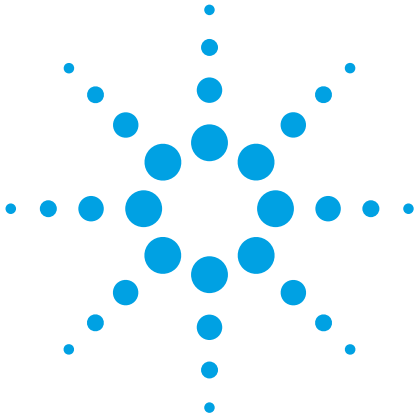

Agilent OpenLAB CDS
Functional Design Specification

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

OpenLAB CDS ChemStation Edition
OpenLAB CDS Shared Services

April 2015

Agilent Technologies

Table of Contents

Table of Contents *continued*

General Description

Overview

Agilent OpenLAB is a family of systems that create and manage analytical information. 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.

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 LC and GC data that can be used together with either OpenLAB CDS ChemStation Edition or OpenLAB CDS EZChrom Edition.

Agilent also offers complementary data management solutions that integrate seamlessly with OpenLAB CDS – scaling from a single workstation to the enterprise. With OpenLAB Data Store you can safely archive, store, and share electronic files in a central repository that can meet the needs of small to medium-sized laboratories. The tight integration of OpenLAB CDS ChemStation Edition with OpenLAB Data Store adds the necessary controls for managing system access, data transfer handling and detailed audit trail functionality. Agilent OpenLAB Data Store ensures secure record keeping, record audit trailing, versioning, as well as provides options for electronic signatures and data archival. OpenLAB Data Store is supported in networked and distributed configurations of OpenLAB CDS and provides several additional benefits:

- PostgreSQL Server or Microsoft SQL Server database support
- Web based data access for search, share, and review
- e-Signatures and audit trail capabilities that facilitate 21 CFR Part 11 compliance
- Chinese and Japanese local language support

Large laboratories face the same and even more demanding information challenges. OpenLAB Enterprise Content Manager (ECM) extends OpenLAB CDS ChemStation Edition into an analytical information management system. OpenLAB ECM provides the same level of security and functionality as OpenLAB Data Store, and scales up to the demands of large laboratories and environments spanning multiple labs. Similar to OpenLAB Data Store, OpenLAB ECM facilitates meeting compliance requirements as mandated by regulations such as 21 CFR Part 11. OpenLAB ECM supports English only content. In addition, OpenLAB ECM provides central storage of data and results from other computer-controlled analytical instruments, organizes results across an analytical operation, and enables organized online storage of files and documents associated with analytical processes.

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.

Supported Instruments

Agilent instruments supported on OpenLAB CDS ChemStation Edition include:

- Agilent 7890 series gas chromatographs
- Agilent 7820A gas chromatographs
- Agilent 6890 series gas chromatographs
- Agilent 6850 gas chromatographs
- Agilent 490 Micro gas chromatographs
- Agilent 1260 Infinity LC modules and systems
- Agilent 1290 Infinity LC modules and systems
- Agilent 1100/1200 Series LC modules and systems
- Agilent 1220 Infinity LC systems
- Agilent 1120 and 1220 Compact LC systems
- Agilent 6100 Series Single Quadrupole LC/MS and CE/MS
- Agilent 7100 capillary electrophoresis systems
- Agilent 35900E series A/D converters

In addition to Agilent instruments OpenLAB CDS ChemStation Edition supports the Waters Acquity and Waters Alliance instruments. Agilent OpenLAB CDS EZChrom Edition supports a wide variety of instruments from other manufacturers.

OpenLAB CDS Configurations

OpenLAB CDS ChemStation Edition is available in a number of different topologies:

- Workstation (standalone)
- Workstations (standalone) connected to a central data repository
- Networked Workstation
- Networked Workstation with a central data repository
- Distributed System with a central data repository

Depending on topology, system size and data management needs the central repository can be OpenLAB Data Store or OpenLAB ECM.

The Networked Workstation and Distributed System are managed using an Agilent OpenLAB Shared Services Server, which provides:

- Central configuration of instrument configuration,
- Central management of users and privileges
- Central management of software licenses
- An overview of the status of all instruments on the system (lab-at-a-glance view)

Agilent OpenLAB CDS ChemStation Edition may be installed and configured in three primary configurations:

- A *workstation configuration* where an Agilent OpenLAB CDS ChemStation Edition workstation directly controls up to four instruments with OpenLAB Shared Services running locally on each PC. The workstation configuration allows direct control of instruments from a standalone PC workstation without requiring server-based network resources. This configuration can optionally do central data management using OpenLAB ECM.
- A *networked workstation configuration* provides direct control of up to four instruments from each Agilent OpenLAB CDS ChemStation Edition workstation with central management of users and licenses on an OpenLAB Shared Services Server. With the networked workstation configuration, instrument control sessions are launched and operated from the individual workstations. The status of each instrument is available system-wide. This configuration can optionally centrally manage data in OpenLAB Data Store or OpenLAB ECM.
- A *distributed system configuration* where instruments are controlled via dedicated Agilent Instrument Control (AIC) servers and access is provided through distributed clients. Users, instruments and licenses are managed on a central OpenLAB Shared Services Server. The distributed system configuration allows each instrument to be accessed from any client on the network. The status of all instruments is available system-wide. Further, running instruments can be accessed across the network. The distributed configuration of OpenLAB CDS ChemStation Edition requires the connection to an OpenLAB Data Store or OpenLAB ECM system.

For distributed- or networked workstation systems, licenses are managed on the central OpenLAB Shared Services Server. This central license management on the OpenLAB Shared Services Server allows for dynamic license allocation. Workstations are licensed individually with licensing for each connected instrument. For more detail see the licensing section of this document.

Central Data Management

For any OpenLAB CDS ChemStation Edition configuration an Agilent OpenLAB Data Store can be added to provide a central data repository for the system. For large enterprises an Agilent OpenLAB ECM scales to their needs. Because both data repositories are tightly integrated with Agilent OpenLAB CDS ChemStation Edition for secure central data storage, Agilent OpenLAB Data Store and OpenLAB ECM specifications are included in this document.

Agilent OpenLAB ECM adds the following functionality:

- Microsoft SQL Server or Oracle databases as the shared central data repository
- Scheduled retrieval, transfer and storage of files from across the network including machines that are not part of OpenLAB CDS ChemStation Edition
- Management of raw data and human readable documents of any data, in any form, from any supplier
- Advanced meta data extraction for keying and searching data
- Secure file management for the entire lifecycle of scientific data including archiving and record retention controls
- Configurable, distributed storage
- An extensive Software Development Kit for product integrations and feature extensibility

Additional software modules for OpenLAB ECM extend the functionality of OpenLAB CDS as whole. Agilent OpenLAB ECM Intelligent Reporter creates a parallel results database to facilitate querying, filtering and reporting CDS results across the entire data repository. Business Process Manager (BPM) allows instantiation and control of records based business processes such as approval and signature of electronic documents.

