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Streamline Laboratory Operations with Sample Scheduler for OpenLab

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Introduction

Many organizations face the challenge of managing analytical requests across laboratories with multiple instruments. Samples must be routed to the appropriate instrument and analyzed in a timely and accurate manner. Manually scheduling samples may result in human errors, inefficiencies, and bottlenecks. Additionally, integrating the various types of instruments with a laboratory information management system (LIMS) can be complex and costly.

Agilent Sample Scheduler for OpenLab is the ideal solution for streamlining sample analysis and managing the analytical workload of a laboratory. Sample Scheduler allows you to easily manage analyses on any networked instrument across an organization, all from a single client. Leveraging its seamless integration with Agilent OpenLab Server, Sample Scheduler provides a single, familiar interface to submit, edit, and review analyses. Lab managers, operators, and analysts can also employ a full lab overview dashboard to assess instrument status and workload from a desktop or mobile device (Figure 1).
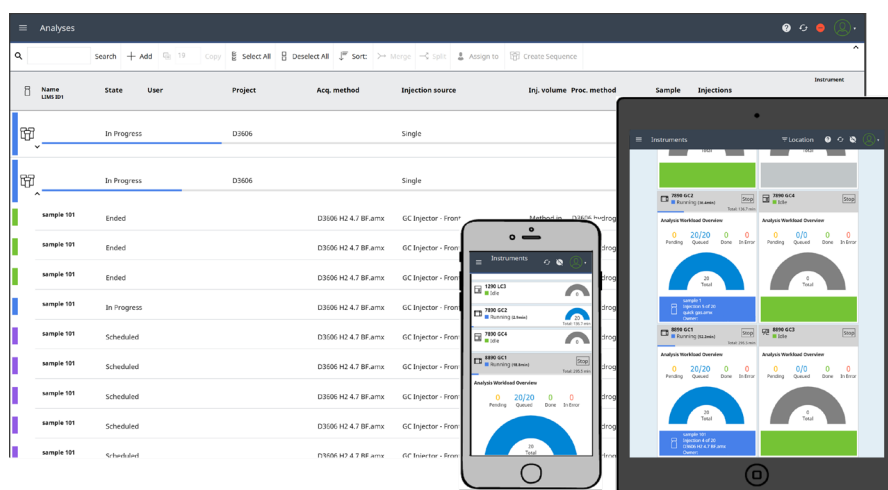

Figure 1. Agilent Sample Scheduler for OpenLab web client shown in browser and in its views on a smartphone and tablet.

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Without Sample Scheduler, a user would have to manually determine which instrument can run a particular analysis and whether that instrument is available. Then, the user would need to access the OpenLab CDS client, launch that specific instrument, and submit a sequence directly to that instrument's sequence queue. This can be cumbersome and time-consuming, especially if there are many instruments and analyses to manage. With Sample Scheduler, the user can focus on a single interface for all their sample submissions. Instruments and personnel can be assigned to specific analyses, and those instruments, along with other predetermined sample parameters, can be automatically set using the analysis autofill triggers.

Sample Scheduler for OpenLab also enables you to schedule runs directly from a LIMS, which can improve data quality and traceability. Costly and time-consuming custom integrations between an existing LIMS and the laboratory instruments are not necessary. Sample Scheduler manages the complexity of interfacing with laboratory instruments right out of the box.

A LIMS only needs to be configured to interface with Sample Scheduler to submit samples for analysis and collect the results from any instrument in OpenLab CDS. In this sense, Sample Scheduler acts as a hub between a LIMS and the instruments.

