

OpenLab CDS Revision 2.8

**Release Notes** 

## Notices

## **Document Information**

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## **Software Revision**

This guide is valid for the 2.8 or lower revisions of Agilent OpenLab CDS software until superseded.

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# 1 Introduction

This document provides a listing of the major feature modifications made in each release of actively supported OpenLab CDS Software including selected add-ons.

Please see chapter 3, **Important Support Information** for references regarding known issues and workarounds.

## 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.

# OpenLab CDS version history

## Version 2.8

2

## Infrastructure Support updates

Workstation Plus uses **Secure Storage** as content management component. New Secure Storage privileges are provided in the Control Panel and are required for data administration and other administrative tasks.

#### Compatibility updates

See the OpenLab CDS Requirements and Supported Instruments guide (CDS\_v2.8\_Requirements\_en.pdf) for full details.

#### Added support for

- Microsoft Server 2022
- PostgreSQL 15.x<sup>1</sup> (Workstation Plus)

#### Removed support of

- Microsoft Server 2016
- PostgreSQL 14.x (Workstation Plus)
- Oracle databases for Shared Services Server.
  Please refer to the ECM XT documentation for changes in general database support.

## Maintenance, Performance and Resiliency

• Improved resiliency when load balancer switches servers: Resiliency and redundancy for client/server customers with OpenLab Server/ECM XT, ensuring operational continuity over a wider range of circumstances. See OpenLab Server/ECM XT Release Notes for more details.

<sup>&</sup>lt;sup>1</sup> OpenLab CDS uses PostgreSQL as part of the Workstation Plus product. The version and installation are determined by Agilent.

- Extend Failover Mode to support remote console access to AIC: When an AIC has lost its connection to a remote OpenLab Shared Services server, users can use remote desktop (or similar) to access the AIC and work in failover mode.
- Performance improvements for Acquisition client, Control Panel (including Activity Log search), and Search (Data Analysis)

### **Data Integrity Enhancements**

- System suitability calculations as described in USP <621> (2022) (relative S/N ratio, resolution using new formula) are available
- Record uncommitted result set changes in Activity Log: Any changes to the results, even if not saved, are recorded in the activity log, including details on what changes were made and the number of times a change was made.
- Enhanced eSignature workflow
- Support of the Authorship concept in eSignature workflows: Option to manage author's rights to sign. E.g., authors (person who modified the results) may sign the record to indicate its completeness for review]
- View Sample Prep method parameters in Data Analysis

### Installation and Backup

- New Backup and Restore tools for Workstation and Workstation Plus (not compatible with v2.7 and earlier)
- Use the Agilent "work area" on a non-default drive location
- Silent, scalable, and resilient installation options for large systems (100 1000+).

#### Language support and Online Help updates

- Online help and selected manuals are available in Korean language from OpenLab Help & Learning (agilent.com)
- Remove Russian from supported languages

## Product-Level Changes for v2.8

## Acquisition updates

Sequence and Single sample usability enhancements

- Support for Agilent LC Sequence override
  - Specific parameters defined in the acquisition method relative to pump and column compartment modules may be overwritten from the sequence table. These parameters are used to perform injections. Requires LC driver v3.7 or greater.
- Enhanced validation of Sequence and Single Sample Parameters
  - New option in Control Panel to validate sequence and/or single sample against specified acquisition method. Modes offered are:
    - On fly: invalid values are highlighted as entered by the user
    - On submit: invalid value prevents sequence submission
    - On demand: User is informed, on demand, when a newer version of the acquisition method used in a pending editing sequence is available. Method is not updated.
- Support to copy/paste sequence lines to and from Excel-like spread-sheets (e.g from LIMS)

Run Queue usability enhancements

- Pause functionality in runs is extended to allow user to choose
  - Pause after current injection (replicates pause after the current one) / as soon as technically feasible -OR-
  - Pause after current sample/line (after all replicates are done)
- Sample name and location (vial number) columns available in run queue
- Columns shown in run queue are user-selectable
- Sequences with aborted injections are tagged in the Run Queue. The total number of aborted injections in a running or completed sequence is available to the user.
- Results are uploaded during *post run* state. Single result sets or the data from each injection of a sequence is processed and uploaded directly after data collection.
- Users can open and view completed result sets in DA while instrument is in *post run* state.

Upload/download the injector program from Sample Prep Method window

• Option in the Sample **Prep Method** window to load sample prep settings from an instrument or download method settings to the instrument.

#### Ad Hoc Mode Enhancements

- New Ad Hoc mode button in layout ribbon bar switches to Ad Hoc mode window
- Options to specify a processing method and to override the printer specified in the processing method with a different one during Ad Hoc mode (instrument initiated) runs

#### ACQ Diagnostics improvements

- Process ID is included in the log entry in the log file
- Option to set the **Verbose** log only on a selected instrument, rather than to all instruments configured on the same AIC.

## Data Analysis updates

MS Spectral Deconvolution for LCMS SQ Data.

The **MS Spectral Deconvolution** feature mirrors the functionality of OpenLab ChemStation with multiple enhancements: Automatic Deconvolution, a new spectral deconvolution results table, and support for an m/z range. Deconvolution can be run for multiple MS Spectra run one at a time. Optional Automatic deconvolution can process data automatically - no need for processing each injection separately. The algorithm is optimized for Agilent unitmass instruments. It provides molecular weight confirmation for large biomolecules. The algorithm is optimized for Agilent unitmass instruments. Manual deconvolution allows deconvolution on an EIC signal.

- New **Spectral Deconvolution Layout** provided with contains the following set of windows for the MS Spectral Deconvolution workflow:
  - Chromatograms Existing Chromatograms window,
  - MS Spectrum Existing window, with new ability to use an m/z range,
  - Components (NEW) shows the mass of each component
  - Deconvoluted Ion Sets- (NEW) shows the ion distribution in separate and overlaid mode

- Spectral Deconvolution Results (NEW) lists the components detected in the spectra of the focused injection. Table is configurable and may be filtered by custom filters (e.g., signal name, RT, component, or mass). Custom filters are retained for each user.
- LC/MS Spectral Deconvolution processing method provides the spectral deconvolution parameters. The processing method parameters are easy to optimize
- New privileges for MS Spectral Deconvolution functionality available in Control Panel.
- Note: MS Spectral Deconvolution is an optional capability and requires a user license. A license is required for all users creating new deconvolution results (using a manual or automated process). Unattended deconvolution, i.e., as part of a sequence, requires one feature license only. Users can view and approve spectral deconvolution data and view and edit the MS Spectral Deconvolution method parameters inside the processing method without consuming a spectral deconvolution user license.

Integrator improvements for Large Molecule Separations (Enhanced ChemStation integrator)

Improved usability and handling of badly separated or wide peaks and noisy signals as common in Biopharma ion exchange applications. Ensures robust and reproducible results for the main compound and impurities.