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

Network Requirements

General Requirements

OpenLAB CDS ChemStation Edition systems rely on network infrastructure in order to support the communication between various system nodes. TCP/IP networking in a LAN is required for all products. This communication is based on standard TCP/IP protocols. In order to provide optimum performance and uptime, the network must meet design criteria for available bandwidth, IP address assignment (IP v4 only), name resolution and appropriate isolation of the lab subnet from the corporate network. IPv6 is not supported and must be deactivated.

When using LAN communications to connect workstations or instrument controllers to an instrument, the connection can be direct using a crossover CAT-5/6 cable or via an isolated switch using standard CAT-5/6 network cabling.

WAN's (wide area networks) are not generally supported. If you plan to implement OpenLAB CDS in a WAN please contact Agilent's Professional Services Organization (PSO) for consultancy services.

For systems configured to use a database external to the OpenLAB Shared Services Server, the network bandwidth between the database and the OpenLAB Shared Services Server must be maximized for best performance. The database and OpenLAB Shared Services Server should be physically connected to the same switch.

For more details on the individual topics outlined below please refer to the *Network Requirements Guides for OpenLAB CDS* (see chapter *Documentation* for the Agilent publication number).

Network Isolation

The communication path between instruments and workstations or instrument controllers is intolerant of latency, competitive traffic or service interruptions. For this reason the instruments and their controllers should be on an isolated network segment. This means there should be no routing within the segment, switching must provide dedicated resources for instrument communication, and the segment should have no other traffic including broadcast messages or network management traffic. Failure to isolate instrument traffic properly may make data acquisition unreliable.

Domain Requirements

Domains support the flow of information and user access rights across machines in the network. Even workstation installations can use a Windows domain-based authentication model. With domain-based authentication individual machines must always be able to communicate with domain components, not just to login but to receive authorization for many routine functions. All machines and instruments within the networked OpenLAB CDS ChemStation Edition system must reside within the same domain or have the appropriate cross domain trusts to allow name based communications between all components in the system.

The domain components necessary to support OpenLAB CDS ChemStation Edition host a variety of services and settings that must be configured appropriately to allow communication across machines.

Firewall Settings

If you are using a third party firewall on the network where OpenLAB CDS ChemStation Edition is installed, you will need to open a list of fixed firewall ports to allow communication between the system components of OpenLAB CDS ChemStation Edition. In addition OpenLAB CDS may use some dynamic ports. More information and detailed lists of required firewall ports for each product are available in the *Networking Requirements Guides for OpenLAB CDS*.

Environments with Proxy Servers

The servers used in an OpenLAB CDS environment (for example, ECM server, Data Store server, or license server) must be accessible via http or https in the network. This might require adjusting the proxy settings.

Computer Hardware and Software Requirements

The terminology for computer hardware in networked systems can be imprecise due to the variety of hardware and operating system combinations available. For the purpose of this specifications document, a PC means a desktop style personal computer running the specified Microsoft Windows operating system. A server is a computer with hardware suitable for continuous service in the networked environment. The version of Microsoft Windows installed on each machine is assumed to be at least "Professional" and not a starter or home edition.

In most cases the personal computer is interfaced to the analytical instruments through a LAN card, in cases where third party hardware is connected, specific interface cards may be required. In addition, there are serially connected instruments (via USB, RS232), e.g., the ELSD can be connected via RS232 directly to the workstation PC. Note that serially connected instruments are not supported on the Agilent Instrument Controller (AIC). Signals from third-party instruments can be acquired via the Agilent 35900E A/D-Converter interface. The separate hardware components that comprise a particular instrument configuration, including third party instrumentation, may need to be coordinated through a remote cabling system for time-critical events such as injection.

The following sections focus on the hardware and software requirements for OpenLAB CDS. For additional information regarding hardware and software requirements please refer to the *OpenLAB CDS Hardware and Software Requirement Guide*. All current OpenLAB CDS manuals with publication numbers are listed in the chapter *Documentation*.

Agilent Original PC Bundles

The Agilent Original Bundle PCs, shipped with many OpenLAB CDS products are computers from Hewlett-Packard, fully tested and qualified to run OpenLAB CDS software. Agilent Original Bundle PCs with Agilent instrument control software offer a one-stop solution for fast and seamless setup of analytical equipment in your laboratory. An Agilent Original Bundle PC comes with ready-to-use pre-installed Agilent software on a high-end computer from Hewlett-Packard with a pre-configured operating system, optimized for use with the specific software product.

To learn more about the Agilent Original Bundle PC please refer to the technical overview *Agilent Technologies Original Bundle PC* (please refer to chapter *Documentation* for publication number). Current hardware specifications can also be found at www.agilent.com/chem/bundlePC.

Agilent provides a selection of workstation PC bundles, optionally including a monitor and printer, and an Agilent Instrument Control (AIC) server bundle. All are equipped with two industry standard LAN interface cards or a 2 port network adapter. Please contact your Agilent Sales Representative for further details on the available products.

Support for Varying Computer Manufacturers

OpenLAB CDS ChemStation Edition has been designed to successfully run on a wide range of compatible personal computers equipped with accessories and peripherals that adhere to the programming standards for the Intel PC platform and Microsoft Windows operating systems. Agilent Technologies has tested OpenLAB CDS ChemStation Edition software mainly on Hewlett Packard equipment. All configuration information listed in the manuals applies to Hewlett-Packard computers and may not be optimized for other vendors' PCs. For a non-Hewlett-Packard computer, use the setup utility program supplied by the manufacturer to configure your computer. Although the software is also designed to be run on other compatible hardware Agilent Technologies will not necessarily accept responsibility for defects solely observed and reported on third party hardware.

Agilent offers a variety of preconfigured Agilent Original Bundle PCs that provide lots of benefits over computers from other manufacturers. For details refer to the chapter *Agilent Original PC Bundles*.

OpenLAB CDS ChemStation Edition Workstations

Unless otherwise stated, workstations are tested and supported with any combination of four instruments (LC's containing DAD and/or FLD count as 2 instruments) with up to one Headspace or CTC Sampler running simultaneously.

OpenLAB Shared Services Server

Agilent OpenLAB Shared Services Servers manage system information in a database. For OpenLAB CDS ChemStation Edition Workstation, this service and associated database is installed and configured automatically during installation of OpenLAB CDS ChemStation Edition.

For networked system configurations, this service and database must be installed explicitly to ensure acceptable performance of the system.

