



Sample Scheduler for OpenLab
Revision 2.6

Release Notes



Notices

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Software Revision

This guide is valid for the 2.6 revision of Agilent Sample Scheduler for OpenLab, until superseded.

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Introduction

This document provides a listing of the major feature modifications made in each release of Sample Scheduler for OpenLab software.

For our Regulated Customers

When any change is made to Agilent software, the validation status of the software needs to be re-established by the user/customer.

Whenever software is changed, a validation analysis should be conducted not just for the validation of an individual change, but also to determine the extent and impact of that change on the entire software system.

The installation of Sample Scheduler for OpenLab on a client/server system with OpenLab CDS will not alter the OpenLab CDS installation. Agilent Technologies confirms that after the installation of Sample Scheduler for OpenLab the functionality of OpenLab CDS is not adversely impacted as a result of the installation.

The transfer of information between an external system and Sample Scheduler for OpenLab needs to be configured, verified, and validated by the user/customer as per defined intended use.

1 Revision 2.6 of Sample Scheduler for OpenLab

Infrastructure

- Support for Windows 10 20H2
- Updated browser support :
 - Removed Microsoft Internet Explorer support
 - Added Microsoft Edge (Chromium based) support (minimum version 89) replacing IE

Compliance

- Renamed privilege **Is a Sample Scheduler user** to **Edit analysis** (affects only new installations)
- Allow login to Sample Scheduler web interface without Sample Scheduler privilege (viewing only)

Installation & Migration

- Integrated Sample Scheduler into the OpenLab Installer (with OpenLab CDS 2.6).
 - All Client/Server OpenLab CDS installations will include Sample Scheduler for OpenLab.
 - The database is installed into the OpenLab Data Repository (OLDR).
 - Upgrades to OpenLab CDS 2.6 will install Sample Scheduler if it was not previously installed.
 - Sample Scheduler web server is always installed on the OpenLab server
 - For Sample Scheduler upgrades the installer must be launched separately.
- Automated creation of Installation logs
- Added optional migration of older Sample Scheduler database into the OpenLab Data Repository "OLDR"
- New Sample Scheduler activation:

Revision 2.6 of Sample Scheduler for OpenLab

- All installations and upgrades require a central activation step before they can be used productively.
- This activation step is done within a browser using the Sample Scheduler web interface.
- Without activation Sample Scheduler can be used for monitoring purposes, but not for sample management (create/edit analyses, submit analyses to instruments etc.).
- Sample Scheduler installation log files are now accessible in OpenLab Control Panel under **Administration > Diagnostics**

Web Interface

- New instrument dashboard monitor function: For viewing purposes, the web interface can be accessed without Sample Scheduler privileges.
- "Transferred" state is now reflected in the web interface
- Improved user guidance with tooltips, context-sensitive online help, and additional information for novice users.
- Updated address of Sample Scheduler web interface to:
<https://<hostname>:52088/openlab/samplescheduler>
- A sequence can be created from any set of selected analyses including different sample types
- Updated sequence view:
 - Updated sequence table to enable default set of table columns. This selection can be modified and is persistent per computer and user.
 - Added input validation, to prevent users from making invalid entries while editing a sequence:
 - A wrong entry is highlighted in red (cell background color),
 - Information on the actual limits or invalid characters is provided for each field (tooltip)
 - Mandatory parameters are marked with an asterisk (*)
 - Modified parameters are marked with a bullet (•) during sequence editing.

General changes

- Opening data in OpenLab CDS 2.6 Data Analysis for reprocessing always opens in the same session of OpenLab DA if
 - The user is the same, and
 - The current DA session is not locked or busy.
- Updated Sample Scheduler **Database Access Reconfiguration Tool** to only install with the Sample Scheduler database
- Sample Scheduler for OpenLab (web interface) can be now launched directly from the Windows start menu
- New Icon in the OpenLab CDS Acquisition client to launch the Sample Scheduler for OpenLab web interface.

Licensing

- The Sample Scheduler LIMS connection license is no longer bundled with the main product. It is now available separately.