- New Gaussian Shoulder/Riders Mode allows more robust integration for wide, poorly separated peaks.
- New Peak Cluster time event allows to allocate a common baseline for a range of badly separated peaks (e.g., in UV-vis workflows for monoclonal antibodies)
- Advanced+ baseline Correction mode minimizes drop shoulders for poorly resolved peaks

#### Integration Optimizer updates

New features in the Integration Optimizer to more effectively auto-integrate chromatography with overlapping peaks. This includes

- Improved workflow for shoulders and rider peaks, provides support for
  - New shoulder Mode: Gaussian Skim (supplements (New) Exponential Skim)
  - New Peak Cluster time event

- Support for Advanced+ baseline Correction mode
- Easily define a common baseline
- Option to choose between area reject and height reject (ChemStation integrator) to allow for excluding peaks by area and determine the area reject value.

Enhanced Calibration and Quantification

- Support of Corrected amount for ESTD and ISTD in Sequence/Compound amounts:
  - New option to set compound multiplier (for purity) and dilution factors to correct the amounts in either the sequence (Acquisition) OR injection list (Data Analysis) tables.
  - The calibration curve is based on the calculated concentrations.
- New option to copy compound and calibration data to another method allows to reuse calibration information in different processing methods.

Enhanced MS Smoothing and Blank subtraction

- Blank Subtraction support for MS data, including ion chromatograms (includes TIC SCAN, TIC SIM, and EICs) to remove noise from the signal.
- Change in the way Gaussian Smoothing of Profile Data settings are applied to the data – updated settings (e.g., width, on/off) are now only applied to new spectra extracted after the change to the method. This change applies to both manual spectral extraction and spectra extracted automatically as part of the processing method. Reprocessing no longer affects the smoothing of spectra previously extracted manually.
- Updated equidistancing algorithm to reduce splining for MS data collected under certain conditions (i.e., low frequency data). The equidistancing algorithm is used as part of chromatographic smoothing for MS data (*Gaussian* and *Moving Average* only), spectral smoothing for MS data, Blank subtraction for MS data (new) and MS Signal Alignment.
   Note: There may be nominal changes to the calculated area of peaks with the updated chromatographic smoothing algorithm when reprocessing data from previous versions.

Import and Export data

- Users with the new **Import raw data** privilege for importing AIA may import data (\*.cdf files) from other CDS software with a compatible data format. AIA standard format is used for exchanging data between CDS.
- Option to import the compound names, retention times, relative retention times, response factors, calibration level amounts from a CSV file or a library

**Note:** Data providence of any AIA file prior to importing into OpenLab CDS cannot be guaranteed and is the responsibility of the Lab to ensure good lab practices.

- Enable export of UV and MS spectrum into .csv file, or export of a calibration curve to an image or clipboard.
- New options for AIA export: Save the file in the result set folder, customize the file name with free text and tokens, and overwrite an existing file.

Enhanced Injection List / Review

- Enhanced precision of displayed value
- Injection list allows to show / hide additional parameters
- Enhance navigation when a compound is selected in the injection list (compound calibration and compound spectra tables in the method and in the compound amount tab in the Injection list)

Enhanced Sample Preparation Methods

- Sample Prep parameters are visible in Data Analysis, and can be reported and printed
- Sample Prep Setpoints are stored with data and are accessible for SDK automation

Extended Data Analysis log

• Available and selected result set version is included into log.

Other MS enhancements

- Reporting and printing of manually extracted MS spectra and associated deconvolution and NIST results
- Support for NIST23 library and associated MS Search

## Reporting / Report Template Editor updates

New barcode snippets

• For QR code and Data Matrix ECC200: Any expression that meets the barcode type requirements will be displayed as barcode or QR in the report

Option to report manually extracted spectra

- Supports UV as well as MS spectra
- Supports multiple manual spectra per peak
- report the manual spectrum in addition to the (default) apex spectrum for a given peak
- New option in report template properties: **Report manual spectra outside a peak** (all spectra snippets)
  - Peak\_RetentionTime is set to the extraction time
  - New dynamic field PEAK\_IS\_VIRTUAL\_SPECTRUMPEAK to filter for these special peaks

#### New MS spectra options

- New option for mass peak labeling: **Simplified mass peak labels** improves visual spectra comparison e.g., for forensics applications
- New option to label only n-largest mass peaks: Supported by all MS spectra snippets except MS Library search and MS deconvolution snippets
- New default template: MS\_Deconvolution\_Short.rdl for reporting of Deconvolution results
- MS Library Search Snippets:
  - New Graphical Only Zoomed snippet allows to zoom MS spectra in % of max abundance
  - New option allows scaling MS spectra in absolute abundance
  - MS library search snippets use same plot control as other MS Spectra
  - Peaks w/o Library search results are no longer reported

Updated or new snippets

- New **MS Deconvolution** Snippets: 5 new snippets to report MS Deconvolution results, including:
  - Deconvoluted MS spectrum plot: Supports shading of m/z range if enabled in deconvolution parameters in the processing method

- Components graph
- Molecular weight table
- Detailed component results table
- Ion sets overlaid or separated
- Updated calibration curve snippets
  - Included both RF definitions on same template
  - Simplified Axis annotation and scaling, and new Axis labels and Axis Scales properties
- Updated fraction collection snippets
  - New **end delay time** allows for variable delay times due to flow gradient setup.

Miscellaneous Reporting changes

- Option to export report header into XLSX file
- Option to display and group recovery fractions in fractions results table
- New icon for "Chart" snippets to better distinguish from MS spectra snippets
- Keyboard shortcut (Ctrl-F5) to refresh the report preview
- Configurable legend text for reference chromatograms
- New dynamic **PEAK** level fields for MS spectra & related result reporting allow to filter-out unwanted spectra and associated results
- Device name in method override parameters snippet
- Hierarchical list of LC instrument modules with sub-modules

## Data System Migration (EZChrom and ChemStation)

Enhanced support to migrate OpenLab ChemStation and OpenLab EZChrom methods into OpenLab CDS.

- Added abilities when retrieving the original result set version of migrated data.
  - Retrieve original version: option to create EZChrom and ChemStation version when opening data
- Import and display manual integration fixes and events (EZ/CS)

## Sample Scheduler for OpenLab integration with CDS

OpenLab CDS package contains the installable for **Sample Scheduler for OpenLab** revision 2.8. See separate Release Notes for details.

#### Instrument control

Extended support for Prep LC systems

- Support pump flow gradients in connection with LC driver 3.4 or higher: option to specify a pump flow gradient to speed up flushing of the columns
- Sample Prep settings used to acquire a sample may be seen in the Data Analysis component

#### LC Driver updates :

- LC Sequence override: supports, with LC driver 3.7 or higher, the ability to override Flowrate, Column Position, Column Temperature, and initial solvent composition as part of the sequence.
- Added Option for Sharing Anonymous Usage Data With Agilent to opt in for Agilent Improvement Program

#### GC driver updates

- Updated Method Resolution Wizard (MRW) in GC Driver
- Access to instrument hosted pages from CDS clients: Enables the use of the existing instrument browser user interface capabilities of the 8890, 8860, and 9000 GC's in OpenLab CDS. Users can use a browser from any system in the network to access instrument pages for an instrument that is hosted on an AIC or Workstation or Workstation Plus

Support of version 1.2 of the 2D-LC Data Analysis Add-On

Provides support for 3D analysis and advanced 2D features such as signal processing enhancements.