The following database software is supported for OpenLAB Shared Services in networked configurations:

- PostgreSQL
- Microsoft SQL Server Standard or Enterprise
- Oracle

OpenLAB CDS ChemStation Edition AICs

In a distributed configuration instruments are controlled via dedicated Agilent Instrument Control (AIC) servers and access is provided through distributed clients. In such a configuration a limit of 10 instruments with 2D detectors can be configured on a single OpenLAB CDS ChemStation Edition AIC. With 3D detectors such as the LC diode array detector or the CE with diode array detection the limit drops to 5 instruments per AIC. For LC/MSD and CE/MSD instruments only 2 instruments are supported per AIC. One LC/MS or CE/MS Single Quadrupole (SQ) instrument is equivalent to four 2D LC instruments. A single AIC can therefore handle two LC/MS or CE/MS SQ instruments and two 2D LC instruments or two LC/MS or CE/MS SQ instruments with one 3D LC instrument.

Each instrument can consist of several modules, as in the case of Agilent modular LC systems. The theoretical maximum number of modules is 31; the recommended maximum number is 14.

OpenLAB CDS ChemStation Edition supports instruments and modules connected exclusively via LAN. (GPIB, RS232, USB or any converter are not supported on AICs.) There is no limit to the number of AICs allowed in an OpenLAB CDS ChemStation Edition distributed system.

Secure Workstation for OpenLAB CDS ChemStation Edition

The Secure Workstation for OpenLAB CDS ChemStation Edition requires Data Store A.02.02 or higher. The required PostgreSQL version is automatically installed with Secure Workstation. A maximum of 2 instruments can be controlled with a Secure Workstation. In case of LC/MSD or CE/MSD the limit is one instrument.

Central Storage Server and Database Requirements

OpenLAB Data Store Server

OpenLAB CDS ChemStation Edition supports the use of OpenLAB Data Store as a central storage location for scientific data. OpenLAB CDS ChemStation Edition and ICP/MS MassHunter Workstation are supported on the same Data Store server. For product version compatibility information please refer to the *OpenLAB CDS Hardware and Software Requirements Guide*.

OpenLAB Data Store is used to store data from different types of instruments. The performance of the system depends on server hardware that can support the number and size of the data files that must be stored on the system. Based on the individual laboratory requirements Agilent recommends differently sized server hardware. OpenLAB Data Store should be installed on a dedicated host machine.

OpenLAB Data Store makes use of a database to manage its information. OpenLAB Data Store can be configured to use an Oracle, Microsoft SQL Server or PostgreSQL database. For complete details about OpenLAB Data Store requirements please refer to the *OpenLAB Data Store Hardware and Software Requirements Guide*.

All current OpenLAB CDS manuals with publication numbers are listed in the chapter *Documentation*.

OpenLAB ECM Server

OpenLAB CDS ChemStation Edition supports the use of OpenLAB Enterprise Content Manager (ECM) as a central storage location for scientific data and other human readable documents.

OpenLAB ECM can also be used to store data from other types of instruments. The performance of the ECM system depends on server hardware, the number of active instruments connected to it and the total number and size of the data files that is stored in the system. Based on the individual laboratory requirements Agilent recommends differently sized server hardware.

OpenLAB ECM must be installed on a dedicated host machine/s. There are several services running in an OpenLAB ECM installation - a Web Server, a File Transfer Server, an Application Server and the Database Server. Often, in smaller installations these services could be combined onto one physical server and for larger installations there will be more than one server to host different services.

Agilent OpenLAB ECM manages information using a database. The database software can be Oracle or Microsoft SQL Server.

For information regarding hardware and software requirements or product version compatibility please refer to the *OpenLAB ECM Hardware and Software Requirement Guide* or the *OpenLAB CDS Hardware and Software Requirements Guide*. All current OpenLAB CDS manuals with publication numbers are listed in the chapter *Documentation*.

Installation

The Master Installer is the central utility to prepare, install, uninstall or add components of OpenLAB CDS. It includes a site preparation tool that checks the system hardware, operating system and installed software. The OpenLAB CDS Installation Wizard provides for a guided installation of the OpenLAB CDS software suite. The Software Verification Tool verifies a successful installation.

The following components are installed by the Master Installer:

- OpenLAB CDS ChemStation Edition Workstation
- OpenLAB CDS ChemStation Edition Networked Workstation
- OpenLAB CDS ChemStation Edition Clients and Agilent Instrument Controllers (AICs)
- Secure Workstation for OpenLAB CDS ChemStation Edition
- OpenLAB Shared Services Server
- OpenLAB Data Analysis
- Connection to central data storage (Data Store or ECM)

In addition the Master Installer has the following capabilities:

- *Upgrade installation* – Installation of OpenLAB CDS on top of an existing system (C.01.03 or higher) resulting in an automatic upgrade.
- *OpenLAB CDS Repair Wizard* – Software installation repair using the repair utility in the maintenance section of the Master Installer.
- *Adding OpenLAB Data Store after an upgrade installation* – Add OpenLAB Data Store components to an AIC or client upgraded from a previous revision.
- *Transform a standalone workstation into a networked workstation* – The installer will add the connection to the OpenLAB Shared Services Server and will register the workstation in the list of instrument controllers.
- *Scripted installation of clients and AICs* – 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 computers.

Installation of OpenLAB CDS requires the installer to be logged into the machine as a domain user that is also a local administrator. This enables the OpenLAB CDS master installer to apply network exceptions to the Microsoft Windows firewall under the domain profile which is necessary to configure a functional system. OpenLAB Data Store and OpenLAB ECM server software is installed separately. Both have their own installer and separate media.

Virtualization

OpenLAB CDS ChemStation Edition, OpenLAB Shared Services Server, instrument controllers and client systems can be virtualized. VMWare ESX hosted virtual machines are also supported for use as OpenLAB Data Store systems. Please contact your Agilent support representative for specific requirements and details.

When using virtual machines as OpenLAB CDS ChemStation Edition clients, Instrument Controllers (AIC's), or networked workstations, the network connections to instruments and application components should be as direct as possible. Each additional router or switch will adversely affect the performance of the entire system. Virtualization of instrument controllers introduces a risk to data buffering functions for the system.

Note that serially connected instruments are not supported under VMware.

Agilent recommends the use of VMWare vSphere software for host machines. All resources for machines hosting OpenLAB components should be reserved in the ESX host, and extra care should be taken to balance a heavy load on disk access and LAN communication on the ESX host server.

For the virtualization of OpenLAB CDS ChemStation Edition the participation of a VMWare application expert is strongly recommended. For more information a technical note *Virtualizing Agilent OpenLAB CDS ChemStation Edition with VMware* is available (see chapter *Documentation*).

OpenLAB Licensing

Agilent OpenLAB CDS ChemStation Edition and Agilent OpenLAB Data Store support the use of a central licensing server for the distribution and tracking of license entitlements. FlexNet Publisher is used for this purpose and is installed with the installation of OpenLAB Shared Services Server components.