2 Revision 2.5 of Sample Scheduler for OpenLab

Infrastructure

- Support for Windows 10 1909
- Most recent browser versions of:
Google Chrome, Internet Explorer, Safari MacOS, Safari iOS

Compliance

- Audit trail logging can be enabled from the Sample Scheduler configuration.
 - By default, audit logging is disabled. Once enabled it cannot be disabled.
- Breaking a session lock in Sample Scheduler provides a confirmation dialog that unsaved changes are lost before closing the session.

Installation & Migration

- Sample Scheduler can be deployed into the OpenLab Data Repository as an alternative to a SQL server database instance.

Web Interface

- A *My Analyses* filter is added to the Start Page.
- A new **Sequence** view for viewing and editing sequences is introduced. It is opened from the **Analyses** view and displays the selected sequence.
 - In the **Sequence** view the sequence header parameters and the sequence line parameters (including custom parameters) can be edited and saved before scheduling the sequence.
- A sequence can be created by applying an OpenLab CDS sequence template to one or more analysis requests. This requires at least revision 2.5 of OpenLab CDS.

Revision 2.5 of Sample Scheduler for OpenLab

- Applying the template creates a sequence as defined by the sequence template. It adds blanks, system suitability samples, control samples, calibration samples etc. in the structure (including bracketing) and with the parameters specified in the template (methods, injection source etc.).
- Parameters that were predefined by the LIMS or a user before applying the template are not overwritten (exception: number of injections as this may conflict with bracketing).

General changes

- In order to connect to multiple LIMS instances Sample Scheduler can be configured to:
 - Receive analysis requests from more than one LIMS and route back results to the same LIMS the requests came from
 - Manage data from multiple LIMS in one Sample Scheduler database instance
 - Show and manage requests from multiple LIMS databases in a single user interface
 - Each LIMS connection requires a license
 - Per LIMS only one distinct method for submitting analysis requests is possible (either XML or SQL), not both
- Single-Sign On with Windows credentials:
 - If enabled in OpenLab control panel, the Sample Scheduler client and configuration will not request credentials on startup if the current Windows user has the appropriate privileges to access the application.

3 Revision 2.4 of Sample Scheduler for OpenLab

Infrastructure

- Support for Windows Server 2019
- Support for Windows 10 1903
- Most recent browser versions of: Google Chrome, Internet Explorer, Safari MacOS, Safari iOS
- Support of OpenLab ECM 3.5 and 3.6 backend

Support of compliant environments with OpenLab CDS

This revision is made to support users and their organizations in implementing the use of Sample Scheduler for OpenLab with OpenLab CDS in environments regulated by 21 CFR Part 11 and Annex 11.

A prerequisite for implementing Sample Scheduler for OpenLab in regulated environments is at least revision 2.4 of OpenLab CDS.

The following features were implemented:

- All relevant changes and activities are logged in the System Activity log in OpenLab Control Panel. The entries can be grouped into the following categories:
 - Automatic changes to analyses or sequences received from a LIMS (e.g. autofill, instrument groups, defaults)
 - Interactive creation of, or changes to an analysis or sequence
 - Changes to the Sample Scheduler configuration
 - Security-relevant activities such as login to or exit the application, session locking and unlocking
- Login ID is replaced by full username in areas visible to the users
- Unique identifiers for sequences (to enable audit trails)

Roles & Privileges

- Analyses can only be assigned to users that have the **Is a user (Sample Scheduler)** privilege
- Privilege to view report in the review view of the Sample Scheduler client

Installation & migration

- Scripted installation
- Upgrade installation from revision 2.0 or higher
- Updated DB migration tool includes instrument groups and notifications

Web Interface – Miscellaneous changes

- New Quick Start guide is available in the Online Help
- Full text search on all analysis parameters
- Single selection mode is now default. Multi-selection can be easily enabled/disabled as needed
- Counter for selected analyses in Multi-selection mode
- Keep the focus on visible analyses during refresh
- Interactive session lock

