agent service (ensure no analysis is currently running on the instruments managed by this Sample Scheduler agent).
 - **b** Restart the Sample Scheduler LIMS agent.
 - c Click Refresh.

Add an instrument in the Control Panel

- 1 Create and configure the new instrument in the Control Panel.
- 2 Start a new session of Sample Scheduler configuration.

13 Maintenance Operations

Instrument Operations

- 3 In the **Instrument management** tab:
 - **a** Assign the Sample Scheduler agent computer name to the instrument and click **OK**.
 - **b** Save.
- 4 In the **Deployment** tab:
 - **a** Restart the Sample Scheduler agent service assigned to the new instrument (ensure no analysis is currently running on the instruments managed by this Sample Scheduler agent).
 - **b** Wait until a Sample Scheduler acquisition agent is created for the instrument managed by the Sample Scheduler agent (especially for the new instrument).
 - c Restart the Scheduler LIMS agent.

Delete an instrument in the Control Panel

- **1** Delete the instrument in the Control Panel.
- 2 Start a new session of Sample Scheduler configuration
- 3 In the **Deployment** tab:
 - **a** Restart the Sample Scheduler agent service that managed the deleted instrument.
 - **b** Restart the Scheduler LIMS agent.
 - c Click Refresh.
- 4 In the Instrument management tab, ensure that the instrument name is no longer listed.

Instrument Operations

Deploy a reconfigured instrument in Sample Scheduler

- 1 Reconfigure the instrument in the Control Panel.
- 2 Start a new session of Sample Scheduler configuration.
- 3 In the **Deployment** tab:
 - **a** Restart the Sample Scheduler agent service assigned to the instrument (ensure no analysis is currently running on the instruments managed by this Sample Scheduler agent).
 - **b** Wait until a Sample Scheduler acquisition agent is created.
 - **c** Restart the Scheduler LIMS agent.

Network and Server-related Operations

Add an AIC after activation

After installing Sample Scheduler on an additional OpenLab AIC, you have to provide the Sample Scheduler agent with valid user credentials.

- 1 Open the Sample Scheduler configuration.
- 2 Go to the Maintenance tab.
- **3** Select **Update OpenLab Services Credentials** and enter user name and password.
- **4** On the additional AIC, make sure that the Sample Scheduler agent service is set to **Automatic (Delayed Start)**.

Connect to another server

If you change the server in your OpenLab system, you will also have to update the OpenLab Services Credentials in Sample scheduler. For details, refer to the Sample Scheduler online help (search for "Update OpenLab Services Credentials").

If in doubt, check the SQL Server connectivity.

Change authentication mode

If you change the authentication mode in the Control Panel, you must also manually update the Sample Scheduler service credentials on each Sample Scheduler computer that was set up with that provider.

Network and Server-related Operations

Back up the Sample Scheduler database

The Sample Scheduler database contains only a few entries that are persisted for a longer time. A risk-based analysis should be done to decide if, when, and how often a backup of the Sample Scheduler database is required.

If you only need to back up the configuration of Sample Scheduler after it is considered final: It may be enough to either print out the configuration from the Sample Scheduler configuration application, or export the data directly from the relevant database tables via SQL Server Management Studio.

If you need to back up data concerning the analyses: Decide how frequently the database should be backed up and how much data would be acceptable to lose in a worst-case scenario.

Consider the following for the database backup strategy:

- Check (either manual or automatic) which analyses have already been performed (for example, the backup still has analyses in Waiting state while the runs have already been carried out successfully) in order to avoid duplicate runs and re-analyses during a database restore.
- Decide on how often a backup should be done.
- Make sure that the backup location is protected against possible disk failures.

Recovery models

Microsoft SQL server supports several recovery models. These models affect what the backup contains, and how the database can be restored from a backup. An administrator needs to decide which recovery model should be used when coming up with a backup strategy.

- · Simple Recovery model
 - No database transaction logs get backed-up. You can only restore back to the point in time when the backup was finished, no further back. The database cannot be reverted to a state before errors occurred (such as user mistakes or applications failures).
- Full Recovery model
 The database and the transaction logs are backed-up. You can restore back to any point in time.
- Bulk Recover model

13 Maintenance Operations

Network and Server-related Operations

The database and the transaction logs are backed-up, however, bulk transactions in the transaction log are compressed. As Sample Scheduler does not use bulk transactions, this recovery model should not be used with Sample Scheduler.