Architecture and deployment

Sample Scheduler for OpenLab can be added to an existing OpenLab Server installation with content management (Figure 2 and see appendix for compatibility). Sample Scheduler integrates with the existing OpenLab Shared Services and user privileges are configured in the control panel. All Sample Scheduler components can be installed within the existing OpenLab Server topology (Table 1). In general, the Scheduler Agent Service is always installed on the Analytical Instrument Controllers (AIC) and the Scheduler client is installed on OpenLab clients. More advanced deployments and details of each service can be found in the Sample Scheduler for OpenLab – Installation & Configuration Guide. This guide, along with other help and documentation, can be found at **https://openlab.help.agilent.com/**.
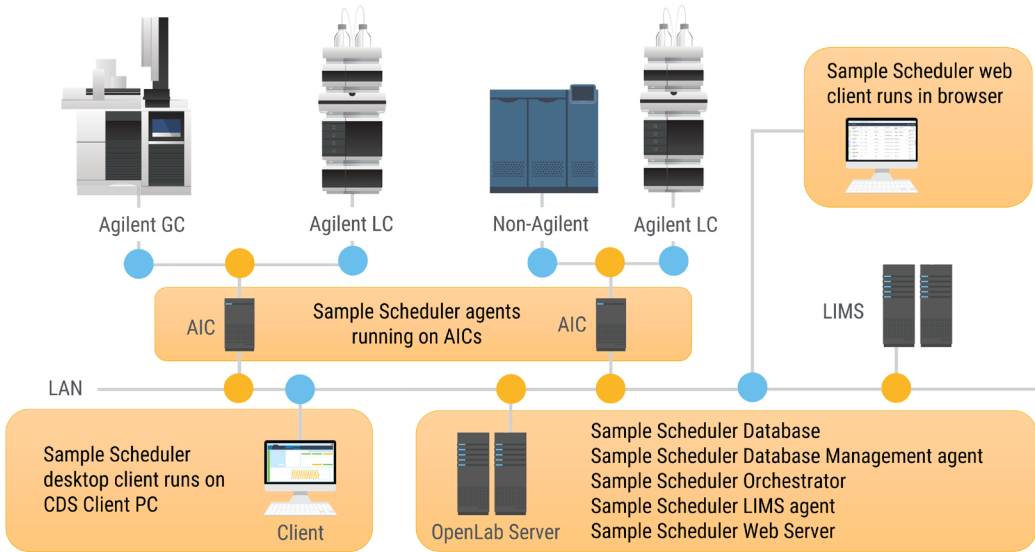

Figure 2. Sample Scheduler for OpenLab topology.

Computer	Scheduler database	Scheduler database Management agent	Scheduler LIMS agent	Scheduler agent	Scheduler client	Scheduler webserver
C1 (Server)	✓	✓	✓	-	-	✓
C2 (AIC)	-	-	-	✓	-	-
C3 (CDS Client)	-	-	-	-	✓	-

Table 1. Minimal Sample Scheduler for OpenLab deployment.

Sample Scheduler for OpenLab is composed of:

- A database
- One LIMS agent
- One or several Scheduler agents
- A webserver
- Multiple instances of the user interfaces: Sample Scheduler configuration, Sample Scheduler client, and web interfaces
- The Database Management agent
- The Sample Scheduler Orchestrator

The LIMS agent:

- Scans the folder in which the LIMS generates the commands or periodically queries the LIMS with a SQL query to retrieve an analysis requests
- Checks the commands' validity
- Transforms valid commands into analyses stored in the database and sends invalid commands into a trash folder located in the LIMS_Commands folder root and, if enabled, notifies the administrator

Scheduler agent: Several Scheduler agents can be installed (one per computer). The role of each Scheduler agent is to manage a pool of instruments.

Each Scheduler agent:

- Requests the Sample Scheduler database to know if there is an analysis to handle on one of the instruments it manages

- Requests the chromatography data system (CDS) to check the instrument license availability and its status
- Initiates an acquisition through a specific agent: the Scheduler acquisition agent (one per instrument)—This specific agent will then handle the acquisition, through the CDS acquisition process, and updates the analysis state

There are four roles available: Sample Scheduler Administrator, Sample Scheduler Analyst, Sample Scheduler Technician, and Sample Scheduler Operator. Each role has different privileges that allow them to perform different tasks related to Sample Scheduler, such as configuring, managing, preparing, and reviewing analyses and sequences. The OpenLab system administrator can edit or create roles and assign them to the Sample Scheduler users.