Language Compatibility

The English version of OpenLAB CDS is validated on Windows English language version and on localized language version of Windows 7 (64bit) and 8.1 (64bit), using default system fonts for Russian.

Localized versions of OpenLAB CDS ChemStation Edition are supported on localized language versions of Windows, using default system fonts (Chinese: SimSun; Japanese: MS UI Gothic).

Non-localized instrument drivers are supported, and will appear in English even when running localized versions of OpenLAB CDS ChemStation Edition.

Localized versions of OpenLAB Data Store are supported on localized language versions of Windows, using default system fonts for English, Chinese, and Japanese.

Printers

The Agilent OpenLAB CDS ChemStation Edition has been designed to work with printers that are compatible with the operating system. The software operates with any Microsoft Windows compatible printer capable of interpreting an escape code language (e.g. PCL) or page description language (e.g. PostScript). The printer may be directly connected to the computer through a parallel or serial interface or connected through a Local Area Network. Serial port printers are supported by the operating system but may exhibit speed performance limitations.

Networked printers must be shared by a network server running a network protocol supported by the Microsoft operating system. Agilent recommends similar printer specifications as offered with our software bundle PCs (see www.agilent.com/chem/bundlePC). Proven black and white printers are the HP LaserJet family using PCL 5e or 6.

Agilent Technologies has not tested all printer and printer driver combinations that are supported in the Windows environment. Print performance and results may vary on other manufacturers' printers and appropriate drivers. Please note that host-based printers (e.g. GDI or PPA printers) impose more processing tasks on the CPU and are not recommended for use with the Agilent OpenLAB CDS ChemStation Edition on-line sessions.

Instrument Communication

OpenLAB CDS ChemStation Edition provides standard LAN-based communication with the instrument, using TCP/IP. All Agilent instrument hardware that is currently supported by OpenLAB CDS is controlled over LAN. For control of some 3rd party instruments OpenLAB CDS additionally supports other communication protocols such as GPIB. Please refer to the instrument specific sections in the chapter *Instrument Control* for details.

LAN Interfaces

The Agilent OpenLAB CDS ChemStation Edition software provides network-based instrument control and data acquisition for network-capable Agilent instruments, optional A/D controllers and some 3rd party instruments. For general networking requirements see also the chapter *Network Requirements*.

Current Agilent instrument hardware is equipped either with an onboard LAN interface or with a G1369C LAN Interface card to connect the analytical instrument to the LAN.

For further information please refer to the *OpenLAB CDS ChemStation Edition Instrument Configuration Guide* (see chapter *Documentation*).

LAN Communication Protocols

Instruments are controlled over LAN using industry standard TCP/IP (Transmission Control Protocol / Internet Protocol). It is necessary to verify correct and stable communication between the PC and analytical instruments connected over the LAN.

For Agilent instruments, the IP address is typically set either from the instrument's front panel, over telnet, or using a handheld control module. Some instruments can use a predefined IP address which is enabled by DIP switches. The IP address is stored in the non-volatile RAM of the module's LAN interface. This is the preferred mode.

For some LAN instruments, the Agilent BootP service is an alternative to assign and administer IP addresses. This method is primarily used for instrument hardware with older LAN cards. For details please refer to the hardware manuals and the *OpenLAB CDS ChemStation Edition Instrument Configuration Guide*.

Additional Hardware Required for LAN Instrument Control

Instruments are connected using industry standard CAT 5/6 twisted pair LAN cabling with RJ45 connectors. An Agilent G2402A 8-port 10/100 auto sensing switch can be used to connect one or more instruments to a PC. A twisted pair 'crossover' cable can be used to make a single connection from one PC to one instrument. This configuration is only suitable for single instrument configurations. This configuration is not supported on Agilent 1100 Series and Agilent 1200 Infinity Series LC/MSD systems.

LAN Transmission Rates

Traffic on the LAN from each instrument is approximately 100 kb per second for a 2D instrument at its maximum data rate.

OpenLAB Control Panel

The OpenLAB Control Panel is the OpenLAB Shared Services client, providing access to instrument management and system administration. All functions in the OpenLAB Control Panel are under system access controls, so the access each user has to the OpenLAB Control Panel is dependent on the roles he has been assigned.

If access control is not required, the OpenLAB CDS can also we used in a mode where user authentication is not enforced. In this mode all functions of OpenLAB Control Panel are available to all users. More details are provided in the section *OpenLAB Control Panel Administration*.

OpenLAB Control Panel functions are divided into views selected through buttons in the lower left pane of the application's user interface. The Instrument view provides a display of the instruments connected to the system, instrument session launch controls, and tools for configuring and managing instruments. The Administration view provides access to system administration functions. In addition, a Projects view is available if OpenLAB ECM Intelligent Reporter or OpenLAB Data Analysis is installed.

OpenLAB Control Panel Instruments

The Instruments view in OpenLAB Control Panel offers an overview of all instruments in the network or on the workstation. It is often referred to as “Lab (Status) at a Glance”.

The Navigation Pane

All instruments connected to the system are displayed in a tree in the Navigation pane on the left of the Instrument view. The Instruments item is the root of the instruments tree. When the root is selected, a table of all instruments connected to the system is displayed in the workspace to the right.

Locations are optional and allow grouping instruments into user-defined groups. Instruments can be created within a location or moved to a location by dragging and dropping. Selecting a location opens a table displaying the same status information for the instruments as the root but limited to those instruments assigned to the location.

The context menu and toolbar buttons enable creating, editing or deleting instruments or locations.

As each instrument or location is created it appears as a named node in the instrument tree. There is always one unique item for each instrument connected to the system. Selecting an instrument item opens an instrument status pane for the individual instrument in the workspace on the right.

Instruments

Selecting the Create button and then “Create Instrument” opens an instrument creation dialog. The dialog begins with a mandatory unique instrument name. Names are unrestricted and can be chosen to match an existing instrument naming scheme. An optional description can be used to label the instrument with more detailed information. The Application field provides a list of available instrument control applications. An instrument controller is then selected. For workstations this is fixed to the local controller. For networked or distributed systems, the controller (networked workstation or AIC) for the instrument is selected from a list of registered controllers available on the system. The instrument type is selected from a list of instrument types. An optional contact field offers space for entry of a contact responsible for the instrument. When OK is selected, the instrument is instantiated and appears in the instrument tree. At this point the instrument can be configured.

Most current instruments can be configured automatically by providing the IP address of the instrument and waiting for the system to locate and identify the instrument. Once modules are identified, they may have optional configuration items that can be accessed by opening each module. Instrument configuration is also available when the instrument is launched to facilitate dynamic configuration for instruments that are operated in more than one configuration.

Instrument control and data processing are performed through associated OpenLAB CDS ChemStation Edition application sessions. Each instrument has an online session which connects to the instrument and an offline session which allows methods and data to be loaded without affecting the settings on the instrument. For workstations, these instrument sessions are running on specific host workstations and can only be run from that workstation. Because the instrument control is running on a specific workstation, this workstation must be running and connected to the instrument whenever data acquisition is active.