Set up the recovery model settings on the database first, before backing up using that recovery model.

For a detailed comparison, refer to the Microsoft documentation: docs.microsoft.com

Backup procedure

After deciding if backups should be done, establish a backup procedure.

For detailed information on the data repository backup of the OLDR server instance, refer to the document *Configuring OpenLab CDS with OpenLab ECM*.

Depending on the SQL server edition, different options are available:

SQL Express

Microsoft SQL Express only offers manually or job triggered backups.

For manual backups, log in to the database server with Microsoft SQL Server Management Studio, right-click the Sample Scheduler database, and select Tasks > Back Up....

For automating the procedure, follow the Microsoft guide on support.microsoft.com

SQL Server Standard or Enterprise

Backups on SQL Server Standard or Enterprise should be automated with the SQL Server agent. To set this up, follow the procedures on docs.microsoft.com

Restore in case of failure

If a database failure occurred, proceed as follows to restore the database to the consistent state of the backup:

13 Maintenance Operations

Network and Server-related Operations

- 1 If the Sample Scheduler configuration is still able to start and display the running agents in the **Deployment** tab, first stop the running Scheduler agents, then log in to the Microsoft SQL Server Management Studio.
- 2 To disconnect all connections to the database and set them offline, execute the following statement in a new SQL query:
 alter database OpenLabSchedulerDB270 set offline with rollback immediate
- **3** After this has finished executing, restore a backup:
 - a Right- click the database, then select Tasks > Restore > Database.
 - **b** Select the backup you want to restore.
 - **c** In case of a Full Recovery model setting on the database, choose the point in time to which the database should be restored to.
- **4** After finishing the restore procedure on the database, log in to the Sample Scheduler configuration and restart all services in the **Deployment** tab.

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About Trobleshooting

NOTE

Some problems are induced by database connection issues. Ensure the database connectivity is all right (see Check Sample Scheduler database connectivity on page 72).

Some errors can be solved by following one of the procedures described in **Configure Firewall for SQL Server** on page 70.

In case of any error, you may refer to the logs generated by the application to understand the reason and perform a corrective action.

Logs are available in the %ProgramData%\Agilent\

Sample Scheduler for OpenLab\Logs folder.

- Command blocked in the LIMS Commands folder or trashed: Agilent.Scheduler.Lims.Agent.<ti>timestamp>.log.
- Acquisition not managed properly:
 Agilent.Scheduler.AgentCore.
 Agilent.Scheduler.Acquisition.AgentCore.
 InstrumentID>.
 timestamp>.log
- Display issue in Scheduler interface:
 Agilent.OpenLab.Scheduler.Client.
- Display issues in Sample Scheduler web interface: Agilent.Scheduler.WebserverService.<timestamp>.log

For details on how the logs are produced, refer to Activity Logs on page 134.

Core Engine Service does not Start

Core Engine Service does not Start

Without the Database Management Service, the following Sample Scheduler services are unable to start:

- · Agilent Sample Scheduler agent
- Agilent Sample Scheduler LIMS agent
- Agilent Sample Scheduler Orchestrator
- Agilent Sample Scheduler Webserver

Both Sample Scheduler services do not start

When the service (Agilent Sample Scheduler agent or Agilent Sample Scheduler LIMS agent) is stopped and cannot be started, with an error listed in the logs, check that:

- the Enterprise path is properly configured in the OpenLab system, and is reachable (that is: No network communication issue). If it is not the case, contact the CDS administrator to solve the issue.
- the user configured in the Sample Scheduler configuration/Maintenance/ Update OpenLab Services Credentials screen has privileges to use all instruments and all projects to be managed by the Sample Scheduler.
- · the Sample Scheduler Webserver is running.

Sample Scheduler agent service does not start

When several Scheduler agents are installed, one or more instruments must be assigned to each agent. If one Scheduler agent has no instrument assigned, the agent automatically stops.

In this case, open the Sample Scheduler configuration, go to Instrument management, and ensure that the agent manages at least one instrument.

14 Troubleshooting

Core Engine Service does not Start

Acquisition agent does not start

If the acquisition agent does not start and is shown red in the configuration, it is possible that the instrument is not properly configured in the Control Panel. Configure the instrument.