Interfaces

Sample Scheduler offers three interfaces for users: configuration, desktop client, and web client. The configuration interface allows the Sample Scheduler administrator to configure Sample Scheduler (e.g., LIMS commands folder path or SQL queries). The desktop client interface is a Windows application that provides full functionality for submitting, editing, and reviewing analyses (Figures 3 and 4).

The web client is a browser-based interface that can be accessed from any device with an internet connection. It provides dashboards of instruments and sample workloads,

Figure 3. Sample Scheduler desktop client analysis table edit view.

as well as the ability to create, modify, assign, prioritize, or cancel analyses (Figures 5 and 6). Both interfaces are seamlessly integrated with OpenLab CDS and share the same analysis table. The web client is ideal for users who want to monitor the status and workload of the instruments from anywhere. It also offers the flexibility to manage their sample analysis workflow in a browser.

Both the Sample Scheduler desktop client and web client can be used as interfaces for all analyses when working with a LIMS. However, these interfaces can also be ignored. With Sample Scheduler operating simply as a bridge between the LIMS and the instruments, the LIMS can manage the entire sample analysis workflow. In either case, the web dashboard can always be used to view the lab and workload.
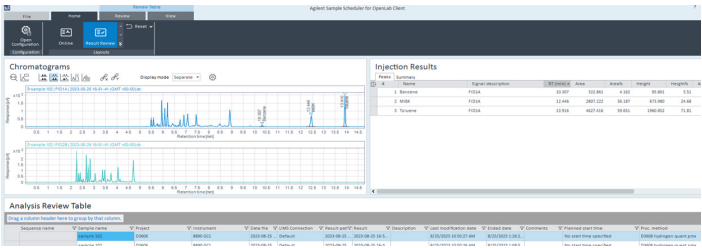

Figure 4. Sample Scheduler desktop client reviewing a completed analysis.
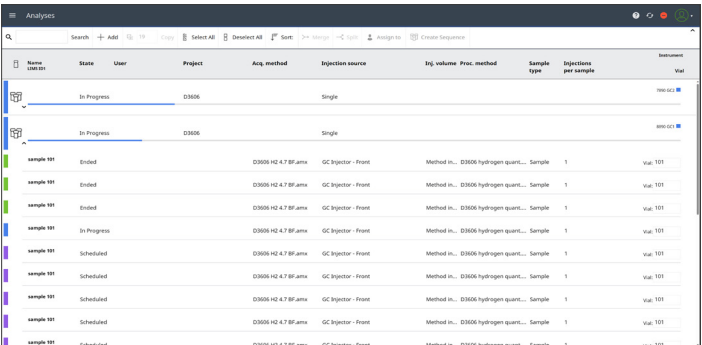