General changes

- Analyses cannot be assigned to an instrument that is locked in OpenLab Control Panel
- New client notification system on configuration changes (if a restart of the Sample Scheduler client is required to become effective)
- Sample Scheduler Service user requires only a minimum set of privileges

4 Revision 2.3 of Sample Scheduler for OpenLab

Time Scheduling

- Schedule single run or sequence with planned start time & date
 - At time of execution time-scheduled analyses get precedence
 - Configurable optional time buffer (in minutes) for time-scheduled analyses, where no other analysis is submitted to the instrument to ensure a timely execution

Infrastructure

- Support for SQL Server 2017
- Support for OpenLab CDS 2.4

Review View

- Contextual ribbon tab for injection results enables filtering of injection results table (display options for identified, unidentified peaks and missing compounds)

Roles & Privileges

- New Sample Scheduler roles:
 - Sample Scheduler for OpenLab Operator
 - Sample Scheduler for OpenLab Technician
- Update to existing Sample Scheduler roles (new installations only):
 - Sample Scheduler for OpenLab Administrator is only responsible for configuration tasks instead of everything
 - Sample Scheduler for OpenLab Analyst is empowered to have an administrative lab manager role

Web Interface - Sequence Support

- Analyses view lists both, single samples and sequences in the queue.
- Sequence viewing and vial editing in the Analyses View
 - Collapsed sequence: Sequence header with global parameters
 - Expanded sequence: sequence lines with line-specific parameters and vial position editor
- Sequence header and sequence line details panel (read-only)
 - Sequence Info tab for sequence headers
 - Analysis Info, Acquisition, Quantitation and Variables tab for sequence lines
 - Favorites tab for both, sequence header and lines.
- Sequence actions for sequences are: schedule, stop, wait, restart, reset and delete sequence
- The numbers shown on the start page item **Analyses Workload Overview** include sequence line counts
- The instrument queues in the Instrument view include sequence line counts
- A sequence progress bar is shown in Analyses view while the sequence is running

Web Interface - Merge & split analyses

- Merge single injections
- Split dual simultaneous injections

Web Interface – Miscellaneous changes

- Lab queue dashboard (locked state) includes sequence headers
- Sorting function to sort sequences by State, Instrument name, User, Project, None
- Bulk assignment of analyses to a user
- New action: Reset analysis or sequence in case of abnormal failure

Revision 2.3 of Sample Scheduler for OpenLab

- Autofill for adhoc samples
- Better readability of injection source in Analyses view
- Show/hide Analyses view toolbar
- Simple user interface: user only sees analyses action buttons he/she has the respective privilege for
- Stop instrument button removed from actions toolbar in Analyses view

General changes

- Priority field is continuously updated
- Token resolution for result name after merging analyses
- Ended date and last modification date displayed in local time

Improved failure resilience & house-keeping

- Minimize time in-between single runs by submitting two at a time to the instrument queue (parallel validation)
- Incompatible Scheduler Agents (wrong version) cannot be activated remotely
- Support of mixed mode projects that can link to both, OpenLab CDS 2.x and EZChrom instruments
- Housekeeping: delete old archived logfiles older than 4 weeks
- Analyses View - Provide error information for single sample analyses in Error state
- Updated DB migration tool



5 Revision 2.2 of Sample Scheduler for OpenLab

General

- Sequence creation via SQL interface:
LIMS SQL connection query supports file-less sequence submission
- Review & Submit:
Results without LIMS ID (adhoc samples) cannot be sent to LIMS
- Autofill can be applied to priority (adhoc) samples that do not come from the LIMS

Sample Scheduler Licensing

- Sample Scheduler for OpenLab now includes access to 1 LIMS and up to 10 instruments
- An Expansion Pack adds access to up to 10 additional instruments. Multiple Expansion Packs can be added
- A LIMS Expansion adds access to an additional LIMS. Multiple LIMS Expansions can be added

Instrument Groups

A new backwards compatible concept replaces the existing alternative instrument / method concept:

- Grouping of Instruments for a certain type of analysis
 - Instrument groups are defined in the Sample Scheduler configuration or by the LIMS
 - Each instrument line in a group consists of the instrument, a project, an injection source, an acquisition method and optionally a processing method
- Users can easily switch between instruments of a group before scheduling the analysis. Parameters are adjusted automatically as defined in the instrument line.
- Instrument groups can be used for single runs and sequences

Web Interface - Usability

- Start page:
 - Link to **Instrument** view filtered by selected instrument status (idle, running, error)
 - **"My instruments"** link to **Instrument** view filtered by the instruments I have scheduled or pending analyses on
- **Instrument** view:
 - Instruments can be filtered by locations defined in OpenLab Control Panel
 - The operator can see the overall queue of an instrument in addition to his own queue of analyses
- **Analysis** view:
 - Queue status at a glance: better visibility of analysis states when the user interface is locked
 - Sorting and Select all / Deselect all functions

Web Interface - Editing

- Adding new analysis requests
 - New analyses can be created using **add** or **copy** function
- User-friendly editing of all parameters from the **Analysis** details
 - Parameters are organized in five tabs:
Favorites, Analysis Info, Acquisition, Quantitation, Variables
 - Analyses in **edition** mode cannot be edited by another user
- User-specific quick access to favorite parameters (**Favorites** tab)
 - Initially populated with meaningful default parameters
 - Centrally stored and managed per user in the Sample Scheduler database
 - Favorites can be centrally defined by the administrator or by the users (based on user privileges)
 - Lab wide restriction of editable parameters for operators: restricted access to Favorites only

Supportability

- Documented upgrade procedure:
The lab can continue to work during the upgrade (non-disruptive upgrade)
 - Scheduled analyses in old database are processed
 - New analyses can be submitted by the LIMS to the new database
 - Database migration tool supports new database
- XML tool to easily create XML sets for demos or testing purposes
- Scheduler agent with no instruments assigned cannot be started

6 Revision 2.1 of Sample Scheduler for OpenLab

General

- Seeing analyses assigned to other users is protected by a new user privilege
- Increased robustness of Sample Scheduler services, if they fail to start during system startup, the system will retry the start
- See elapsed and remaining runtime of a running sample in the Sample Scheduler client to estimate when the instrument will be available again
- Sample Scheduler user matches CDS user
- The user that schedules a run in Sample Scheduler automatically becomes the user of record

Analysis Table

- For Incomplete analysis requests missing values are highlighted
- Dual simultaneous injections coming from a LIMS can be split
- The result path can be specified using tokens
- During editing the Analysis Table sorting, grouping or filtering is not applied until the user has finished editing
- A sequence marker "S" indicates that a row in the Analysis Table corresponds to a sequence
- A user can assign an unassigned analysis to himself or release an analysis that was assigned to him to other users by setting the user to "unassigned"
- Only the instruments that are assigned to a Scheduler Agent are shown in the instrument dropdown list in the Analysis Table of the Sample Scheduler client
- Use of default values for sample custom parameters as defined in OpenLab Control Panel

Result Review

- In Result Review analyses can be opened in the Data Analysis via context menu or Ribbon toolbar
- Sign-Off workflow: Results can be reviewed in the Sample Scheduler Result Review view before they are submitted to a LIMS
- Review of pdf reports in Result Review view

Configuration

- The Sample Scheduler Configuration has a new function "collect and zip local log files" to collect all Sample Scheduler client log files automatically
- Remote reconfiguration of Sample Scheduler agents from Sample Scheduler configuration (update database location and credentials)
- The Sign-off for LIMS is enabled in the Sample Scheduler configuration