RC.NET Instrument Driver	Driver Software Revision	Installed by default
Agilent LC & CE	3.7	•
Agilent LC/MS SQ	3.0	•
Agilent ELSD	1.8	
Agilent GC	4.0	•
Agilent 7697A-8697 Headspace	4.0	
Agilent GC/MS SQ	1.5	•
Agilent Micro GC	2.4	
Agilent Gas Analyzer	2.8	
Agilent G1888 Headspace	01.09	
Agilent 35900E A/D Converter	2.4	•
Agilent SS420X A/D Converter	1.2	•
Agilent Data Player	2.5	•
Agilent CTC PAL 3	2.7	
Agilent CTC PALxt	1.08	

Agilent Instrument driver packages shipped with OpenLab CDS 2.8:

See the OpenLab CDS media for more details on final component versions.

## **Non-Agilent Instrument Control Drivers**

Support for non-Agilent instruments in OpenLab CDS continues to expand.

For the most current list of supported non-Agilent instruments visit the FAQ page *"What instruments are supported in OpenLab CDS?"* on the Agilent website www.agilent.com.

## Compatibility updates with Agilent Software versions

Shipped with OpenLab CDS	Version	Comment
OpenLab Server / ECM XT	2.8	Secure Storage as content management component
Test Services	3.6	
Sample Scheduler for OpenLab	2.8	Installed by OpenLab Installer, requires activation
Add-on Independent releases	Package version	Comment
OpenLab Shared Services Server	3.7	with ECM 3.x deployments only
RTL Wizard	4.0	part of GC driver package
GPC/SEC Software for OpenLab CDS	1.7	
Peak Evaluation	4.0	part of GC driver package
Match Compare	A.01.03.5	
NGA-RGA	2.8	

OpenLab CDS 2.8 is prepared to support current and/or future versions of the following Agilent products. See the respective product release notes for more information on the required versions!

Independent releases	Comment
Allotrope ADFExport for	
OpenLab 1.4	Check the respective product documentation
WalkUp v4.3	for the required compatible version. Previous versions might require
Data Analysis 2D-LC v1.2	uninstallation.
Online LC monitoring 1.3	Agilent multisampler with integrated bar- code reader
SLIMS	Check SLIMS documentation for supported
	versions

## Version 2.7

## Infrastructure Support updates

See the OpenLab CDS Requirements and Supported Instruments guide (CDS\_v2.7\_Requirements\_en.pdf) for full details.

### Compatibility updates

Added Support for:

- Windows 11 (64-bit): 21H2 (Enterprise or Professional)
- Windows 10 (64-bit): 20H2 or greater (Enterprise or Professional)<sup>2</sup>
- OpenLab Server/ECM XT 2.7, includes Basic Server product
- .NET 4.8 (minimum required) .NET 6.0 (installed by default without removing previous versions)
- PostgreSQL 14.1 (Shared Services, Content Management, and Data Repository)
- Amazon Web Services (AWS): Tested releases until April 2022
- Microsoft Azure: Tested releases until April 2022

Removed support of

- Windows 10 (P + E) 2004 and 20H1, and Windows 10 (E) 1909
- Oracle 18C, SQL 2014
- Internet Explorer

<sup>&</sup>lt;sup>2</sup> For support of LTSC/LTSB check FAQ on OpenLab CDS product page:

https://www.agilent.com/en/support/software-informatics/analytical-software-suite/chromatography-data-systems/openlab-cds/faq-openlab-cds-ltsc

## Reduced number of firewall ports required open to run an OpenLab CDS + OpenLab Server/ ECM XT system

With the release of CDS v2.7 and Server/ECM XT 2.7, communication between various OpenLab Components is moving towards well accepted standard ports 443 (TLS) and 80. See the OpenLab CDS Requirements Guide for full details on the required ports.

**Note**: These changes only apply to OpenLab components version 2.7 or greater. OpenLab Server/ ECM XT 2.7 maintains backwards compatibility with previous versions of CDS. The communication requirements for use with these versions are documented in the respective Requirement guides.

## Compatibility with Agilent Software versions

Note: These are independent releases

- OpenLab Server / ECM XT v2.7
- Sample Scheduler for OpenLab v2.7
- OpenLab Shared Services Server 3.6 (with ECM 3.x deployments only)
- Test Services v3.5
- WalkUp 4.2
- RTL Wizard 3.7.x
- NGA-RGA 2.7
- GPC/SEC Software for OpenLab CDS v1.6
- Peak Evaluation 3.7.x
- Allotrope ADFExport for OpenLab v1.3.1

Compatibility prepared for the subsequent product versions that will release after OpenLab CDS 2.7 (see the respective release notes for detail):

- EZChrom Migration
- SLIMS
- Match compare
- 2D-LC
- Online LC monitoring

## **Data Integrity Enhancements**

Standardized display of usernames with user-ID

• Usernames are displayed in the format **Full Name (userid)** in all OpenLab CDS applications, audit trails and activity logs

Improved Audit Trail

- For methods and cc files, reviewing or adding a manual entry to the audit trail does not trigger a new version.
- Audit trail logs a 'Saved method' event if a processing method gets linked to a result set or if a master method is updated.
- File type is provided in the audit trail header
- Rollback of changes in method is logged in audit trail (without updates of method version)

Sample Prep method (.smx) is now saved with results and can be included in a report

Improved traceability when exiting Failover mode:

• Change of username from general (System) to machine name of AIC for activity log entries when reconnecting to system.

## Enhanced OpenLab installer

Usability enhancements

- System Preparation Tool (SPT) launched automatically during installation.
- Option to navigate between launcher tabs using key "Tab" and "Shift+Tab"; "Enter" or "Space" to select the tab
- During upgrade, installer shows tiles for installed topology only
- New command keys enhance silent mode:
  - Cmd key "CheckStatusOnly" to avoid automatic change of Windows settings during SPT runs in silent mode
  - Ability to set key "DBAdmin", "DBpassword" in cmd or tags <AdminName>, <ObfuscatedPassword> via configuration file

## **Branding updates**

- Installer UI refresh
- Update Launch Icon, splash screen, and login screens

## **Online Help updates**

- New, additional cloud version of the Help and Learning platform accessible at <a href="https://openlab.help.agilent.com">https://openlab.help.agilent.com</a>. Adds direct access of updated English and localized user-guides.
- New help format supports favorites

## Product Level Changes for v2.7

## **Control Panel**

Added software status in instrument view

- New optional software status column\_is available in the instruments panel: Color codes indicate one of the following SW states:
  - Default (ok state)
  - Collecting data from instruments
  - Waiting for user action
  - Paused (because user is doing something)
  - Disconnected from hardware
  - Error state

#### Added Privileges

- New Activity Log Access privilege
  - Required for view access to the Activity Log.
  - Upon upgrade the **Activity Log Access** role is assigned automatically to all existing users and groups.