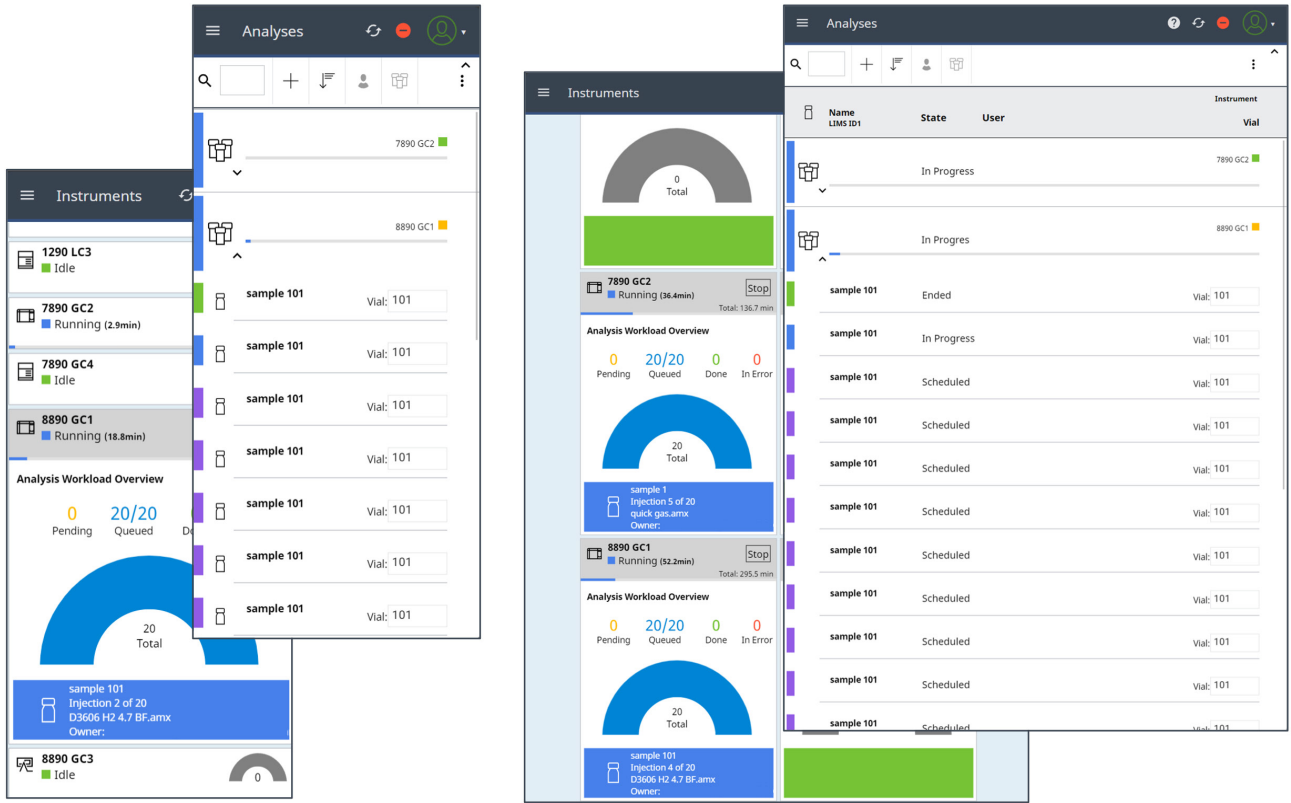**Figure 5.** Sample Scheduler web client editing an analysis.

Figure 6. Sample Scheduler web client views across smartphone and tablet.

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Bidirectional LIMS Connection

Labs often transcribe their information manually, a time-consuming, labor-intensive, and error-prone process. For example, the samples that are registered in LIMS are tagged with a LIMS ID. These LIMS IDs are manually transcribed to a CDS either in the form of sequences or single runs. The results are then manually transcribed to LIMS to be reported on the certificate of analysis. With Sample Scheduler, a bidirectional OpenLab CDS and LIMS integration means that all information is transferred electronically from LIMS to OpenLab CDS and back. This ensures a seamless and human-error-free process. This solution consists of three components: OpenLab CDS, Sample Scheduler for OpenLab, and any LIMS (Figure 7).

Sample Scheduler supports two types of LIMS:

– LIMS that can 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 Sample Scheduler

