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

OpenLAB CDS ChemStation Edition C.01.04
OpenLAB Shared Services A.01.04
Differential Specification from C.01.03

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.

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.01.04.
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 21: This port is used for Agilent OpenLAB Data Store FTP.
- Port 80: This port is used by OpenLAB Data Store or OpenLAB ECM.
- Port 443: This port is used for Agilent OpenLAB Data Store HTTPS.
- Port 8081: This port is used by Agilent OpenLAB Data Store support.

Computer Hardware Requirements by Role

OpenLAB Data Store General Requirements

OpenLAB CDS ChemStation Edition revision C.01.04 and Shared Services revision A.01.04 support the use of OpenLAB Data Store revision A.01.01 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 (64-bit). The database requires SQL Server 2008 R2.

OpenLAB Data Store Server Hardware Requirements

For a laboratory with 5 or fewer instruments running concurrently, the following hardware is recommended:
- CPU - 2 x (Intel Xeon 2.4 GHz 4 Core)
- Memory - 16 Giga Bytes (GB) (1333 GHz)
- DISK – OS, DB, Indexes - 2 x (300 GB 15K rpm SCSI) RAID 1
- DISK – Data - 3 x (1 TB 7.2K rpm SATA) RAID 5

This configuration can store up to 2 Tera Bytes (TB) of data, which is considered sufficient for 3 years of normal use for 5 LC or GC instruments.

For a laboratory that has 15 or fewer instruments running concurrently, the following hardware is recommended:
- CPU - 2 x (Intel Xeon 3.0 GHz 6Core)
- Memory - 24 Giga Bytes (GB) (1333 GHz)
- DISK – OS, DB, Indexes - 2 x (300 GB 15K rpm SCSI) RAID 1
- DISK – Data - 4 x (2 TB 7.2K rpm SATA) RAID 5

Master Installer

Master Installer Updates

- Master Installer now supports installation on top of an existing C.01.03 system resulting in an automatic upgrade.
- Master Installer now supports the installation of either Data Store or ECM for central data storage system components including servers, AICs, and clients.
- Software installation repair is now supported using the repair utility found in the maintenance section of the Master Installer.
- A new additional software installation tool is now available in the maintenance section of the Master Installer. This currently only supports the addition of OpenLAB Data Store components to an AIC or client upgraded from a previous revision.
- Scripted installation of clients and AICs is now supported. An XML file may be exported at the end of installer parameter definition which can then be used to install an identical configuration on other machines.
- The Master Installer now supports the new OpenLAB Data Analysis (currently available only for standalone workstations)

OpenLAB Control Panel Administration

Links

A link to an OpenLAB Customer Survey is now included in the link list

Licenses

The licensing user interface has added features to simplify license management.

- The name and MAC address for the license server are displayed.
- Each license file installed is displayed with the associated host name, MAC address, and validity status
- Tool icons copy the MAC address for the PC to the clipboard or save it to a file to make it easy to provide the correct MAC address to create a new license or reassign a license.
- There is now a tool in the OpenLAB license administration dialog linking directly to the Agilent SubscribeNet site to generate license files.

Methods and Sequences

Some instruments allow parameters to be controlled on an instrument keyboard or a handheld controller. Since the ChemStation or the instrument may have the most current parameters, users can now select whether to download parameters to the instrument or upload them from the instrument when the ChemStation starts. In addition, when the parameters are uploaded from the instrument they can update the last method loaded in the ChemStation or create a new method with the instrument parameters.

Data Acquisition

Analysis Control

New single injection naming expands automatic naming from a simple prefix counter to pattern based naming that can combine any or all of the following elements:

- Date
- Time
- User Name
- Instrument Name
- Sample Name
- Counter
- Computer Name

Data Analysis

Time-Based Integration Events

Area sum ranges in integration now use the integration algorithm to set the baseline rather than drawing the baseline from the beginning point to the endpoint of the range.

Three new integration events allow control of the source of the baseline start and end when complex chromatograms may have long periods when the elution of compounds from the column prevents baseline from returning to zero. Set Baseline from Range uses a sophisticated algorithm to set a baseline from the beginning to the end of the selected range. Set Low Baseline from Range is similar but applies a correction to correct for higher noise. Use Baseline from Range allows the baseline determined for the range to be projected forward or backward from the range.

Area Sum Slice allows the area above a baseline set for the range to be sliced into sections to estimate the portion of the areas within each slice.

Peak Performance Calculations

A new Interactive Peak Performance tool opens a detailed display of peak performance information for the selected peak. The parameters for the calculations and the values to be included can be configured through settings dialogs.

Peak performance calculations now include relative retention time, Resolution, Number of theoretical plates, S/N ratio, and Peak-to-valley ratio according to European Pharmacopeia and Japanese Pharmacopeia. These values can be reported using Intelligent Reporting.

