



Agilent OpenLAB CDS ChemStation Edition for GC, LC, LC/MSD, CE, CE/MSD, and A/D Instruments

OpenLAB CDS ChemStation Edition C.01.05 OpenLAB Shared Services A.01.05 Differential Specification from C.01.04

Functional Design Specification

General Description

Agilent OpenLAB is a family of systems providing analytical information creation and management. OpenLAB CDS ChemStation Edition provides instrument control, data acquisition, and data evaluation for GC, LC, LC/MSD, CE, CE/MSD and A/D instruments.

OpenLAB Data Analysis is a new data analysis product for 2D-LC and GC data that can be used together with either OpenLAB CDS ChemStation Edition or OpenLAB CDS EZChrom Edition.

Agilent OpenLAB Enterprise Content Manager (ECM) provides central data storage and data organization that extends OpenLAB CDS ChemStation Edition into an analytical information management system. OpenLAB ECM allows central storage of data and results from OpenLAB CDS ChemStation Edition and other computer-controlled analytical instruments, organizing results across an analytical operation, and providing organized online storage of files and documents associated with analytical processes. OpenLAB CDS ChemStation Edition is tightly integrated with OpenLAB ECM. The integration of OpenLAB CDS ChemStation Edition with OpenLAB ECM adds the necessary controls for managing system access, data transfer handling and audit trail functionality, while Agilent OpenLAB ECM ensures secure record keeping, audit trailing, versioning, electronic signatures and data archival. OpenLAB ECM is proven to satisfy compliance needs as mandated by regulations such as 21 CFR Part 11.



Small to medium-sized chromatography laboratories face many of the same demanding information challenges as large laboratories. OpenLAB Data Store is a central repository where you can safely archive, store, and share electronic files in a repository that can scale down to meet the needs of smaller laboratories. Use of Data Store storage is supported in networked and distributed configurations of OpenLAB CDS and provides several benefits for your system:

- Central Storage with security for small to medium sized labs
- Handles localized Chinese/Japanese content
- Web based data access for search, share, and review
- 21 CFR 11 compliant e-signatures and audit trail

Agilent OpenLAB CDS ChemStation Edition uses LAN communication to combine servers, workstations and instruments into a unified data system. When instruments do not support LAN communication, the instrument is connected to a workstation, which provides network connectivity to the system.

An exhaustive specifications document was created for revision C.01.02, this document only contains changes introduced with revision C.01.05.

Agilent OpenLAB CDS offers two distinct instrument control and data processing applications: OpenLAB CDS ChemStation Edition and OpenLAB CDS EZChrom Edition. This specification document covers Agilent OpenLAB CDS ChemStation Edition. Agilent OpenLAB CDS EZChrom Edition is covered in a separate document.

The following sections break the system down and detail the capabilities and specifications for each functional element.

Network Requirements

Firewall Settings

- Port 9753: (default) used for all task-based messaging communication between acquisition controllers and chromatography clients. It is configurable during AIC registration. It is required that all ports designated during AIC registration be opened for access.

Computer Hardware Requirements by Role

OpenLAB Data Store General Requirements

OpenLAB CDS ChemStation Edition revision C.01.05 supports the use of OpenLAB Data Store revision A.01.02 as a central storage location for scientific data.

OpenLAB Data Store Database Server

The server for OpenLAB Data Store can run on Windows 2008 R2 SP1. The database requires SQL Server 2008 R2 SP1.

OpenLAB Data Store Server Hardware Requirements

The following table summarizes the recommended hardware for a small (5 instruments) and large (15 instruments) server configuration for three years:

	Small Server Configuration*	Large Server Configuration †
CPU	2 x (Intel Xeon 2.0 GHz 4 Core) or 1 Intel Xeon 3.0 GHz 6 Core	2 x (Intel Xeon 3.0 GHz 4 Core)
Memory	8 GB (1333 GHz)	12 GB (1333 GHz)
Disk1: OS, DB, Indexes	2 x (150GB 7.2K rpm SATA) RAID 1	2 x (250GB 15K rpm SCSI) RAID 1
Disk2: Data	3 x (150GB 7.2K rpm SATA) RAID 5 (300GB of total space)	3 x (500GB 7.2K rpm SATA) RAID 5 (1TB of total space)
Network	1 GB	1 GB

* Recommended configuration for a laboratory that has 5 or less concurrent instruments running at any time. This configuration can store up to 300 GB of data, which is considered sufficient for 3 to 5 years of normal use for 5 LC or GC instruments.