Sample Scheduler performs the following actions for both command types: collecting the command, checking its validity, and creating an analysis in the Sample Scheduler database.
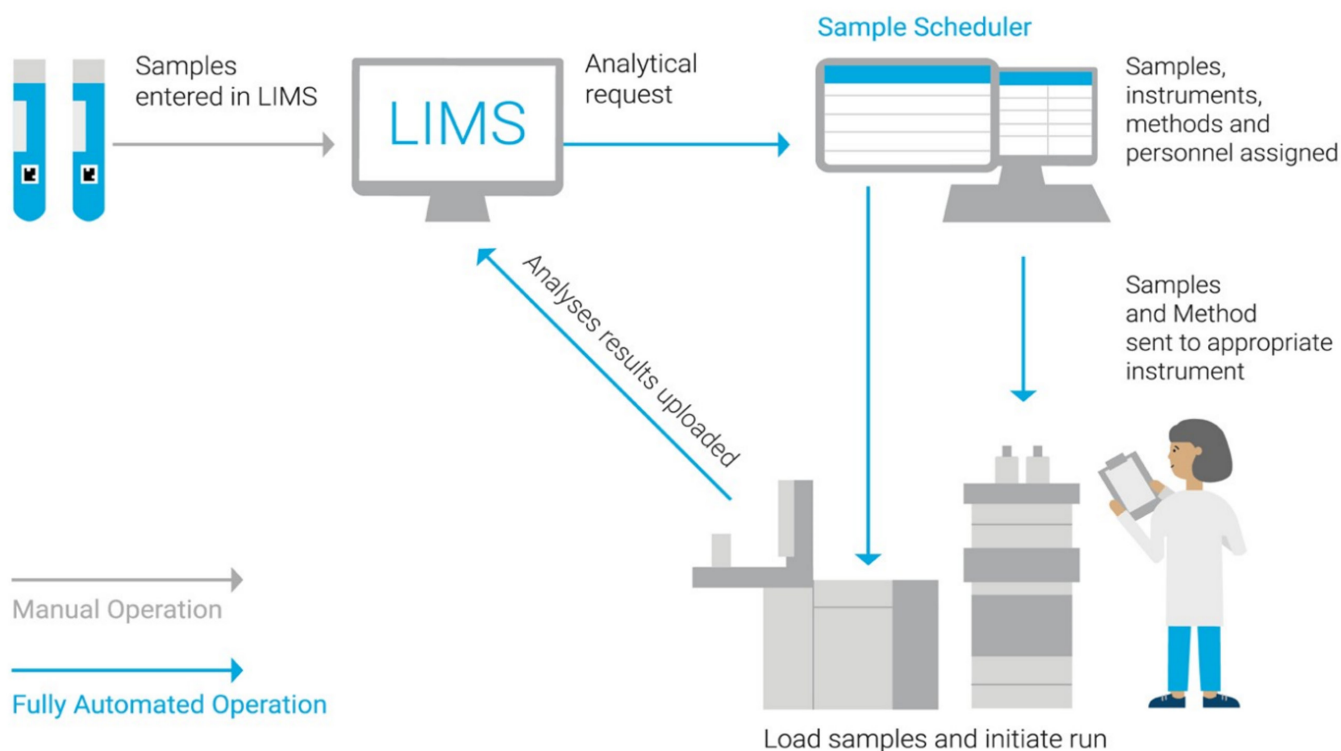

Figure 7. Sample Scheduler web client editing an analysis.

XML Commands

The structure of an XML file is defined to fit the CDS instrument/method architecture. Sample Scheduler for OpenLab manages two types of XML files: XML commands and XML actions. XML commands handle the analysis of a sample in OpenLab CDS, while XML actions initiate an action, such as deleting an analysis or creating a sequence. The XML schema are described in the Sample Scheduler for OpenLab Command Guide. The most basic XML command can be seen in Figure 8. This XML example demonstrates the minimum set of parameters that need to be defined in an XML to allow OpenLab CDS to perform the analysis. To use this command, ensure 'OpenLab default user', 'Default sample name', and 'Default result name' are assigned valid values in the Sample Scheduler configuration.

More advanced commands can be built upon the example above or built upon several other example XML files included in the Agilent Technologies/Sample Scheduler for OpenLab/Documentation/xml folder, such as: calibration samples, dual injection, and sample customer parameters.

```
                    XML commands - Basic_Command.xml
1   <SchedulerCommand>
2     <Identifier>LIMS_ID</Identifier> <!-- Sample Identifier generated by the LIMS -->
3     <Tasks>
4       <Task>
5         <InstrumentMethods>
6           <InstrumentMethod>
7             <InstrumentName>OpenLabValidInstrument</InstrumentName>
8             <!-- Valid OpenLab Instrument Name -->
9             <AcquisitionMethodName>OpenLabValidMethod.amx</AcquisitionMethodName>
10            <!-- Valid OpenLab Acquisition Method Name -->
11          </InstrumentMethod>
12        </InstrumentMethods>
13        <Towers>
14          <Tower>
15            <InjectionSource>InjectionSourceName</InjectionSource>
16            <!-- Injection Source - Front or Back -->
17            <SampleInfo>
18              <UseMethodInjectionVolume>true</UseMethodInjectionVolume>
19              <!-- Use injection volumne in acquisition method? -->
20              <Vial>1</Vial> <!-- Autosampler vial position -->
21            </SampleInfo>
22          </Tower>
23        </Towers>
24      </Task>
25    </Tasks>
26  </SchedulerCommand>
27
```

Figure 8. Minimal XML parameters required to submit a command to Sample Scheduler from a LIMS.