- Other new privileges: (see respective sections on details about the related functionality)
  - Request access
  - Cancel my pending runs: Delete pending runs submitted by me
  - Run single sample: Control Single injection runs
  - Modify instrument configuration in CDS Client

## Acquisition

New "Ad Hoc mode" allows instrument-initiated runs

• Controlling user may initiate runs "ad hoc" from the Agilent GC instrument: CDS is made aware and can acquire data. Ad Hoc mode restricts access to Agilent LCs and GCs for other users.

Centrally Managed Unattended Printing

- Option to create common, shared folders ("printers") to use for centralized, unattended printing if used in conjunction with a 3<sup>rd</sup> party print management software package.
- Users may choose from a predefined list of printers to assign for specific print tasks (e.g., print injection reports) or summary reports
- Option to override the printer specified in the processing method.

New Wait sequence line type.

- Allows the user to specify that the sequence will wait until
  - User resumes
  - Wait Timeout triggers automatic resume
- Option to specify method for the instrument as part of the **Wait** line (e.g., to flush the system when changing methods)
- While acquisition is waiting, additional samples may be added to a sequence. The user can
  - Scan Barcodes while sequence is waiting
  - Update & resume sequence with one click

Tokenized result path (structured acquisition result storage)

• Pre-defined tokens may be appended to the result path (e.g., Date, injection source, instrument name), to enhance data organization and search for results.

New print/export option for sample prep methods

• Report provides the same options as the Acquisition Method report. It offers printing or exporting method parameters and audit trail.

Ability to request access to an item that is blocked by another user

• Requires **Request access** privilege. The original, blocking user can deny the request. In case of no response after 60 seconds, the blocked item is released automatically.

Change of instrument configuration in the Acquisition Client:

• Requires **Modify instrument configuration in CDS Client** permission. Note: Requires LC&CE driver version 3.5 or higher to use the whole feature set.

Productivity and Usability enhancements

- Easy refresh of an injection list (without closing the tree) provides ability to select newly acquired data only (single run workflow)
- Sorting of single-sample data by project or sequence
- Enhanced "Home" project feature for easy access from Data Processing view
- New "Save and close" option allows easy clean-up of tree-view
- Support large number of files in the Sequence
- User-configurable Run Queue table persistent per user and per instrument
- New Active and History tabs display acquiring runs separately from completed runs.
- Sample/Sequence **Stop** options are limited to those supported by the instrument configuration.
- Enable continuous use of snapshot feature for single runs: Supports faster workflows without need to close and open a new DA instance.

## **Data Analysis and Reporting**

**Enhanced Calibration** 

- Calibration may be based on time-based group as reference (if using linear curve models or fixed response factors)
- Calibration Coefficient of determination (r2) calculations can be validated for all calibration modes

Added option to scale detector response for peak area or height before calibration and quantification

- Facilitates  $\sqrt{peak area}$ ,  $\sqrt{peak height}$ ,  $\log_{10}(peak area)$ ,  $\log_{10}(peak height)$
- Use of area correction for CE
- Scaled responses are shown in the injection results, custom calculation, and reports

Extended token list in Injection Reports

- New token Result Path (e.g., year/month/day/instrument name etc.) allows for structures defined at acquisition time to be used for report copy operations.
- Option to include the new result path token in processing method enables to structure exported reports and exported data.

Different detectors can use the same compound name in compound table of the processing method

• A compound may be identified with the same name in multiple signals. It is possible to create results for dual column confirmation applications.

Possibility to define calibration level specific ISTD amounts in the processing method to simplify sequence setup.

• Option to choose for method level amounts to override those from the sequence table and in the injection list.

Enhanced Integration Optimizer

• Added option for fine tune of the integration using timed events

• Added time programming and advanced functions, such as Overlays, fine tune existing processing methods, or the option to optimize different retention time ranges independently for timed events

Enhanced support of 2D-LC (may require additional product)

- Support Custom Calculation for 2D-LC
- Support 2D-LC and 2D-GC data with integration optimizer
- Store and use 2D column information
- Peak Purity provided for 2D peaks
- Support in AMX method import

Extended custom calculations and reports

• Compound specific multiplier

## Mass Spec related improvements

Enhanced Automatic Spectrum Extraction

• Added ability to use either identified peaks or all peaks.

Enhanced the MS Peak Purity

• Changed the graphical presentation in Peak Details to show components. This applies to both Separate and Overlaid modes.

Add\Update now adds compounds to the compound table with a TIC SCAN signal instead of an EIC signal.

## Enhanced method-import from EZChrom

• Improved DA methods import now includes calibration curves, timed groups, and history points.

## Expanded support of Capillary Electrophoresis (CE)

In conjunction with LC&CE Driver 3.5 the following workflows are supported:

#### Acquisition

- Configure the 7100 Agilent CE or CE/MSD instruments using instrument type Agilent LC & LC/MS.
- Connect to the CE instrument, create methods, and run analyses using CE specific soft configuration options.
- Review CE analytic data with same feature set as for LC.
- Create reports from CE data with same feature set as for LC.
- Capillary Zone Electrophoresis (CZE) workflow (with or without corrected area and CE specific calculations).

Data Analysis updates

- Data Analysis allows for scaled responses using various options.
- Audit trail is supported with CE.

Automation for method developments, including user vials/sequence overwrite.

## Sample Scheduler for OpenLab integration with CDS

Balance integration - from Sample Scheduler to Data Analysis:

- Digital transfer of weighing results from balance (LabX balance) to OpenLab CDS, via lab balance bridge
- Barcode-driven balance workflow with Sample Scheduler integration
- Meta Data transfer with or linked to results from Sample Scheduler to OpenLab CDS Data Analysis
- Audit trails provide seamless documentation of entire workflow

Instrument dashboard that is integrated with OpenLab CDS is available in localized versions:

• Provides overview of instruments from a mobile device or PC

## Enhancements to Backup and Restore for Workstation Plus

- Temporary files are now stored in the database backup location.
- Added retries mechanism for backup finalization
- Added detailed progress tracking for the verification procedure
- Created a console application for PostgreSQL customization to support incremental backups
- Added installation of the Restore Utility and launch icon. Restore utility may be launched from the Start menu
- Updated launch icons for Backup and Restore utilities

## **Driver Updates**

Agilent Instrument driver packages shipped with OpenLab CDS 2.7:

RC.NET Instrument Driver	Driver Software Revision	Installed by default
Agilent LC & CE	3.4 *	•
Agilent LC/MS SQ	2.5	•
Agilent ELSD	1.8	
Agilent GC	3.7	•
Agilent GC/MS SQ	1.4	•
Agilent Micro GC	2.3	
Agilent Gas Analyzer	2.7	
Agilent G1888 Headspace	B.01.09.2	
Agilent 7697A-8697 Headspace	3.3	
Agilent 35900E A/D Converter	2.3	•
Agilent SS420X A/D Converter	1.2	•
Agilent Data Player	2.4	•
Agilent CTC PAL 3	2.5	
Agilent CTC PALxt	B.01.08	

\* LC&CE driver version 3.5 or higher is required to use the extended CE workflow, for non-RC.Net Method Import (2DLC), and the whole feature set provided by the **Modify instrument configuration in CDS Client** permission.