XML Command Management

XML Command Management

Command file got stuck in the LIMS_Commands folder

When commands are blocked in the LIMS_Commands folder, check that the Agilent Sample Scheduler LIMS agent is started. If it is not the case, start it. If it automatically stops again, read the Agilent.Scheduler.Lims.Agent.<ti>timestamp>.log to understand the reason.

Command File is not Archived in the Processed **Folder**

Check that the processed folder defined in the Sample Scheduler configuration exists. If that is not the case, create it.

Command is rejected in the trash folder

Check the Agilent.Scheduler.Lims.Agent.<timestamp>.log stored in the %ProgramData%\Agilent\Sample Scheduler for OpenLab\Logs folder located on the computer where the LIMS agent is installed. The root cause likely is an invalid value, a syntax error, or the absence of a mandatory parameter.

Missing LIMS Database Notification on Successful Command Processing

Unable to notify LIMS database

You may have defined SQL queries in the Sample Scheduler configuration in order to notify the LIMS database about a command that has been handled. If a momentary loss of connection occurs, the LIMS database is not notified. The Sample Scheduler could handle again the same command, then trash it as it detects an analysis with the same name already exists.

In this case you get the following message in the LIMS agent log:

```
| Info | Notifying LIMS database for VALID command Id 3...
```

 \mid Warn \mid Unexpected result while notifying LIMS database on try 1/5

...

| Warn | Unable to notify LIMS database, connection state is 'Closed'

| Warn | Delete Analysis - no analysis found in the database

| Warn | Try to reopen 'Closed' LIMS database connection...

| Warn | Unexpected result while notifying LIMS database on try 2/5

...

[|] Warn | Unable to notify LIMS database,

^{&#}x27;System.Data.SqlClient.SqlException' occurred with message 'A transportlevel error has occurred when sending the request to the server. (Provider: TCP Provider, error: 0 - An existing connection was forcibly closed by the remote host.)'.

The SQL query cannot update the command in the LIMS database

You may have defined SQL queries in the Sample Scheduler configuration to notify the LIMS database about a command has been handled. The Sample Scheduler is expected to update the command in the LIMS database. In some cases, the update could fail (note that five update attempts are performed). The following message is displayed in the LIMS agent log:

```
| Info | Notifying LIMS database for VALID command Id 1...
```

| Warn | Notification has been successfully sent to LIMS database but no row was affected.

```
| Warn | Unexpected result while notifying LIMS database on try 1/5
```

 \mid Warn \mid Notification has been successfully sent to LIMS database but no row was affected.

```
| Warn | Unexpected result while notifying LIMS database on try 2/5
```

| Warn | Notification has been successfully sent to LIMS database but no row was affected.

```
| Warn | Unexpected result while notifying LIMS database on try 3/5
```

| Warn | Notification has been successfully sent to LIMS database but no row was affected.

```
| Warn | Unexpected result while notifying LIMS database on try 4/5
```

| Warn | Notification has been successfully sent to LIMS database but no row was affected.

| Warn | Unexpected result while notifying LIMS database on try 5/5

Import of XML files fails although they are valid

If the number of licenses is insufficient, all attempts to import XML files will be trashed when the XML-based LIMS agent starts. Check if number of LIMS connection licenses is the same or more than the number of LIMS connections specified in the Sample Scheduler configuration. Add the required number of licenses before you restart the import.

Analysis got Stuck During Life Cycle

Analysis stays in Scheduled state

- Check that the instrument on which the analysis is launched is assigned to a
 Sample Scheduler agent in Scheduler configuration/Instrument management.
 If it is not the case, assign it to a Sample Scheduler agent, then restart the
 corresponding Scheduler agent in the Sample Scheduler configuration/
 Deployment tab. If the analysis still not starts, end the AcquisitionServer.exe
 (OpenLab CDS service) in the task manager, to release the connection with
 the instrument.
- Check that the user defined in the OpenLab services credentials in the Sample Scheduler configuration still exists in the Control Panel and that he has the privilege to use the instrument and the project on which the analysis is launched. If it is not the case, update the credentials with a user who can access all relevant instruments and projects to perform analyses with Sample Scheduler.