XML Actions

Sample Scheduler can also handle XML files that are not intended to create an analysis, but instead perform an action such as canceling an analysis or creating a sequence from a group of analyses (Figures 9 and 10).

```
            XML commands - Cancel_Experiment_Command.xml
1   <SchedulerAction>
2     <Identifier>LIMS_ID</Identifier>
3     <Type>Delete</Type>
4     <LimsConnection>ValidLIMSConnectionName</LimsConnection>
5   </SchedulerAction>
```

Figure 9. Cancel experiment XML command.

```
              XML commands - Create_Sequence_Command.xml
1   <?xml version="1.0" encoding="utf-8" ?>
2   <!-- If you do not specify the encoding, the file is treated as UTF-8 -->
3   <SchedulerCreateSequenceAction>
4     <SequenceName>MySequence</SequenceName>
5     <SequenceState>Scheduled</SequenceState>
6     <Identifier>MySequenceIdentifier</Identifier>
7     <LimsConnection>MyLimsConnection</LimsConnection>
8     <User>OpenLAB User</User>
9     <Identifiers>
10      <Identifier>MySequenceLine-1</Identifier>
11      <Identifier>MySequenceLine-2</Identifier>
12      <Identifier>MySequenceLine-3</Identifier>
13      <Identifier>MySequenceLine-4</Identifier>
14      <Identifier>MySequenceLine-5</Identifier>
15    </Identifiers>
16  </SchedulerCreateSequenceAction>
```

Figure 10. Create sequence XML command.

The "LimsConnection" parameter refers to the LIMS connection configured in the LIMS tab of the Sample Scheduler configuration. Multiple LIMS connections can be configured if needed. Included with the Sample Scheduler installer is also a tool for generating XML files (Figure 11). The XML file generator enables an administrator to generate test XML commands for setting up the Sample Scheduler system. The tool can be found on the installation media in the folder Support/Xml_tool.

Figure 11. XML tool to generate test XML files.

Command collection via SQL query

Sample Scheduler provides a generic tool to gather analysis orders from the LIMS database (that handles SQL queries). The configuration is done in the LIMS tab of the Home ribbon. Both analyses and sequences can be submitted to Sample Scheduler via SQL query. They are automatically assigned the LIMS connection from the configured LIMS database. As all LIMS databases are different, it is up to your database system administrator to configure the parameters detailed in the Sample Scheduler for OpenLab – Installation & Configuration Guide to fit your LIMS database structure. Example SQL queries are also available in the Sample Scheduler installation directory.

Review and submit to LIMS

Sample Scheduler provides the option to wait for sample review before submitting to a LIMS. This choice can be configured in the LIMS tab of the Sample Scheduler configuration. A folder path is specified here for a LIMS to collect the processed results reports. This path must be defined on the computer where the Sample Scheduler LIMS agent is installed. Analysis results from across all connected instruments can be aggregated in a single view and the data can be individually reviewed before submission. This review screen not only shows the final results, but also allows the user to view the chromatograms via a familiar chromatogram window (Figure 12).
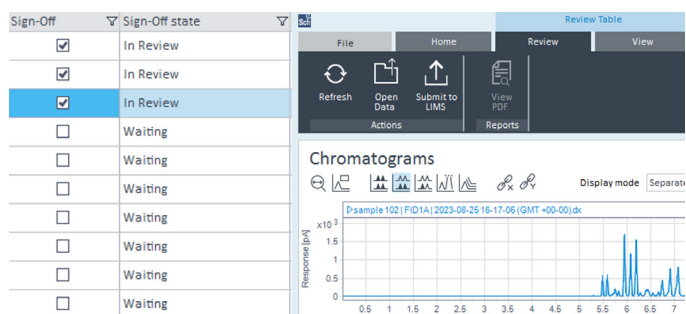

Figure 12. Results review, Sign-Off for LIMS, and Submit to LIMS.

