



Agilent OpenLab CDS  
Version 2.4

## Release Notes

# Notices

## Manual Part Number

M84410-90011 Rev. 2.4  
February 2019

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## Software Revision

This guide is valid for the 2.4 revision or higher of Agilent OpenLab CDS software until superseded.

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### CAUTION

A **CAUTION** notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in damage to the product or loss of important data. Do not proceed beyond a **CAUTION** notice until the indicated conditions are fully understood and met.

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# 1

## Introduction

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

References to product documentation regarding known issues and workarounds are also provided.

### **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.

## 2 OpenLab CDS

### 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>1</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.

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<sup>1</sup> for support of the most current versions check with your Agilent representative

## Version 2.4

### 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

## Version 2.4

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 have the ability to 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 in the event that it may be displaying confidential or sensitive information in its tests or descriptions.

## Version 2.4

### 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	x
Agilent ELSD	A.01.07 (build 12)	
Agilent LC/MS SQ	2.2.2260	x
Agilent GC	3.0.532	x
Agilent GC/MS SQ	1.3 (build 54)	x
Agilent 490 Micro GC	B.01.12.1.2125	
Agilent Headspace	B.01.07.3	
Agilent 35900E A/D Converter	2.3 (build 53)	x
Agilent SS420X A/D Converter	A.01.01 (build 65)	x
Agilent Data Player	2.2.6	x
Agilent CTC PAL 3	A.01.04.1	
Agilent CTC PAL-xt	B.01.08	

## Non-Agilent Instrument Control Drivers

For the most current list of supported non-Agilent instruments visit the OpenLab CDS product page at: [www.agilent.com/chem/openlabcds](http://www.agilent.com/chem/openlabcds)

## LC/MSD Driver Update

Method Editing with Gain

- Method editing now supports Gain instead of EMV. EMV from previous methods will be 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

## Version 2.4

- 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

# 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 color 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.

## Version 2.3

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 the most current list of supported non-Agilent instruments visit the OpenLab CDS product page at: [www.agilent.com/chem/openlabcds](http://www.agilent.com/chem/openlabcds)

## 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 2.2

- 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 (including ch)
- AIA
- Support for Match Compare for OpenLab\*

## Version 2.2

### 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 USB 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



# Version 2.1

## Infrastructure Support Changes

### OpenLab CDS Workstation

- Introduction of a second Workstation product: File based Workstation (secure/non-secure). In addition to the Workstation Plus (with Content Management – formerly referred to as “OpenLab CDS Workstation”) a new lower footprint Workstation with file-based storage is now available. Optionally the project folders can be protected against modifications from outside OpenLab CDS.

### Windows 10 support

- Workstations, Clients and Agilent Instrument Controllers can run under Windows 10 (Windows 7 and 8.1 still supported).

## Acquisition

### Dual simultaneous injection

- User can create a dual simultaneous sequence for high throughput on a dual tower Agilent GC.

### Dynamic instrument configuration

- User can perform limited configuration changes to the configured instrument from within the acquisition client without reconfiguring the instrument from Control Panel, such as LC autosampler capillary configuration, GC inlet liner and syringe configuration, GC column configuration, moving injector from front inlet to back inlet on a 7890 GC etc. With this feature, the instrument also does not need to be reconfigured after firmware updating.

### Printing from Acquisition client:

- Previewing and printing acquisition method and sequence table from acquisition client is available. Acquisition method and sequence table need to be saved to allow printing. User can save both report as PDF, word, or excel, alternatively, print from a printer. Configuration report printing is also allowed from instrument status dashboard.

## Version 2.1

Method parameter overriding capability:

- LC/MS Acquisition Method Override Columns (source parameters and fragmentor) and Compound Amounts are columns introduced in sequence table where users can override the method parameters during acquisition or for post run data processing.

Simultaneous SIM & SCAN acquisition for LC/MS

Lamp off after run:

- Introduced a global instrument setting that allows to automatically turn LC detector lamps off after a definable idle time after a run.

## Data Analysis

Blank subtraction

- Use the blank subtraction to calculate a clean chromatogram with contribution of the analytes only.

Qualifier ion support

- The presence of qualifier ions in the correct amount relative to the target ion gives evidence of correct target compound identification.

Store manual integration in method

- Ability to copy manual integration corrections into the linked Processing Method.

DA search tool

- On Workstations w/ Content Management and Client/Server systems, users can search results by text or by time period.

Higher quality reports

- Vector graphics replace bitmaps (chromatograms and spectra). Added long term storage pdf report format (PDF/A-1b format).

## Version 2.1

### Driver Updates

All driver packages are updated to new software revisions. Some new RC.net Drivers are included:

Driver packages (revision) installed with OpenLab CDS version 2.1:

Agilent LC	A.02.14
Agilent LC/MS SQ	A.01.01
Agilent GC	A.03.02
Agilent GC/MS SQ	A.01.01
Agilent 35900E A/D	B.01.01.15272
Agilent SS420x Interface (NEW)	A.01.01
Agilent Data Player	A.01.02

Other RC.NET drivers included on USB media:

CTC PAL3	A.01.03
PAL XT	B.01.08
ELSD	A.01.05
Agilent 490 Micro GC	B.01.12
Agilent Headspace	B.01.07

### Non-Agilent Instrument Control Drivers

- Includes driver support for Waters Acquity and Acquity H-Class systems (v A.1.2)
- Includes support for Bruker/Varian CP-3800/3900 and Scion 430/450/456 GC instruments (A.02.01)
- Includes support for Valco Instruments Valves: EMHCA-CE, EMHA-C, EMTCA-C (A.01.01)
- Further 3rd party instrument support (released independently and not on CDS 2.1 install media)
- Shimadzu GC and LC (planned)

## Version 2.1

- Thermo Accela / Surveyor LC (planned)
- Waters e-Alliance LC (planned)



## 3 Version History

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

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

You may also visit [www.agilent.com](http://www.agilent.com) for up to date issue information for all Agilent software products.

## 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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Edition 02/2019

M84410-90011