With a distributed system, instrument control sessions run on their assigned AICs and an instrument’s online and offline sessions are accessed through Remote Desktop Services from any OpenLAB CDS client. Only one client is allowed to access a specific instrument session at a time. With instrument control running on the AIC, an operator can disconnect from a running instrument at one client location and move to another client and reconnect later without affecting ongoing automated acquisition.

For any selected instrument, the Create Shortcuts button will add a shortcut to launch the online and offline sessions for a given instrument to the desktop of the local computer.

There are also data analysis (DA) only instrument types for all techniques available.

Instrument Status Displays

When a location is selected in the navigation pane, all of the instruments in the location and all locations beneath it are displayed in a single instrument status table. Each row has a color coded status, with the colors:

- Grey – Not Connected
- Green – Connected and Ready
- Yellow – Connected and Not Ready
- Red – Error
- Magenta – Injecting
- Blue – Running
- Teal – Sleep (7890B GC) and Standby

By default all status columns are displayed including:

- Location
- Application
- Type
- Controller
- Description
- Last Configured By
- Last Configured
- Created
- Used By
- Remaining Time

Selecting Edit Columns allows configuration of this table. Unchecking an item removes it from the table. A selected item can be moved up or down the list to move the corresponding column to the left or the right in the table.

Selecting an individual instrument displays a status page with expanded display of the same information provided in the instrument status table along with an instrument activity log. The activity log is an overview of activities on the instrument for the last 24 hours. This is a portion of the information stored in the permanent instrument logs.

Instrument Privileges

Instruments are created with a default privilege setting of "Inherit Privileges from Parent". This means instrument access privileges are set from the level above and ultimately from the instrument root. This means privileges set in the Administration view are automatically applied to each instrument.

If users are to have access to some instruments but not others or to have different privileges on different instruments, the privileges can be set at any level in the instrument tree. With inheritance active, privilege adjustments to locations apply to all locations and instruments within the location.

Privileges are changed by selecting the item and then selecting Edit Privileges. When the "Inherit Privileges from Parent" option is unchecked, the parent privileges can be copied down to the item or set from scratch. Users or User groups can then be explicitly assigned or removed and the specific roles added or removed. User privileges are detailed in the *OpenLAB Control Panel Administration* sections.

Instrument Session Locking

The OpenLAB Control Panel and the OpenLAB CDS ChemStation Edition sessions can be locked manually or be set to lock based on a timeout after the configured period of user inactivity. Users can lock OpenLAB CDS ChemStation Edition "Privately" (only the current user or an administrator can open the session) or "Non-Privately" (any valid user can open the session).

The Timeout period can be set in the OpenLAB Control Panel in the Security Policy section of the Administration view. On each installation, the "OpenLAB CDS ChemStation Edition Administration Tool" which is available from the Windows Start Menu, can set the locking mode for time-based and manual locking. The OpenLAB CDS ChemStation Edition Administration Tool also allows administrators to set the option "Break session lock". This allows any user to break a private session lock (set by another user or time-based). This may be useful in an emergency situation if an instrument needs to run 24/7 and any operator needs to be able to break a session lock.

Selecting the Lock button from the toolbar or "Lock" from the context menu will lock an open session. The operator opening the session must supply login credentials based on the authentication configured for the system.

Locations

Locations are created with a name and have an associated description. Locations can be created within locations to create a multi-level hierarchical organization for the instruments. Instruments can be created in a location or directly under the Instruments root node.

Locations cannot be deleted when they have content so locations or instruments within a location must be deleted or moved before the location is deleted.

OpenLAB Control Panel Projects

The Projects view in the OpenLAB Control Panel is used to add, edit, or remove projects. A project is the set of directories that store related methods, data, sequences, and templates. Project Groups can be used to arrange projects to match the organizational structure.

The Projects view is not automatically available for OpenLAB CDS ChemStation Edition. OpenLAB CDS ChemStation Edition does not utilize projects by itself. As soon as an application is installed that requires projects the Projects view appears in OpenLAB Control Panel. Projects are necessary when using OpenLAB Data Analysis (data analysis project) or OpenLAB ECM Intelligent Reporter (reporting project).

To use OpenLAB Data Analysis with OpenLAB CDS ChemStation Edition it is necessary to configure one project for each ChemStation instrument. On the OpenLAB Data Analysis tab the paths to the related Data, Method, and Template subfolders of the instrument folder can be set.

The ChemStation projects can also be managed in a Project Group. For a project groups, administrators can automatically create one project for each configured instrument within this group when selecting Create Projects for ChemStation Instruments from the properties toolbar.

When a Data Analysis only client without OpenLAB CDS ChemStation Edition is installed, users can create one OpenLAB Data Analysis project containing the paths to the relevant data, methods, and templates.

OpenLAB Control Panel Administration

The Administration view in the OpenLAB Control Panel provides a display of configuration and settings and tools to modify the OpenLAB Shared Services configuration. The navigation pane on the left allows users to select a given section. Corresponding tools and workspace appear for each selection.

The items available in the navigation pane will depend on the user's privileges. All users can see My Settings, the Local Configuration, and the System Activity Log.

My Settings

This section allows each user to check his information and access to the system. Selecting "My Settings" will display fields that can contain the user's Name, Email Address, and Contact Information. Depending on the authentication mode selected, these may reflect settings returned to OpenLAB CDS from the selected authentication provider (OpenLAB Shared Services, Windows domain, Windows local or OpenLAB ECM).

The Group memberships and Roles assigned will be displayed. This display can help not just determine a user's OpenLAB CDS settings but also the information returned to OpenLAB CDS in the authentication process.

"My Settings" is only available when user authentication is enabled.

Local Configuration

This item displays the URL for each available OpenLAB Shared Services Server. Depending on the system topology the OpenLAB Shared Services may be local or accessed on a central server. For networked workstation and distributed systems, the "Local Configuration" item displays the server selected for the current connection, and the current connection status. OpenLAB Shared Services Servers can be added, deleted or edited. When information for a server is entered, you can test the connection to make sure the server is available. The server should be configured and available on the network before it is added to the system.

The local instance can be connected to any valid server in the list. This can reassign the relationship between workstations or clients with available OpenLAB Shared Services Servers or it can be used to connect to a remote OpenLAB Shared Services Server for administration.

For a networked workstation configuration an administrator can configure the local OpenLAB Shared Services as a fallback option. In the event of a network- or server outage, this allows the user to select the option "Switch to Failover Mode" during the startup of OpenLAB Control Panel, thereby switching to the local instance of OpenLAB Shared Services. This local instance of OpenLAB Shared Services needs to be prepared ahead of time by an administrator with licenses and instrument configurations. This effectively makes the local instance a standalone workstation until an OpenLAB Shared Services Server connection is restored.