See the OpenLab CDS media for more details on final component versions.

## **Non-Agilent Instrument Control Drivers**

Support for non-Agilent instruments in OpenLab CDS continues to expand.

For the most current list of supported non-Agilent instruments visit the FAQ page "*What instruments are supported in OpenLab CDS*?" on the Agilent website www.agilent.com.

## Version 2.6

## Infrastructure Support updates

Cloud Services supported: OpenLab CDS with ECM XT as backend can run in an Amazon Web Services (AWS) or Microsoft Azure cloud environment. For details see your Agilent representative.

#### Compatibility updates

Workstations, Clients, and Instrument Controllers (AICs) are now supported on:

- Windows 10 64-bit, Enterprise (1909 or greater), or Professional (2004 or greater)<sup>3</sup>
- OpenLab Server / ECM XT 2.6, includes new Basic Server product

See the CDS Requirements guide for full details.

## Communication port and protocol changes

OpenLab CDS with OpenLab Server or OpenLab ECM XT now utilizes secure https communication protocols between clients (e.gs OpenLab CDS Clients, AICs, and web browsers) and the server application. To ensure appropriate authentication of the applications, Agilent OpenLab can utilize any existing commercially signed digital certificate OR supplied OpenLab self-signed certificate as part of system configuration.

<sup>&</sup>lt;sup>3</sup> For support of LTSC/LTSB, and the most current versions check with your Agilent representative.

## System / Installation

Enhanced System Preparation Tool (SPT)

- This SPT is now integrated in the installer and runs as the first step. It may still be launched prior to installation
- SPT steps and progress shown in installer UI
- Mandatory settings are checked, and OS settings are updated if possible or identified as requiring manual correction before installation proceeds
- The user can choose the recommended actions
- SPT report provides instructions how to update the setting manually before installation of the CDS

New dedicated installation workflow for Shared Services Server

• New workflow is used specifically for deployments connected to OpenLab ECM 3.x

## Updated data integrity features

- Updated wording or category of audit trail and activity log entries
- Added entries to the audit trail

## **OpenLab Control Panel updates**

Added Privileges for OpenLab CDS

- Disable/enable calibration points (default in built-in role Chemist, Technician, Everything)
- Use integration optimizer (default in built-in role Chemist, Everything)
- Integration optimizer: Display peak results (default in built-in role Everything)

Added Privileges and Roles for Workstation Plus New Privilege:

• Delete Content Of Project

New Roles:

- Project Content Deletion
- Content Management Administrator

# Sample Scheduler for OpenLab delivered on OpenLab CDS media

Sample Scheduler for OpenLab is installed via OpenLab installer

Instrument dashboard available with OpenLab CDS (C/S only)

- Provides overview of instruments from a mobile device or PC
- Displays available instruments
- Shows status information and instrument errors

By activating the software and adding instrument licenses the instrument dashboard is turned into a full *Sample Scheduler for OpenLab* installation: This management tool includes a simple user interface for submitting analyses, time scheduling capabilities for unattended maintenance and calibration procedures, and more productivity features.

Launch Sample Scheduler for OpenLab (C/S only)

• New launch button for fast access from within the Acquisition client or the Windows start menu

## Migration Tools for OpenLab

No longer part of the OpenLab installer.
 It is now available on the media in Setup > Tools > Migration

## QualA

New QualA 3.4 release (Test Services) delivered with OpenLab CDS. See separate QualA Release Notes for details on feature updates

## **Updated Branding**

Redesigned launch Icons, splash screens and login screens, to adjust to new Agilent branding

## Product Level Changes for v2.6

## Acquisition

Changes to Run Queue and Sequences

- Option to save each sample in a sequence as unique result set
- Edit currently running sequence when run queue is paused
- Sequences in progress can now be stopped to add priority samples or address a tray loading mistake
- Runs are shown separately on Active or History tab

Changes to the dual simultaneous injection workflow

- Unique table fill down possible for front and back injections
- Sequence table can be filtered to display only the front or back channel
- Option to save front and back samples to separate result sets
- Option to save each sample in a dual simultaneous sequence as unique result set

Improved snapshot and result review feature

Once opened from the online signal window or sequence table, a snapshot/review instance can remain open for further snapshots taken in the context of the same sequence.

Added Reference Chromatogram in Acquisition

• Allows to visualize the reference chromatogram within the real time plot

## **Data Analysis and Reporting**

Unique calibration curve handling

- A new quantification mode for calibration runs. When acquiring new sequences, the new function provides the option to post-pone processing and reporting until an uninterrupted series of calibration injections is finished. This mode needs to be activated in the project. When reprocessing data acquired with immediate processing or data acquired with an earlier version of OpenLab CDS, the quantification results for the intermediate calibration injections will be different
- In addition to the back quantification of calibration standards, deactivation of a single calibration point now gets automatically applied to all loaded calibration and sample injections where the corresponding calibration was used

## New Integration Optimizer Wizard

- The integration optimizer helps find a suitable set of integration events. It allows integration parameters to be tuned via sliders (peak width, slope sensitivity, height reject, peak separation modes) and the resulting integration to be previewed in real-time in the **Chromatograms** window
- It enables easy deployment of integration settings to the lab

## Reference Chromatogram

• Added option to define a reference chromatogram in the processing method and display up to 5 signal specific reference chromatograms in the chromatogram window

Enhanced compound management in the calibration tab

• New column in compound table provides the option to sort compounds by signal names and retention times

Enhanced visualization of sample types

• Added coloring in the injection list analogous to Acquisition context

Miscellaneous updates to reporting

- User can choose separate acquisition method parameters to use in both Acquisition and DA reports
- Added ability to report MS Peak Table via a new snippet

## Mass Spec related improvements

Update to Sample Purity

- Updated design of results table for sample purity analysis, to allow faster screening of results
- Added signal column: sample purity results can be viewed by signal
- Added sample purity results filter
- Added copy and export capabilities from the sample purity table
- Updated sample purity report to reflect the updated sample purity results table
- Added columns to the target table to show RT and Adducts.