Many of the calculations have been adjusted and improved. The formulas and algorithms are detailed in the OpenLAB ChemStation Edition Reference to Operation Principles publication number M8301-90023.

OpenLAB Data Analysis A.01.01

Support for OpenLAB Data Analysis A.01.01 was introduced post-release of OpenLAB CDS A.01.04 (in November 2012). With OpenLAB Data Analysis, Agilent introduces a new data analysis package. The first release is specially designed for data analysis in Chemical and Petrochemical laboratories and in the Hydrocarbon Processing Industry. OpenLAB Data Analysis features intuitive operation, easy sample review and fast reprocessing of large sets of chromatographic data. OpenLAB Data Analysis is a new data analysis product for LC and GC

data that can be used together with OpenLAB CDS ChemStation Edition. It 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.

Reporting

Intelligent Report Items

Tables now support double rows. Multiple row controls enable a second header line and/or table detail line providing the flexibility to detail header information and to stack 2 rows to enable more fields within the same table width.

Individual report items may be locked to protect their definition in the report template. The privilege to lock and unlock items is a new privilege which can be assigned to a user or a role. This allows validated calculations to be locked to prevent accidental or intentional modification while allowing users access to less critical elements in the report.

User parameters can now be defined within a report template. Parameters are given a variable name, the data type is selected and text for a user prompt can be defined.

These parameters can be internal to the template so no prompts are displayed but the values defined in the template parameters can be set to adjust the behavior of the template for different reports. Multiple value parameters can be defined so the user selects from a list when the report is opened. Parameters always have default values so a defined value is available if the template is called through automation and the user cannot select or provide a value.

Previewing Intelligent Reports

In addition to PDF and XLS formats, Intelligent Reports can be exported to Microsoft Word DOC format and TXT format.

In larger and more complex reports, locating specific injections or injection types can become tedious. A new Document Map pane acts as a navigation tool for report views. The Document Map shows the injections in the results set and enables direct links from a specific injection to results in the report.

Automating Intelligent Reporting

For the naming of a Sequence Summary report an additional token LIMS ID has been introduced.

Automation

Queuing Sequences

Single injections initiated with the Run Method control are now placed into the run queue. A Queue Method control has been added so single injections may be added to run queue with sequences and EasySequences.

Good Laboratory Practice

Secure Data Storage and Result Revisions

With file-based data storage alone, the current results and the logs are properly preserved but the complete revision history is not recorded. When OpenLAB Data Store is configured as the central repository, the complete revision history is preserved. At the completion of a set of operations, the result set is zipped into an SSIZip and saved to the OpenLAB Data Store as a new revision. Once the data are stored in OpenLAB Data Store, each operation that modifies the data will result in a new revision once the data are uploaded again to OpenLAB Data Store.
A transaction log is maintained in OpenLAB Data Store detailing each data transaction with the identity of the operator, the dataset and a date and timestamp.
When a user requests a dataset to be returned to the OpenLAB CDS client for reporting or, recalculation or reprocessing they can view a list of previous revisions and select the revision to be returned.
For those specifically concerned with 21-CFR Part 11 compliance please consult the document Integration of Agilent OpenLAB CDS ChemStation Edition with OpenLAB Data Store - Compliance with 21 CFR Part 11 (5991-1470EN).

Agilent OpenLAB CDS ChemStation Edition for GC

Instruments

Updated Agilent GC Drivers, 78xx Driver Version 4.02, 68xx Driver Version 6.11
- Support for the 7650 Injector with 78xx GCs (G4567A)
- New menu item to extend run for 68xx GC
- GC Tray user interface enhanced (RC.NET only)
- Method Audit Trail and Method Resolution Audit Trail

Agilent OpenLAB CDS ChemStation Edition for LC

Updated Agilent LC Drivers (RC.NET Drivers A.02.05)
- Improved status dashboard for enhanced control and interaction
- 1290 Quaternary Pump (G4204A)
- 1220 Infinity LC with DAD (G4294B)
- Flexible Cube (G4227A)(Standalone Driver)
- Universal Interface Box II (G1390B)
- ISET 2 (Emulation for Waters Alliance systems, generic HPLC devices)

3rd Party Drivers: Support for Waters Acquity

Support for Waters Acquity drivers was introduced post-release of OpenLAB CDS A.01.04 (in October 2012). The Waters Acquity driver allows the control of the following Waters Acquity and Acquity H-Class modules in OpenLAB CDS ChemStation Edition C.01.04:
- 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

Documentation

Accessing OpenLAB Documentation and Manuals

New html-page for OpenLAB CDS Documentation can accessed from the START menu > All Programs > Agilent Technologies > OpenLAB CDS Documentation. Documentation installed from the product CD is organized into views and lists with links that directly open each document selected.

To learn more about OpenLAB CDS, visit us at **www.agilent.com/chem/openlabcds**

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