System Configuration

System Settings

"System Settings" control the configuration of user authentication and data storage for the system. OpenLAB CDS supports the following authentication providers:

- *No Authentication* – eliminates the requirement for users to provide any credentials to access the system. The generic user name SYSTEM will be used for logs and reports.
- *Internal* – the user accounts are created by and stored within OpenLAB Shared Services.
- Windows Domain – Domain users and groups defined in the Active Directory services can be granted access to the OpenLAB CDS with the Windows domain controller providing user authentication.
- *Windows Local* – Local Windows users and groups can be granted access to the OpenLAB CDS with the local Windows operating system providing user authentication.
- *OpenLAB ECM* – Users and groups for the OpenLAB CDS are administered through OpenLAB ECM. OpenLAB ECM allows the creation of built-in users defined and authenticated through the built-in database account. Alternatively, it is possible to grant Windows domain users access to OpenLAB ECM and OpenLAB Shared Services with the Windows domain controller providing user authentication. Both modes can be mixed.

When OpenLAB ECM is chosen as the authentication provider, OpenLAB ECM becomes the storage type and the OpenLAB ECM database becomes the storage location for OpenLAB CDS ChemStation Edition.

Instrument Status Refresh

The refresh interval can be set for instruments and for the full system. The interval can be set to zero to disable status refresh.

Activity Log Settings

By default, the system is installed with the detailed System Activity Log disabled. The log can be enabled but once enabled cannot be disabled.

The System Activity Log contains information on the various events associated with the OpenLAB Shared Services or with specific instruments. You can filter the list in order to view only the events of a specific type, in a specific time range, created by a specific user, or containing a specific description.

The following types of events are recorded:

- System
- Instrument Management
- Instrument
- Project Management
- Instrument Controller
- User
- Group
- Security
- Printer
- License

The system activity log can be exported, printed and selections can be copied to the clipboard.

Email Server

Not applicable for OpenLAB CDS ChemStation Edition.

Security Policy

With OpenLAB ECM as the authentication provider, the core security policy is controlled in OpenLAB ECM. An inactivity timeout can be configured. After the selected period of inactivity the application interface will lock.

With Windows domain (or local) as the authentication provider, the core security policy is controlled by Windows domain (or local). An inactivity timeout can be configured. After the selected period of inactivity the application interface will lock.

With OpenLAB Shared Services as the authentication provider, the administrator can set a "Minimum password length", "Password expiration period" and a "Maximum number unsuccessful login attempts before the account is locked". The administrator can set an "Account lock time", which determines how long the account is frozen after a user has exceeded the maximum unsuccessful number of login attempts.

Users

Users may be imported from the authentication provider or created in OpenLAB Shared Services. Users can be assigned to groups defined within OpenLAB Shared Services.

For each user there is a checklist of roles available in OpenLAB CDS ChemStation Edition. Each role may be assigned or removed for the user. Alternatively users may inherit roles from the groups they have been assigned to.

Groups

Groups defined by the authentication provider can be imported and added to the access list for the OpenLAB CDS. Additionally, local groups can be defined to group users on the OpenLAB CDS access list to simplify role assignment.

For each group there is a checklist of roles available in OpenLAB CDS ChemStation Edition. Each role may be assigned or removed for the group.

Roles

Roles are a defined set of OpenLAB CDS privileges given a name and description. A set of predefined roles are available at installation. Each role (with the exception of the *Everything* role) may be edited to add or remove specific privileges. New roles can be added with user-defined names and privileges. Privileges are broken into privilege groups. For a role the privilege group may be selected or the privileges individually.

The table below lists each role and the checkmarks indicate the privileges assigned by the role. For better overview, the privileges are logically grouped by the privilege group name.

Role Name	Everything	System Administrator	Instrument Administrator	Project Administrator	Instrument User	OpenLAB CDS ChemStation Edition Administrator	OpenLAB CDS ChemStation Edition Lab Manager	OpenLAB CDS ChemStation Edition Analyst	OpenLAB CDS ChemStation Edition Operator	DA Chemist	DA Technician
Administration											
Manage Printers	●	●									
Edit Activity Log Properties	●	●									
Create Administrative Reports	●	●									
Manage System Components	●	●									
Manage Security	●	●									
Manage Instrument Controllers	●	●									
Unlock Any Locked UI	●	●									
Instrument Management											
View Instrument or Location (not editable)	●		●		●						
Manage Instrument or Location	●		●								
Manage Instrument or Location Access	●		●								
Run Instrument	●		●		●						
Service Instrument	●		●								
Project Management											
View Project or Project Group (not editable)	●			●		●	●	●	●	●	●
Manage Project or Project Group	●			●							
Edit Content of Project	●			●							
Manage Project or Project Group Access	●			●							
E-Signature											
Signature Sign Data Files	●			●							
OpenLAB CDS ChemStation Edition Control											
Run Acquisition	●						●	●	●		
OpenLAB CDS ChemStation Edition Data											
Delete Data	●					●	●				
Manual Integration	●					●	●	●			
Save Data to Storage	●					●	●	●	●		
OpenLAB CDS ChemStation Edition Instrument											
Modify Instrument Configuration	●						●				

Role Name	Everything	System Administrator	Instrument Administrator	Project Administrator	Instrument User	OpenLAB CDS ChemStation Edition Administrator	OpenLAB CDS ChemStation Edition Lab Manager	OpenLAB CDS ChemStation Edition Analyst	OpenLAB CDS ChemStation Edition Operator	DA Chemist	DA Technician
OpenLAB CDS ChemStation Edition Logbook											
Clear Logbook	●					●	●				
Save Logbook	●					●	●	●			
OpenLAB CDS ChemStation Method											
Edit Calibration Table	●						●	●			
Delete Method	●					●	●	●			
Edit Integration Events	●						●	●			
Edit Ion Labels	●										
Edit System Suitability	●							●			
Enable Audit Trail	●					●	●				
Modify Instrument Method	●					●	●	●			
Modify Method Properties	●					●	●	●			
Perform Method Recalibration	●						●	●			
Save Method Changes	●					●	●	●			
OpenLAB CDS ChemStation Edition Report											
Preview/Print Report	●					●	●	●	●		
Modify Report	●						●	●			
Lock/Unlock Report template items	●						●				
OpenLAB CDS ChemStation Edition Security											
Break Session Lock	●					●	●				
Take over ChemStation Remote Session	●					●	●				
Command Line	●					●	●				
Manage Transfer Queue	●					●	●				
Modify Storage Transfer Preferences	●						●				
OpenLAB CDS ChemStation Edition Sequence											
Delete Sequence	●					●	●	●			
Edit Sequence Summary	●						●	●	●		
Reprocess	●						●	●			
Save Sequence Template	●						●	●			
Delete Entries from Run Queue	●						●				
Change Priority in Run Queue	●						●	●	●		