Web Interface

- The Analysis view is a list view of all or a subset of single run analyses
 - The vial position of a single run analysis can be edited in Waiting state
 - All analysis and acquisition parameters of a single run can be viewed in a Details panel
 - The following actions can be applied to one or more analyses (single runs): Schedule, Wait, Restart, Stop, Stop Instrument, Delete
- The Instrument view is a concise view on all instruments and their states in the lab (lab at glance)
 - The instrument tile in collapsed mode shows: instrument name, instrument type (icon), instrument status, minimized half-circle radar
 - In "Running State" the following information is shown in addition: Elapsed runtime, expected runtime, run progress bar
 - The instrument tile in expanded mode shows an enlarged half-circle radar and a status-related colored information area with instrument status details
- From the Start page the user can navigate to a filtered queue of analyses
 - A Lab Manager Start page provides a numerical overview of the workload of all instruments in the lab and a graphical overview (half-circle radar) of the queue of analyses for the entire lab
 - An Operator Start page shows the current workload of the logged in user in a graphical overview (half-circle radar)
 - The half-circle radar graphically shows today's workload and is the access point to the daily work filtered by pending analyses that require a user action, queued analyses and analyses in error state.
- Responsive Web Design - The Sample Scheduler Web UI can be viewed on a mobile device as well as on a desktop PC

Instrument Support

- GC/MS and LC/MS support: same functionality as for GC and LC data, no SQ MS data analysis functionality in Sample Scheduler Result Review

Infrastructure Support

- SQL Server 2014 & 2016 support
- OpenLab CDS 2.2 support
- Supported configurations with Sample Scheduler for OpenLab revision 2.1:
 - OpenLAB CDS 2.1 SR1 Client Server System
 - EZChrom A.04.07 SR1 and SR2 Distributed System with Filesystem backend
 - EZChrom A.04.08 Distributed System with Filesystem backend
 - EZChrom A.04.08 Update 2 with OpenLab Server 2.1 SR1 as backend
 - OpenLAB CDS 2.2 Client Server System
 - OpenLAB CDS 2.1 SR1 Client Server System + EZChrom A.04.08 Update 2 Distributed System with a single OpenLab Server backend
 - Changes for EZChrom Users
- The following new features will become available for EZChrom users:
 - Review of results from within Sample Scheduler
 - Sample name and Sample Scheduler ID (required to maintain an analysis in Sample Scheduler and ensure uniqueness) are now separate parameters (like for OpenLAB CDS 2.x)
 - Separate sample names for front and back injection in dual simultaneous injection
 - No need to update the LIMS - support for both, old XML schema from Sample Scheduler for EZChrom A.02.0x and new XML schema from Sample Scheduler for OpenLAB 2.x
 - Merge GC front and back injection analyses in Waiting state to be executed as dual simultaneous injections
 - Splitting dual simultaneous injections that were previously merged
 - Use of multiple methods in a sequence
 - Open EZChrom data files in EZChrom Client Review Mode (only first of multiple injections)
- The following features are no longer available:
 - Quickstart is replaced by the "Add analysis" function

Revision 2.1 of Sample Scheduler for OpenLab

- Mixed Mode
 - A project is dedicated to one CDS type "EZChrom" or "OpenLab CDS"
 - New Analysis table column "CDS type" differentiates between "EZChrom" and "OpenLab CDS" analyses
 - Mixed mode is only possible with an OpenLab server backend, no Advanced File System support
 - One Shared Services backend (revision 2.1 or higher) for common user, project, instrument management etc.
 - The Sample Scheduler configuration and Sample Scheduler client can be installed and used either on an EZChrom or OpenLAB CDS client
 - The installation supports installing the Sample Scheduler components on both OpenLAB CDS and EZChrom AICs and Shared Services originating from an EZChrom or and OpenLAB CDS Distributed System

Migration

- Migration path for an EZChrom A.04.0x / Sample Scheduler A.02.0x C/S system to Sample Scheduler for OpenLab revision 2.1 and a supported CDS system

User Information

- New configuration online help is integrated into the Sample Scheduler Configuration client as HTML help
- Backup & restore procedure for SQL server database described in the Installation & Configuration Guide
- New user manual: *Guide for former Sample Scheduler for EZChrom Edition User* with mapping table of old and new XML commands and SQL queries

In This Book

The manual provides the feature updates introduced with each revision of Sample Scheduler for OpenLab

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