† Recommended configuration for a laboratory that has 15 or less concurrent instruments running at any time. This configuration can store up to 1 TB of data, which is considered sufficient for 3 to 5 years of normal use for 15 LC or GC instruments.

Master Installer

Master Installer Updates

A new additional software tool to transform a standalone workstation into a networked workstation is now available in the maintenance section of the Master Installer. The tool will add the connection to the OpenLAB Shared Services Server and will register the workstation in the list of instrument controllers.

Methods and Sequences

Users can now review acquisition methods in the Method & Run Control view using the Acquisition Method Viewer. The viewer does not load the method to the instrument and does not trigger method resolution.

Data Analysis

Data Analysis Workflow for Single Samples

The Navigation Table now shows the acquisition method as well as the data analysis method for single samples. The system automatically loads the respective master method for a single run. A fly-over indicates the path to the data analysis method.

Last Result Mode

The Last Result Mode can now be accessed from the View menu or via the new icon in the Data Analysis view.

Using the Last Result Mode, it is now possible to save the data analysis parameters last used from the DA.M method into a master method. The user has three options:

1. To update any master method with the data analysis parameters,
2. To update the corresponding master method with the data analysis parameters, or
3. To save as new master method by combining the data analysis parameters with acquisition parameters from any master method.

In the Last Result Mode, users may only modify the data analysis method DA.M and create a report when saving the modified data analysis parameters to a master method.

Recalculate Mode

The Recalculate menu now lists the same actions that are provided by the icons. In the Preferences, the user has the choice whether to automatically load the master method used for the last data analysis. This option is applied for the loading of single runs.

OpenLAB Data Analysis A.01.01

With OpenLAB Data Analysis, Agilent introduces a new data analysis package, that includes all standard tasks required for analyzing two-dimensional GC and LC data. In the first release, it mainly addresses the needs and applications of Chemical and Petrochemical laboratories. OpenLAB Data Analysis features intuitive operation, easy sample review and fast reprocessing of large sets of chromatographic data. It can be used together with OpenLAB CDS ChemStation Edition and is a separate application installed via Master Installer. Direct interaction with ChemStation (i.e. automatic processing with OpenLAB Data Analysis during data acquisition) is only possible via a macro in the run-time checklist of the method. During processing, OpenLAB Data Analysis does not alter any ChemStation raw data or methods, but only writes new results into the .acaml file. The content of the .acaml files is displayed in the ChemStation in the Review view only. Therefore if ChemStation data was processed in OpenLAB Data Analysis, there is no impact on the results displayed in ChemStation. Only in the Review view, there will be no results available until the data is reprocessed in ChemStation again.

OpenLAB Data Analysis is supported on Windows 7 SP1 (32bit and 64bit) only. It requires RC.NET Framework 4.0. It is supported on stand-alone workstations without central data storage only. The software does not provide features for compliance with regulations like GLP or 21 CFR Part 11. There are no qualification services available.

Reporting

Intelligent Reporting

Intelligent Report Items

Table columns can now be formatted using conditional formatting based on expression results. Expressions may include custom variables and parameters.

Users can now select to include EMF counters and advanced run information in reports.

Display or Printing of Chromatograms

- A new printing option optimizes the printout of chromatograms for black and white printers. All signals are drawn in black color.
- The drawing of baselines has been improved.
- For a series of overlaid signals, user may now choose to limit the peak annotation to a single signal or annotate all.
- Users may turn off bitmap data compression for high detector sampling rates. This option does not affect the acquired raw data. Switching off data compression improves the display and printing of the signal.
- The new reporting option "fraction delay" allows correcting for the delay time between fraction collector and detector when marking the fractions in the chromatogram printout.
- Printing performance has been improved by reading audit trail information from the ChemStation register files instead of the ACAML file. For users this has no visible impact, the audit trail still gets reported as expected.