Role Name	Everything	System Administrator	Instrument Administrator	Project Administrator	Instrument User	OpenLAB CDS ChemStation Edition Administrator	OpenLAB CDS ChemStation Edition Lab Manager	OpenLAB CDS ChemStation Edition Analyst	OpenLAB CDS ChemStation Edition Operator	DA Chemist	DA Technician
OpenLAB CDS ChemStation Edition View Access											
Access Companion View	●						●				
Access Data Analysis View	●					●	●	●			
Access Diagnostic View	●					●	●				
Access Method and Run Control View	●					●	●	●	●		
Access Retention Time Lock	●										
Access Retention Time Search	●										
Access Review View	●					●	●	●			
Access Tune View	●						●				
Access Verification View	●						●				
Access Report Layout View	●					●	●	●			
Enable Batch View	●						●	●			
OpenLAB Data Analysis											
Edit Sample Information	●									●	●
Reprocess Data	●									●	●
Create new Method	●									●	
Save Processing Method	●									●	
Edit Integration Parameters	●									●	
Edit Identification Parameters	●									●	
Edit Calibration Parameters	●									●	
Edit Report Templates	●									●	
Lock/Unlock Report Items	●									●	
Do Manual Compound Identification	●									●	●
Do Manual Integration	●									●	●
Update DA Master Method	●									●	

Links

OpenLAB Shared Services stores and displays a link list for users of the system. Links can point to any URL accessible through the network configuration used to implement the system. There are predefined links to the following websites:

- Agilent Informatics Software Portal
- Agilent Support
- Agilent's Website
- OpenLAB Customer Survey

Tools allow administrators to create, edit, delete or hide the links in the list. Each link is defined as a text label and a link URL. Optionally, an .ICO file can be selected to associate an icon with each link.

Licenses

OpenLAB Control Panel administers all licenses that are required for instrument modules and add-ons. When starting an instrument, OpenLAB CDS automatically checks whether the required licenses are available in the license pool, and reserves the licenses needed to operate the instrument. When stopping the instrument, the freed licenses can be used by other instruments. This licensing strategy introduced with OpenLAB CDS enables more effective use of licenses. Licenses for instrument control, drivers and add-ons are floating licenses.

The OpenLAB Shared Services use a 3rd party tool called FlexNet Producer Suite from Flexera to manage the licenses. The license server can be local, on an OpenLAB Shared Services Server, or on a separate Flexera license manager server.

The MAC address and name of the current license server are displayed in the user interface. All installed licenses are listed.

OpenLAB CDS provides the following license types:

- Core license
- Instrument Control license
- Driver license
- Add-on license

The OpenLAB CDS ChemStation Edition core license enables data analysis, automation and customization functions (no instrument control) for the following separation techniques:

- Gas chromatography (GC)
- Liquid chromatography (LC)
- Capillary electrophoresis (CE)
- Analog data acquisition with external event protocol (A/D)

One OpenLAB CDS ChemStation Edition core license is required for each OpenLAB CDS ChemStation Edition PC or AIC and is shared by all required sessions residing on the same machine. Networked Workstations or Distributed Systems also require one Shared Services Server license for each OpenLAB Shared Services Server in the system.

Each instrument driver license product contains an instrument control license and an instrument driver license. The license server counts the licenses in use, so starting an instrument control session consumes a license and closing the session releases it to the license pool. This means it is not required to have a license for every instrument but the system will limit the number of concurrently active instruments to the number of instrument licenses.

There are three add-on licenses:

- 3D UV,
- MS Data Analysis and
- MS Bioanalysis and Deconvolution.

One of these licenses is required per instrument. Sessions without a 3D UV license will have spectral data acquisition and processing disabled. MS Data Analysis is mandatory for MS OpenLAB CDS ChemStation Edition sessions; the MS Bioanalysis and Deconvolution license enables the optional deconvolution features.

There is a 60-days Startup License for the system. The expiration period starts with the installation of an application. In order to run the data system software after that period, you must install the appropriate licenses. License purchases provide an authorization code to enable creation of the appropriate license file or files from Agilent's SubscribeNet online service. The 'Get License' tool in the OpenLAB license administration dialog links directly to the Agilent SubscribeNet site.

Licenses are specific to the computer they are installed on. Each license file installed is displayed with the associated host name, MAC address, and validity status in the licensing user interface. Licenses may be returned and reissued for a different computer when a hardware change is required. To make it easy to provide the correct MAC address to create a new license or reassign a license, the licensing toolbar includes tools to copy the MAC address for the PC to the clipboard or save it to a file. The license can be returned and reissued twice.

In Summary, the License Management in OpenLAB Control Panel provides the following functions:

- Add license files to the license server.
- Navigate to the license monitor and view the properties of all licenses installed on a given license server.
- Remove license files from the license server. This may be useful if an invalid license file has been added.
- View or change the license server.
- View, copy, or save the MAC address of the license server.
- Navigate to the Agilent Electronic Software and License Delivery web page (Agilent SubscribeNet site) to get a license.

For more details related to licenses please refer to the current *OpenLAB CDS Administration Guide* (see chapter *Documentation*).

Instrument Controllers

OpenLAB Shared Services administers instrument controllers. For standalone or networked workstations, the local PC is the instrument controller. For distributed systems Agilent Instrument Controllers (AICs) run on one or more independent servers.

A status table lists all the instrument controllers assigned to the Shared Services Server. For each instrument controller the table displays:

- Name
- PC Name
- Type
- Network Status
- Location
- Comments

The OpenLAB Shared Services instrument controller management tools allow the administrator to perform a series of management functions.

Instrument controllers may be deleted from the Shared Services Server. Each instrument controller can be pinged to determine its ability to respond on the network. A report can be generated providing the detailed configuration of an instrument controller. To easily access and collect diagnostic information, a detailed list of the log files on each instrument controller can be launched. All or selected files can be marked on the list and written to a single file.

Diagnostics

Version

The version section displays the software version and builds for client and server.

Installed Components

The installed components section displays a table of the detailed software components installed including the following information:

- Component Name
- Description
- Assembly version
- File Version
- Product version

Some or all of the rows may be selected and copied to the clipboard to export the information for diagnostics purposes during a support call.

The server tools provide means to diagnose the OpenLAB Shared Services Server. It can be pinged to determine its ability to respond on the network. A detailed server report can be created.

A service mode for advanced diagnostics, restricted to Agilent access, opens the Agilent OpenLAB Diagnostics Dashboard. The dashboard can modify the local or remote log configuration and create local system diagnostic reports.

Log Files

All local or server log files or a subset of them can be selected and saved for diagnostics, during a support call or for documentation purposes.