Sample Scheduler for SLIMS

Agilent SLIMS is a laboratory information management system designed to help organize and optimize laboratory operations. Tapping into a wealth of prebuilt plug-ins and packages from the SLIMS Store, SLIMS can be quickly and easily deployed to streamline and organize your lab operations. One of the essential features of SLIMS is the Sample Scheduler submit analysis integration. Instead of using customized XML or SQL to facilitate analytical requests to Sample Scheduler, this feature handles all the communication between SLIMS and Sample Scheduler. SLIMS's core integration with OpenLab Server allows syncing of all instruments configured in OpenLab Shared Services.

Once your instances of OpenLab Server and Sample Scheduler are authenticated within SLIMS, a two-way connection is created (Figure 13). SLIMS will connect to OpenLab Shared Services and synchronize all instruments, projects, and methods (Figure 14). This information is then made available in SLIMS for submitting analysis via the Submit Sample Scheduler analytical workflow. Within this workflow, SLIMS will leverage the Sample Scheduler configuration and can automatically identify the proper instrument based on the nature of the analytical request. With this two-way connection, SLIMS is aware of the instrument status and availability (Figure 15). Finally, the results from the analysis can be uploaded to SLIMS (Figure 16). To learn more about SLIMS, visit **https://www.agilent.com/chem/slims**.
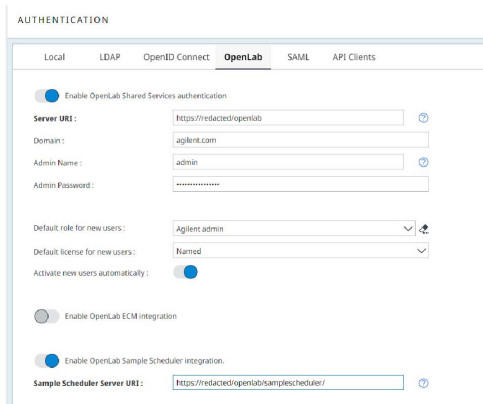

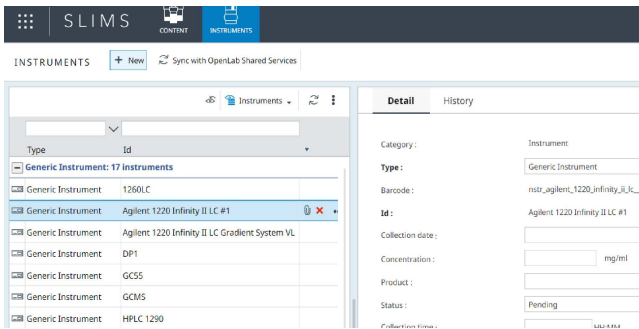**Figure 13.** Shared Services and Sample Scheduler authentication within Agilent SLIMS.

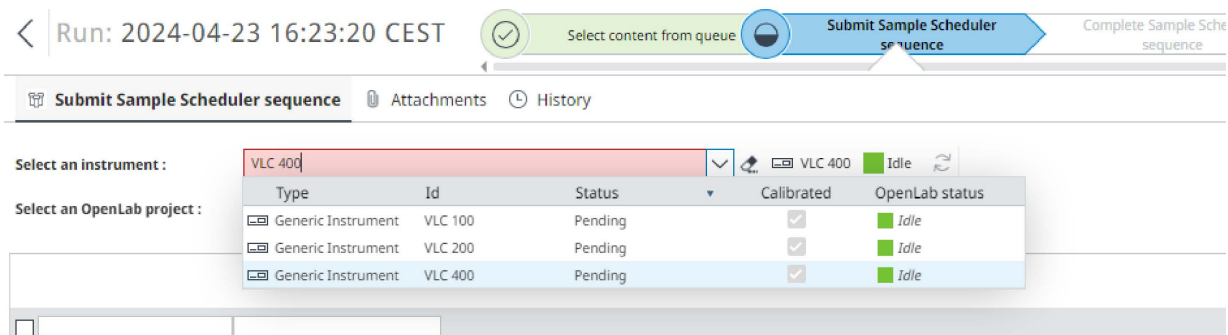**Figure 14.** Instrument synchronization within Agilent SLIMS.