Analysis stays in Submitted state

Before starting an analysis, the Sample Scheduler acquisition agent checks for the instrument license and uses it during operation. If an analysis stays in **Submitted** state, check that an *Agilent OpenLab Sample Scheduler Expansion Pack* license is available. In the web browser, insert the following address: http://<name of the License Server>:8090.

If no license is available (because the instrument is currently running), the Sample Scheduler acquisition agent tries to obtain a license in a loop (in a time interval of 30 seconds). After 15 attempts the analysis turns into the **Error** state.

The users defined in the **Notification** tab will be informed about the missing license (by email and/or on the Notification screen of the Sample Scheduler client).

Analysis got Stuck During Life Cycle

Analysis blocked in the Sample Scheduler database

When an analysis is blocked in the Sample Scheduler database, connect to the Scheduler client, select the analysis, and click **Reset**. To be able to reset the analysis, you need the privilege **Reset analysis**. The analysis will be either turned into **Error** or **Waiting** state (according to its state while it was stuck in the database).

Analysis turns into Error/Waiting on Error

Analysis turns into Error/Waiting on Error

Analysis turns into error after having been stopped from the CDS

When an analysis running in the Sample Scheduler is stopped via the CDS, it turns into Error state in the Scheduler. Then the other scheduled analyses on the same instrument turn into Waiting on error state. The Scheduler is not informed that the acquisition has been stopped from the CDS; it is only informed that the acquisition didn't go up to the end, which is an abnormal behavior from its point of view

Reschedule the analyses that have been put into Waiting on error state. To avoid this error, do not stop an acquisition via the CDS that has been launched from the Sample Scheduler.

Analysis passes from Scheduled to Error or Waiting on Error state

When an analysis passes from **Scheduled** to **Error** or **Waiting on error** state, it can be due to an instrument error, a connection issue between Sample Scheduler and OpenLab CDS. You can access the reason of the error in the Sample Scheduler client by clicking the **State** cell of the **Error** analysis. A message extracted from Sample Scheduler logs and the OpenLab system logs is displayed explaining the reason why the analysis turned into Error.

Client or configuration connection issues

If you get the User is not authenticated message when connecting either to the Sample Scheduler client or Sample Scheduler configuration, check that the user name still exists in the Control Panel and that the password is correct.

14 Troubleshooting

Analysis turns into Error/Waiting on Error

If you get the **User 'Username' is not administrator** message when connecting to Sample Scheduler configuration, check that the user has the **Is an administrator** (Sample Scheduler) privilege in the Control Panel under **Administration**.

Analyses are not displayed in the Sample Scheduler client

The user connected to the Sample Scheduler client can only see the analyses launched on the instruments/projects he has access to.

If the user access privileges have been modified in the Control Panel (allow the user to use an instrument and/or project) while a Sample Scheduler client session is still open, the changes are not considered. The user cannot see the analysis associated with the new instrument/project in the Sample Scheduler client. The OpenLab user instruments/projects access privileges are loaded only at the Sample Scheduler client opening. To load the new instruments/projects access privileges, close and reopen the Sample Scheduler client. The analyses will be visible

Loss of connection

A loss of connection can be caused by database, network related or instance specific errors.

When the message box Agilent Sample Scheduler Client (or Configuration) has stopped working shows up, you may have lost the connection with the Sample Scheduler database. Verify if the connection mode and /or the credentials have been modified. Please read the Agilent.OpenLab.Scheduler.Client, or Agilent.OpenLab.Scheduler.Configuration logs for more information. If analyses were running, they will be turned into the Error state. The corresponding Scheduler agent log will show the message Impossible to update agent instance Computer name: ComputerName, agent Id: scheduler agent.....

For more information about changing these parameters on the SQL Server, refer to the sections of Switch SQL server authentication mode on page 61 and Edit or add system administrator on page 64.

14 Troubleshooting

Analysis turns into Error/Waiting on Error

Critical error when saving configuration

When getting the following critical error on saving configuration: Configuration value could not be modified in database, and no connection is established to the database (Not connecting message in the status bar), check that the connection mode and the credentials have not been modified for Sample Scheduler database. For SQL Server, refer to Switch SQL server authentication mode on page 61 and Edit or add system administrator on page 64.

