

# **Agilent OpenLab CDS** Version 2.3

**Release Notes** 



# Introduction

This document provides a listing of the major feature modifications made in each release of the Agilent OpenLab Chromatography Data System (CDS) product.

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.

# OpenLab CDS 2.3

# Infrastructure Support

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 rawdata (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 the most current list of supported non-Agilent instruments visit the OpenLab CDS product page at: <a href="https://www.agilent.com/chem/openlabcds">www.agilent.com/chem/openlabcds</a>

# OpenLab CDS 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, Enterpirse 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 (including ch)
  - 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 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

For the most current list of supported non-Agilent instruments visit the OpenLab CDS product page at: <a href="https://www.agilent.com/chem/openlabcds">www.agilent.com/chem/openlabcds</a>

# OpenLab CDS 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 refered 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.

#### 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).

# **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	A.01.01
(NEW)	
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)
- Thermo Accela / Surveyor LC (planned)
- Waters e-Alliance LC (planned)

## **Known Issues**

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

You may also visit <u>www.agilent.com</u> for up to date issue information for all Agilent software products.

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