Figure 15. Submit Sample Scheduler analysis workflow within Agilent SLIMS.

Content	Analyte	Area	Value	CDSLink	Value entered on	Status					
00000929	Aspirin	100	157.56 ng/ml	https://ol2003a/openlab-stora...	07/02/2025 11:56:55	Verified	Q	✓	🗑	🔗	✗
00000930	Salicylic Acid	15.92	3.03 ng/ml		07/02/2025 11:57:34	Verified					
00000930	Aspirin	84.08	133.28 ng/ml	https://ol2003a/openlab-stora...	07/02/2025 11:57:34	Verified					
00000930	Salicylic Acid	15.92	2.52 ng/ml		07/02/2025 11:57:14	Verified					
00000930	Aspirin	84.08	133.06 ng/ml	https://ol2003a/openlab-stora...	07/02/2025 11:57:14	Verified					

Figure 16. Results imported from OpenLab CDS report to Agilent SLIMS.

Conclusion

Agilent Sample Scheduler for OpenLab is a powerful application that can help streamline laboratory operations and improve productivity. It allows you to easily manage analyses on any networked instrument across an organization, all from a single client. Using its integration with Agilent OpenLab Server, it provides a single, familiar interface to submit, edit, and review analyses. Lab managers, operators, and analysts can also employ a full lab overview dashboard to assess instrument status and workload from a desktop or mobile device. Sample Scheduler for OpenLab saves time, money, and prevents transcription errors by automating the routing of sample information through your workflow. It also enables you to schedule analyses for any instrument supported in OpenLab. This means that a variety of instruments from multiple vendors can all be connected to a LIMS without the need for custom configurations to each instrument. With Sample Scheduler for OpenLab, you can focus on a single application for all your analysis submissions and information routing needs.

Appendix

OpenLab help documentation and manuals can be found at **https://openlab.help.agilent.com/**

Sample Scheduler for OpenLab version 2.7 is compatible with:

– OpenLab CDS 2.5 client/server system with a content management system

– OpenLab CDS 2.6 client/server system with a content management system

– OpenLab CDS 2.7 client/server system with a content management system

– OpenLab CDS EZChrom Edition A.04.09 or OpenLab EZChrom A.04.10*

– Distributed System with Content Management, ECM XT, ECM 3.5 Update 6, or ECM 3.6

– SLIMS 6.7, 6.8, and 6.9

– Installation on a standalone workstation is not supported

Sample Scheduler for OpenLab version 2.8 is compatible with:

– OpenLab CDS 2.7 client/server system with a content management system

– OpenLab CDS 2.8 client/server system with a content management system

– EZChrom is no longer supported

– Distributed System with Content Management, ECM XT, ECM 3.5 Update 6, ECM 3.6, or Secure Storage

– SLIMS 6.8 and 6.9

– Installation on a standalone workstation is not supported

*In an environment regulated by 21 CFR Part 11 and Annex 11, Sample Scheduler for OpenLab is only supported in combination with OpenLab CDS 2.5 or higher. A configuration with EZChrom is not supported in a regulated environment.

Mixed configurations using ECM XT or OpenLab Server are supported with OpenLab CDS versions 2.5 or 2.6 with OpenLab CDS EZChrom Edition A.04.09 or OpenLab EZChrom A.04.10.*

References

Sample Scheduler for OpenLab Revision 2.7 – Installation and Configuration Guide. *Agilent Technologies user manual*, publication number D0014638 Rev. A, **2022.**

Bidirectional LIMS and OpenLab CDS Integration with Agilent Sample Scheduler. *Agilent Technologies technical overview*, publication number 5994-3153EN, **2021**.

To learn more about Sample Scheduler for OpenLab, visit:

www.agilent.com/chem/sample-scheduler