Update to MS spectrum window

- Added a movable threshold selection to hide unwanted m/z values
- Added maximum abundance window to identify the most abundant m/z

Added MS Spectral Smoothing

• Option to apply the Gaussian smoothing algorithm to an MS Spectrum displayed in profile mode

Enhanced SIM data functionality

- Extract Chromatogram
- Add ion as compound to the method
- Add ion as qualifier to the compound

Added support for NIST/EPA/NIH EI-MS Library, 2020 release (NIST20)

### **Enhancements to Backup and Restore**

- Added automated Restore for Workstation Plus. Restore Utility is available from the Start Menu and provided on the media (Setup > Tools)
- New tools for all-in-one and 2-server topologies of OpenLab Server and ECM XT will allow users with limited technical skills to automate a scheduled back up and perform a restore when necessary
- Incremental backups are supported

#### Added basic CE and CE/MS Support

OpenLab CDS v2.6 supports basic CE release with LC & CE Driver 3.2 or higher

- Configure the CE instrument as part of the instrument type "Agilent LC"
- Connect to the CE instrument, create methods, and run analyses
- View CE monitor signals in Online Plot
- Review CE analytic data with same feature set as for LC
- Create reports from CE data with same feature set as for LC

## **Driver Updates**

Agilent Instrument driver packages shipped with OpenLab CDS 2.6:

RC.NET Instrument Driver	Driver Software Revision	Installed by default
Agilent LC & CE	3.3	•
Agilent LC/MS SQ	2.4	•
Agilent ELSD	1.8	
Agilent GC	3.5	•
Agilent GC/MS SQ	1.4	•
Agilent Micro GC	2.2	
Agilent Gas Analyzer	2.6	
Agilent G1888 Headspace	B.01.09.1	
Agilent 7697A-8697 Headspace	3.1 *	
Agilent 35900E A/D Converter	2.3	•
Agilent SS420X A/D Converter	1.2	•
Agilent Data Player	2.4	•
Agilent CTC PAL 3	2.3	
Agilent CTC PALxt	B.01.08	

\* The two HSS drivers may be co-installed on one system. Installing 3.1 or higher will upgrade both B.01.09 and B.01.10 drivers. To keep G1888 control install B.01.09.1 after the upgrade.

See OpenLab CDS Requirement guide (CDS\_Requirements.pdf) for details.

## **Non-Agilent Instrument Control Drivers**

Support for non-Agilent instruments in OpenLab CDS continues to expand.

For the most current list of supported non-Agilent instruments visit the FAQ page "*What instruments are supported in OpenLab CDS*?" on the Agilent website www.agilent.com.

## Version 2.5

#### Infrastructure Support

OpenLab CDS version 2.5 is supported in the following configurations: Workstation Plus, Workstation with file-based storage, and Client/Server.

Workstations, clients, and Agilent Instrument Controllers (AICs) are supported on:

• Windows 10, Enterprise or Professional, 64-bit (version 1809 or higher<sup>4</sup>)

Additionally, for networked deployments, clients  $^{\rm 5}$  and AICs  $^{\rm 6}$  are supported on:

- Windows Server 2016, Standard or Datacenter, 64-bit
- Windows Server 2019, Standard or Datacenter, 64-bit

#### **Russian Language Support**

• OpenLab CDS Workstation with file-based storage and OpenLab Workstation Plus now support Russian language.

#### Systems Management Software Support

• Supports installation and updates deployment of select components of OpenLab CDS using systems management software, such as Microsoft System Centre Configuration Manager (SCCM).

<sup>&</sup>lt;sup>4</sup> For support of the most current versions check with your Agilent representative.

<sup>&</sup>lt;sup>5</sup> In virtual environments

<sup>&</sup>lt;sup>6</sup> AICs are supported but not recommended on Windows Server 2016 or 2019, Standard or Data Center

#### System Preparation Tool

• Performs an automatic check of PC requirements required to use OpenLab CDS, identifies errors encountered, and provides associated warnings. Automatically updates most required Windows settings as needed and generates an outcome report.

#### **Product Level Changes**

#### Introduction of core purification workflows

- OpenLab CDS now supports the use of Agilent Purification LC systems with fraction collection.
  - Includes UV signal triggered collection; time and volume-based collection and manual.
  - Includes delay volume collection calibration.
  - Includes pooling and recovery collection.

Note does not support Mass based purification.

#### Support for Single Sign-on

• Support for SSO on OpenLab CDS Systems using Windows domain authentication including card key access. Eliminates the need for multiple logins from valid users once they have logged in with their Windows credentials.

# Introduction of Method Status labels to ensure that only approved methods can be used to acquire and process data.

- Ability to configure and enforce which methods are available for use within a project according to designated method status label.
  - Generic = default status. Users can be restricted from using this type of method.
  - Approved = Select users can be restricted to only see and "use Approved" methods.
  - Obsoleted = marked as no longer in use. Users cannot use this method type if Method Status is active for a project.
- New privileges introduced to define who can
  - change the associated status label of a method
  - use generic status methods

#### Automatic Collection and Storage of Column Information

- OpenLab CDS now collects and saves column information as provided by instrument. This includes columns using RFID column tags. Column tags used in Agilent hardware and consumables will now auto-propagate information into the result set data available for search and reporting. Certain information may be automatically populated for further data analysis calculations
  - For LC: Use of RFID column tags requires an Agilent Infinity II LC series column compartment and appropriate columns.
  - For GC: Requires an Agilent 8890 or Intuvo 9000 GC with a J&W column with Smart ID Keys.

#### Inclusion of the eMethod software tool with OpenLab CDS

• Allows the import of available eMethods from Agilent to OpenLab CDS.

## Acquisition

#### Added injection types for GC dual injection sequence

• Ability to run samples with "Manual/External" or "No Injection/Instrument Blank" as injection sources in the same dual sequence.

## **Data Analysis and Reporting**

#### Integration parameters for individual MS signals

- Ability to setup integration parameters for individual MS signals similar to existing chromatographic signals.
- Total Ion Chromatogram (TIC) Single Ion Monitoring (SIM), TIC Scan, SIM and EIC (Extracted Ion Chromatogram).

#### Normalized amount calculations

• Ability to easily apply NORM calculation using custom calculator. Supports % and ppm calculation corrected for different sample volume inputs.

#### Enhanced report generation and export capabilities.

- Ability to generate more than 2 reports automatically using a Data Analysis method.
- Reports can now be named and saved to locations using tokens allowing for automated routing /printing using 3rd party applications.

#### MS spectrum overlay

• Ability to overlay multiple color-coded MS Spectra to compare MS Spectra from different samples.

#### Split TIC SIM signal by Polarity, Fragmentor, and Gain for MS data

• Ability to view separate TIC SIM signals based on Polarity, Fragmentor, and Gain to provide unique information for each of these different analytical conditions.

#### Data exported in AIA. NetCDF standard format now includes MS spectra.

#### Export of files in Analytical Studio Reviewer (ASR) file format

• Ability to generate files in ASR format to allow OpenLab CDS data to be viewed in MassHunter Analytical Studio Reviewer. Plate view is not currently supported.

## **Backup tool for WorkStation Plus**

# New utility provides users with enhanced data backup and restore including the ability to:

- Set up scheduled data backups
- Perform immediate data backup
- Supports cold backup or hot backup

#### New PowerShell script enables one step data restore

## Hot backup support for Client/Server

New procedure for hot backup and restore of the OpenLab Server and ECM XT system. Hot backup can be performed while the system continues to acquire and analyze data.

## **Driver Updates**

Agilent Instrument driver packages shipped with OpenLab CDS 2.5

RC.NET Instrument Driver	Driver Software Revision	Installed by default with OpenLab CDS 2.5
Agilent LC	3.1	Х
Agilent ELSD	1.8	
Agilent LC/MS SQ	2.4	Х
Agilent GC	3.2	Х
Agilent Micro GC	2.1	
Agilent Headspace	B.01.09	
Agilent GC/MS SQ	1.4	Х
Agilent 35900E A/D Converter	2.3	Х
Agilent SS420X A/D Converter	A.01.01	Х
Agilent Data Player	2.3	Х
Agilent CTC PAL 3	2.1	
Agilent CTC PALxt	B.01.08	

## Non-Agilent Instrument Control

For a current list of supported non-Agilent instruments visit the FAQ page "What instruments are supported in OpenLab CDS?" on the Agilent website.