14

Impossible to Start Sample Scheduler Services

When you cannot start either the Sample Scheduler LIMS agent service or the Sample Scheduler agent service, and you get

the Invalid OpenLab Authentication Ticket message in the corresponding log file:

- 1 Check if the ticket is correct:
 - a Open the Sample Scheduler configuration
 Maintenance/ Update OpenLab Services Credentials, define the credentials and click Save.
 - **b** Start again the Sample Scheduler agent service or Sample Scheduler LIMS agent service.
 - **c** If it still does not start, and OpenLab is configured in *Windows domain* authentication mode, perform step 2.
- 2 Check on all computers where either a Sample Scheduler agent or a Sample Scheduler LIMS agent is installed that the Shared Services are defined by their IP or as: ComputerName.DNSdomain (for example, MyComputerName.mydomain.com). If it is not the case, modify them.
 Open Shared Services Maintenance > Server settings > Add server. Define the correct server, and set this server as default.

Multiple Main Instances in an Enterprise Topology

Multiple Main Instances in an Enterprise Topology

In some instances of load balanced system or scalable Enterprise topologies with multiple servers (CM2/CM3/Index servers), the **Deployment** screen may show multiple instances of the following Sample Scheduler services:

- Scheduler LIMS agent
- Scheduler Webserver

This may happen when the load balancer is configured as the primary OpenLab Shared Services (OLSS) server on multiple servers.

For proper usage of Sample Scheduler, activate the services on the active OpenLab Shared Services server only. Deactivate them on all other servers.

Dashboard Does Not Open After Reinstallation With New Database

Dashboard Does Not Open After Reinstallation With New Database

If you have already opened a Sample Scheduler session before an upgrade, data is cached within the browser session.

This prevents login after upgrade. Empty the browser cache after upgrading.

15 Appendix A: Parameter Mapping to CDS

Table 15: Mapping of XML Parameters used in Sample Scheduler for OpenLab, OpenLab CDS

Parameter in OpenLab CDS
SampleName
ProcessingMethod
AcquisitionMethod
Injectionsource
SampleDescription
Vial
UseMethodInjectionVolume
Volume
SampleAmount
Dilutor1
Dilutor2
Dilutor3
Dilutor4
Dilutor5
Multiplier1
Multiplier2
Multiplier3
Multiplier4
Multiplier5
Description
SampleType

Parameter in Sample Scheduler for OpenLab	Parameter in OpenLab CDS
CalibrationRuntype	CalibrationRuntype
Level	CalibrationLevel
InjectionsPerSample	InjPerVial
n/a	n/a
Datafile	n/a
SamplePrepMethodName	SamplePrepMethod
n/a	n/a
Target1	Target1
Target2	Target2
Target3	Target3
Target4	Target4
Target5	Target5
InternalStandardAmount1	InternalStandardAmount1
InternalStandardAmount2	InternalStandardAmount2
InternalStandardAmount3	InternalStandardAmount3
InternalStandardAmount4	InternalStandardAmount4
InternalStandardAmount5	InternalStandardAmount5
LimsID1	LimsID1
LimsID2	LimsID2
LimsID3	LimsID3
SampleCustomParameters	SampleCustomParameters in selected Project

16 Appendix B: Components and Features

 Table 16: Sample Scheduler installable features and included components

Feature	Included components
Sample Scheduler agent	Sample Scheduler agent service (1 per AIC) Scheduler Acquisition agent process (1 per connected instrument) Sample Scheduler Services Controller service (max. 1 per machine)
Sample Scheduler LIMS agent	Sample Scheduler LIMS agent service Sample Scheduler Services Controller service
Scheduler database	A database (SQL Server or OpenLab Data Repository) Sample Scheduler Database Management agent service Sample Scheduler Services Controller service (max. 1 per machine)
Sample Scheduler client	Sample Scheduler configuration user interface Sample Scheduler client user interface Sample Scheduler Services Controller service (max. 1 per machine)
Sample Scheduler web interface	Sample Scheduler Webserver service Sample Scheduler web interface Sample Scheduler REST API Sample Scheduler Orchestrator service

In This Book

This guide describes the requirements, installation, configuration and maintenance of the *Sample Scheduler for OpenLab* software revision 2.8.

In addition, it contains information on LIMS commands, XML structures, and troubleshooting hints.

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