Agilent OpenLAB Data Store

Lab Applications Module

A new feature called Sample Submission has been introduced. Users may now:

- Request an analysis - Prepare a chromatography sequence and assign it to the analyst through Data Store.
- Accept and complete the analysis - The analyst receives the sequence, runs the acquisition on an instrument controlled by Agilent OpenLAB CDS, and stores the results into Data Store.
- Review results - Import the results, review, approve or reject them in Data Store.

Lab Journal

The new Lab Journal offers laboratories an easy way to track their samples, manage lab assets, such instruments and columns, and capture important lab events without a more costly enterprise-level asset management system. For instruments it lists the status, events such as maintenance, scheduled instrument service, replacements and calibrations. Lab Journal also keeps an inventory of vital supplies.

Privileged users may review the history of events that occurred on a specific instrument or column. Usage statistics per instrument, column or method over a user-defined period of time make the review easier.

Data Store User Interface

The Data Store user interface has been enhanced to support the new applications.

Agilent OpenLAB CDS ChemStation Edition for GC

Updated Agilent 78xx GC Driver, Version 5.01

- Support for new Agilent 7890B GC instrument
- Updated Column Configuration, including the ability to lock the column
- New Syringe and Liner Configuration
- Support for the 7667A Mini TD for 7820A GC
- GC Calculators integrated into the method editor
- Updated Columns Database
- New Syringe and Liner Databases
- New Keypad Lock Options

Resource Conservation (7890B)

Users may now reduce gas and power consumption with the new Resource Conservation functionality. The instrument can be put to sleep manually or by scheduling the time of the Wake and Sleep methods.

Early Maintenance Feedback EMF (7890B)

User-defined EMF counters can now be set in OpenLAB CDS based on the configuration of the GC. Warnings and Service Due notifications are provided based on the configured thresholds. EMF Exceptions can be printed on Intelligent Reports.

Barcode Scanning (7890B)

Barcode scanning enables automatic transfer of column, liner and syringe information into the method.

Autosampler (ALS) Error Handling

The handling of ALS errors has been improved.

Agilent Parts Finder

The new Agilent Parts Finder Tool is tightly integrated with OpenLAB CDS ChemStation Edition. It can be called from the Instrument menu in the Method and Run Control view and allows users to quickly locate the part number and add it to the parts list or favorites and then print the parts list or save it to a file. The parts finder supports the 7693A and 7650A ALS, 7890A and 7890B GC.

Agilent OpenLAB CDS ChemStation Edition for LC

Updated Agilent LC Drivers (RC.NET Drivers A.02.07)

Support for Agilent 1260 Preparative LC Systems including:

- 1260 Isocratic Preparative Pump (G1361A)
- Cluster of up to four 1260 Isocratic Preparative Pumps (G1361A)
- Cluster of up to three Fraction Collectors (G1364A/B/C or G5664A) and additionally one as Recovery Fraction Collector (G1364A/B/C or G5664A)
- 1260 Dual Loop Autosampler (G2258A)
- 1260 Preparative Autosampler (G2260A)

3rd Party Drivers: Support for Waters Acquity

The Waters Acquity driver allows the control of the following Waters Acquity and Acquity H-Class modules in OpenLAB CDS ChemStation Edition C.01.05:

- ACQUITY Sample manager
- ACQUITY Binary solvent manager
- ACQUITY Column manager (CM)
- ACQUITY H-Class Sample manager FTN
- ACQUITY H-Class Quaternary solvent manager
- ACQUITY H-Class Column manager (CM-A)
- ACQUITY H-Class Column manager AUX
- ACQUITY and ACQUITY H-Class Sample organizer
- ACQUITY and ACQUITY H-Class TUV detector
- ACQUITY and ACQUITY H-Class PDA detector
- ACQUITY and ACQUITY H-Class PDA eLambda detector
- ACQUITY and ACQUITY H-Class Fluorescence detector
- ACQUITY and ACQUITY H-Class ELSD detector

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