## Version 2.4

#### Infrastructure Support

OpenLab CDS version 2.4 is supported in the following configurations: Workstation Plus, Workstation with file-based storage, and Client/Server.

Workstations, Clients, and Agilent Instrument Controllers (AICs) are supported on:

- Windows 10, Enterprise or Professional, 64-bit (version 1703, 1709, or 1803)<sup>7</sup>
- Windows 7 SP1, Enterprise or Professional, 64-bit

Additionally, for networked deployments, clients and AICs are supported on:

- Windows Server 2012 R2, Standard or Datacenter, 64-bit
- Windows Server 2016, Standard or Datacenter, 64-bit

New support for OpenLab ECM as networked security repository for OpenLab CDS. Supported OpenLab ECM software:

- OpenLab ECM Version 3.5 Update 6 or later is required
- OpenLab ECM Version 3.6

No operating system support has been removed since v2.3.

#### Acquisition

Priority sample submission

• Ability to add priority sample. Users can submit priority samples that will acquire after the current injection is completed.

<sup>&</sup>lt;sup>7</sup> for support of the most current versions check with your Agilent representative

Edit pending sequences

• Ability to edit pending sequence. Users can preview the pending sequence and modify all pending lines of the sequence without disruption to the run queue.

Support for multiple gain acquisition with LC/MSD

• Ability to acquire data with different gain settings for the same mass to allow increased throughput (see LC/MS Driver Update for details).

SIM ion override

• Allows users to specify target SIM Ion other than what is currently defined in the acquisition method at time of sequence submission.

Reasons for aborting (see Data Integrity Enhancements for details)

Control client (see Data Integrity Enhancements for details)

### Data Analysis and Reporting

Support for MS profile mode

• Acquire and view MS data in profile mode with quantitation through extracted chromatograms from spectrum peak.

Improvements to custom calculator expression editor

- Adoption of common scripting standards to provide improved readability
- Autofill and error highlighting
- Indenting and inline help

Multi MS library searching

• Ability to select up to 10 libraries in processing method to search spectrum in the NIST format Library

Automated batch export functionality of CSV file

• CSV file includes mass, peak area, peak height, and retention time.

Automatic calculation of UV purity sensitivity value

• Ability to have the purity threshold calculated automatically for all compounds in the method based on the sensitivity set for a compound.

Signature order and locking results on sign (see Data Integrity Enhancements)

#### **Data Integrity Enhancements**

Improved signature workflow support

- Ability to enforce customizable signature paths
- Ability to approve/reject multiple at the same level

Signature order and Locking results on sign

 Administrators now can configure and enforce a signature order. When enabled, signatures in Data Analysis will have to follow the order and meaning as prescribed in the project's signature settings. An additional enhancement in the Signature Settings page allows for all results to be automatically locked upon the first signature.

Reasons for aborting

 If reasons are enabled for Results modification, the user will now be prompted for a reason when they intentionally abort a run queue item.

**Obscure Locked Windows** 

 If OpenLab CDS is locked, the text in the application is blurred if it may be displaying confidential or sensitive information in its tests or descriptions.

#### Control Client

• In a multi-user environment, users with the privilege to manually control an instrument can "take control" of an instrument to modify its settings. Other users can still submit runs to the instrument run queue, but only one user can be modifying these settings at a time. This reduces mistakes in user overlap and allows changes to the instrument settings to be correctly attributed to the person who is in-control.

#### Add-ons

Introduction of QualA add-on for OpenLab CDS WorkStation Plus and Client/Server

• New software qualification tool allowing customers to self-perform software qualification assessments for future minor software releases.

Version 1.4 of Migration Tools for OpenLab add on to support workstation to workstation upgrades to CDS 2.4 from the following software:

- ChemStation C.01.05, C.01,06 or C.01.07
- EZChrom A.04.05, A.04.06 or A.04.07

Support for creation and automated export of Allotrope files in OpenLab CDS WorkStation and Client/Server software. The Allotrope Data Format (ADF) files are a universal data format, a detailed description of the Allotrope Data Format and its structure is available on the Allotrope Foundation web site (https://www.allotrope.org).

- Automated creation of Allotrope Data Format when result set/injection completes. Consists of the LC-UV analytical raw data (chromatograms + spectra) plus metadata and the original OpenLab CDS files.
- Manual export of result set or sequence

#### **Driver Updates**

Agilent Instrument driver packages shipped with OpenLab CDS 2.4

RC.NET Instrument Driver	Driver Software Revision	Installed by default with OpenLab CDS 2.4
Agilent LC	A.02.19 SR3	х
Agilent ELSD	A,01.07 (build 12)	
Agilent LC/MS SQ	2.2.2260	Х
Agilent GC	3.0.532	Х
Agilent GC/MS SQ	1.3 (build 54)	х
Agilent 490 Micro GC	B.01.12.1.2125	
Agilent Headspace	B.01.07.3	
Agilent 35900E A/D Converter	2.3 (build 53)	Х
Agilent SS420X A/D Converter	A.01.01 (build 65)	Х
Agilent Data Player	2.2.6	х
Agilent CTC PAL 3	A.01.04.1	
Agilent CTC PALxt	B.01.08	

## **Non-Agilent Instrument Control Drivers**

For a current list of supported non-Agilent instruments visit the FAQ page "What instruments are supported in OpenLab CDS?" on the Agilent website.

## LC/MSD Driver Update

Method Editing with Gain

• Method editing now supports Gain instead of EMV. EMV from previous methods is reset to Gain=1. Using constant gain in methods relieves the user from controlling delta EMV change in a regulated environment.

Two Scan Types with Method Manual Resolution

• The driver now designates two scan types: Single Ion Monitoring (SIM) and Scan. The "Scan" scan type will persist throughout the run. If there are Scan method discrepancies, the Manual Resolution window with hover-over tips will appear for users to adjust their method. Additionally, users can check the "Target points per second" box to specify the

number of points across the peak. The driver software will automatically calculate the scan time and dwell time to meet the "Target points per second" setting.

Time Segments in Audit Trail but Not in UI

• Since the scan will be run throughout the time segments, the audit trail reflects time segment changes although the UI no longer shows time segments as an option.

Distinguishing Scan Traces with Overlapping Masses

• When there are overlapping masses in multiple "Scan" scan segments and if all the parameters (fragmentor, gain, polarity) are the same, users will not be able to distinguish the scan trace that the overlapped mass came from in Data Analysis. If any of the above parameters is different, users will be able to distinguish the spectrum data based on the parameters shown in DA.

## Version 2.3

OpenLab CDS version 2.3 is supported in the following configurations: Workstation Plus, Workstation with file-based storage, and Client/Server.

Workstations, Clients, and Agilent Instrument Controllers are supported on:

- Windows 10, Enterprise or Professional, 64-bit, version 1607 or later
- Windows 7 SP1, Enterprise or Professional, 64-bit

Licensing updates

• OpenLab CDS version 2.3 requires an update to the license file from SubscribeNet when upgrading.

Functional verification following upgrade installation

#### Acquisition

LC shutdown options in run queue allows users to set shutdown actions Shifting of runs/sequences in the run queue

• Users can edit the order of pending items in the run queue.

Ability to display all users currently using the same instrument

Automated sequence summary report

• Ability to specify the sequence summary report(s) at the time of sequence submission.

Graphical display of sample location

• Optionally display the location of your samples in a sequence table when using most Agilent LC injectors.

#### **Data Analysis and Reporting**

Extract 2D (UV) signal from 3D matrix

• Ability to define specific chromatogram extraction parameters and identify and quantify compounds from extracted chromatograms.

Isoplot UI for interactive spectra and signal extraction

• Ability to display a 3D UV matrix as an isoplot and to provide tools for method optimization.

MS peak purity

 MS Peak Purity for SCAN and SIM/SCAN data. Users can setup in the processing method to calculate MS peak purity for identified peaks or all peaks.

Mass annotation

• Ability to label the UV and MS chromatogram peaks with base peak m/z.

Chromatogram smoothing

• Ability to setup the smoothing parameters in the processing method.

Loading methods from another project

• Allows authorized users to browse to another project, open a method and save a copy of that method to their current project or link it to a result set.

Overlay chromatograms from different projects

• Allows users to load data from other projects to compare results.

MS tune report

• Ability to display the MS tune report for selected injection from the injection tree.

Enhanced conditional formatting and Reporting

• Improved conditional formatting for tables, fields, and matrix including multiple colour choice.

Automated export of ChemStation and AIA Files

• Ability to define automatic export of raw data (ANDI/AIA, CH) during a running sequence as part an automatic processing method.

Load ChemStation/EZChrom Method

• Users can open a result set from ChemStation or EZChrom (option to have multiple methods imported and linked automatically).

OpenLab CDS data analysis updated to true native 64-bit support for handling of large files/data.

#### **Driver Updates**

Driver packages (revision) installed with OpenLab CDS version 2.3:

Agilent LC	A.02.19
Agilent LC/MSD	A.01.02.35
Agilent GC	B.01.03
Agilent GC/MSD	A.01.02
Agilent 35900E A/D	2.3.0
Agilent SS420x Interface	A.01.01
Agilent Data Player	A.02.01

Other RC.NET drivers included on USB media:

CTC PAL3	A.01.04
PAL XT	B.01.08
ELSD	A.01.07
Agilent 490 Micro GC	1.12.3
Agilent Headspace	B.01.07.2

#### **Non-Agilent Instrument Control Drivers**

For a current list of supported non-Agilent instruments visit the FAQ page *"What instruments are supported in OpenLab CDS?"* on the Agilent website www.agilent.com.

## Version 2.2

#### Infrastructure Support

OpenLab CDS version 2.2 is supported in the following configurations are Workstation Plus, Workstation with file-based storage, and Client/Server.

Workstations, Clients, and Agilent Instrument Controllers can run under the following:

- Windows 10, Enterprise or Professional, 64 bit
- Windows 7 SP1, Enterprise or Professional, 64 bit
- Windows 8.1, Enterprise or Professional, 64 bit

#### Acquisition

Automated creation of sequence result folder and name

Project enhancements supporting template file sharing

• Ability to share sequence and templates within multiple projects.

Failover state for operational continuity

• Allow submission of samples through the AIC in case of network connectivity failure occurs.

Method translation from 68xx to 78xx and Intuvo

• Ability to open acquisition method created on a 68xx and use on 78xx or Intuvo.

#### **Data Analysis**

Snapshot via Data Analysis

- Ability to view, process and print from a sample that is being acquired. Translation and import of MSD ChemStation data format to OpenLab CDS Enhancement to user permissions and version access in Data Analysis
- Auto-lock result set when e-signing
- Version label will not change when a result set is signed or locked

- User can sign a locked result set
- Load older version of a processing method & single run result sets where available
- Enhancements to user privilege control for MS functionality

Enhancements to reporting

- Zoom in/out of report preview with mouse wheel
- Ability to add any data field in header or footer
- Use of complex custom fields in filter, grouping and sorting expressions
- More formatting settings for custom tables
- New option to remove duplicate peaks when using named groups
- Ability to define sorting of a repeated table

Integrated template documentation tool

• Allows the template author to document the design of the report template.

Enhancements for MS data include:

- Report single values of method override parameters in table and single fields
- Print graphical qualifier results (limit lines) and missing qualifiers

#### Add-ons

The following add-ons are supported with OpenLab CDS (\*additional licenses may be required):

- Support for Sample Scheduler for OpenLab
- Support for Gel Permeation Chromatography (GPC)\* add-on
- Manual export of data files in legacy formats:
- ChemStation Edition \*.D
- AIA
- Support for Match Compare for OpenLab\*

### **Driver Updates**

Driver packages (revision) installed with OpenLab CDS version 2.2:

Agilent LC	A.02.16.6
Agilent LC/MSD	A.01.02
Agilent GC	B.01.02
Agilent GC/MSD	A.01.01
Agilent 35900E A/D	2.3.0
Agilent SS420x Interface	A.01.01
Agilent Data Player	A.01.02
Other RC.NET drivers included on USE	3 media:
CTC PAL3	A.01.03
PAL XT	B.01.08
ELSD	A.01.07
Agilent 490 Micro GC	B.01.12
Agilent Headspace	B.01.07.2

### **Non-Agilent Instrument Control Drivers**

- Includes driver support for Waters e-Alliance, Alliance, Acquity and Acquity H-Class LC instruments
- Includes support for Bruker/Varian CP-3800/3900 and Scion 430/450/456 GC instruments
- Includes support for Valco Instruments Valves: EMHCA-CE, EMHA-C, EMTCA-C
- Includes support for Shimadzu GC and LC instruments
- Includes support for Thermo Accela / Surveyor LC instruments

# 3 Important Support Information

For known issues and workarounds in the OpenLab software at the time of release see the Software Status Bulletins (SSB), which can be found online at:

http://www.agilent.com/en-us/support/software-informatics/openlab-software-suite/openlab-chromatography-data-system-(cds)/m84xx

Software Support Lifecycle Policy

Check the Agilent Software Support Lifecycle Policy at https://www.agilent.com/en/support/agilent-openlab-software-support-lifecyclepolicy so you can schedule the updates to keep your version up to date.

#### **Agilent Community**

To get answers to your questions, join over 10,000 users in the Agilent Community. Review curated support materials organized by platform technology. Ask questions to industry colleagues and collaborators. Get notifications on new videos, documents, tools, and webinars relevant to your work.

https://community.agilent.com/

#### Agilent on the web

Visit Agilent's website Lab Informatics Software - OpenLab Software Suite | Agilent for up-to-date issue information on Agilent's Analytical Software suite.

## In This Book

This document provides a listing of the major feature modifications made in each release of OpenLab CDS Software.

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