Administrative Reports

Administrative reports allow detailed system configuration information reports to be created. The following reports types are available:

- *Instrument Controllers Report* – listing the name, address, connected instruments and status of each instrument controller
- *Instruments Report* – listing details of the configured instruments
- *Projects Report* – listing all projects and related details, assigned users and groups, and their roles and privileges
- *Roles and Privileges Report* – listing all roles and their associated privileges
- *System Report* – listing instruments, assigned users and groups, and their roles and privileges
- *Users and Groups Report* – listing instruments, user and groups and their roles

The Create Report tool opens the report as a PDF, the Export XML tool saves reports as XML export files.

OpenLAB Shared Services Maintenance

OpenLAB Shared Services includes an additional tool, the OpenLAB Server Utility which is available from the Windows Start Menu to manage the Activity Log entries. This tool allows activity log event records to be exported and then optionally purged. The entire Shared Services database may also be archived either in total, or incrementally from the database. Archives may also be restored in the future.

In addition, if Windows domain security is being used, the credential used to interrogate the domain control may be configured.

Methods and Sequences

The Agilent OpenLAB CDS ChemStation Edition analytical method fully describes how a particular analysis is performed. It contains all the parameters for instrument control, data acquisition and evaluation, including integration, quantitation and reporting. The system may be set up for automated analysis of a number of samples using the same or different methods. The control file for this operation is called a sequence template and holds sample information for the individual samples, references to the method to be used for each injection and specifications for automating recalibration.

With the creation of Result Sets enabled (Unique Folder Creation ON), when the acquisition based on the sequence template begins, a copy of this sequence template and of all required methods are placed into a uniquely named folder which also receives all data files and log files thereby creating a result set. As the data is processed, integration, identification and quantitation results are saved to files in Agilent Common Analytical Markup Language (ACAML) into the result set, thereby creating a self-contained, transportable result set for the entire analytical process.

For more details please refer to *Agilent OpenLAB CDS ChemStation Edition Concepts and Workflows* guide (please refer to the chapter *Documentation*).

Instrument Parameters

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 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.

System Configuration

Dynamic Instrument Configuration

In addition to the instrument configuration tools in the OpenLAB Control Panel, OpenLAB CDS ChemStation Edition can prompt for instrument reconfiguration at the start of each session or from a menu item in the OpenLAB CDS ChemStation Edition. These features enable ‘plug and play’ like dynamic instrument configuration when modules are added or removed from the instrument.

Data Handling and User Access Configuration

With OpenLAB CDS ChemStation Edition, the “OpenLAB CDS ChemStation Edition Administration Tool” is used for secure configuration of each OpenLAB CDS ChemStation Edition. This supports different OpenLAB CDS ChemStation Edition configurations attached to the same OpenLAB Shared Services and/or Data Store or ECM server.

Login

In a networked workstation system, if the authentication provider or the OpenLAB Shared Services Server are not accessible, a user can fall back to an emergency mode by connecting to local OpenLAB Shared Services. The local OpenLAB Shared Services should be set up for this emergency scenario ahead of time. This allows users to access the system even if the authentication provider or OpenLAB Shared Services Server are not accessible.

The time-based lock or the Lock button in the OpenLAB CDS ChemStation Edition UI can be set to lock privately so only the session owner or a system administrator can open a locked session.

Data Handling and Audit Trail Configuration

The features described in the following, with the exception of method and sequence audit trails, require an OpenLAB Data Store or an OpenLAB ECM server (in the following referred to as "central data storage") to be part of the system.

OpenLAB CDS ChemStation Edition can be set to allow users to configure the settings in the OpenLAB CDS ChemStation Edition Preferences dialog for an individual OpenLAB CDS ChemStation Edition session. Alternatively, the administrator can set these settings for an entire workstation or AIC using the OpenLAB CDS ChemStation Edition Administration Tool.

OpenLAB CDS ChemStation Edition can be set to always transfer data to the central data storage for any combination of the following events:

- After Acquisition
- After Reprocessing
- After Any Data Modification (Full Tracking)
- Import after Reprocessing: import OpenLAB CDS ChemStation Edition data acquired outside the system or data from self-assembled result sets into the central data storage

OpenLAB CDS ChemStation Edition can be set to open the data transfer queue when the software is started to make sure data transfer issues to the central data storage are noticed.

OpenLAB CDS ChemStation Edition can be set to delete local data already safely transferred to the central data storage each time the OpenLAB CDS ChemStation Edition session closes.

The audit trails for methods, sequences and results can be enabled in the OpenLAB CDS ChemStation Edition Preferences dialog for an individual OpenLAB CDS ChemStation Edition session. Alternatively, the administrator can set these settings for an entire workstation or AIC using the OpenLAB CDS ChemStation Edition Administration Tool. The sequence audit trail is automatically enabled with the results audit trail. In addition the method audit trail can be enabled for an individual method. Note that once an audit trail has been enabled, it cannot be disabled. The sequence audit trail is started with the acquisition or re-processing.

Configuration Profiles

Each OpenLAB CDS ChemStation Edition workstation can be set to

- Only connect to the OpenLAB Shared Services Server and use the settings defined in OpenLAB Shared Services (user authentication, roles, privileges etc.) without any connection to a secure central storage, or
- Connect to OpenLAB Shared Services Server and the secure central storage to enable data transfer to and from the storage, in addition to the communication with OpenLAB Shared Services.

Logging profiles can be set to adjust the type and depth of the logging of OpenLAB CDS ChemStation Edition operation.

Data Model

Memory Data Model

The OpenLAB CDS ChemStation Edition software is designed around a data model based on a memory structure called a register. Registers are multi-purpose structures that can hold analytical data and information for both two dimensional (e.g., time/intensity) and three dimensional (e.g. time/intensity/wavelength) analyses.

OpenLAB CDS ChemStation Edition provides, commands and functions to construct, expand, extract and, where it does not alter primary data, edit registers. Registers hold information about their contents in register headers. The registers are further subdivided into one or more objects. Typically an object holds data that describes an analytical measurement, such as a chromatography signal. Each of these objects have their own header with information about the analytical measurement such as the data file name, injection date and time, sample name, and tables. Tables are used to hold different types of data as one block of information. For example, the quantification process in a calibrated method constructs a quantification table that contains peak numbers, compound names, compound amounts and retention times.

Like other parts of the registers, tables may be user-defined and have the functionality of database tables with the additional benefit of being directly associated with the base piece of analytical information from which they were derived.

Result Set

The information created in the memory of OpenLAB CDS ChemStation Edition in the course of data acquisition and processing is written to files in the sequence data folder to create a complete result set for the sequence. The files used to store the information and their purposes are detailed in the *Agilent OpenLAB CDS ChemStation Edition Reference to Operation Principles* (Please refer to the chapter *Documentation*).

The calculated results for each analysis, the signals, calibration and selected method information is written to Agilent Common Analytical Markup Language (ACAML), a variant of Extensible Markup Language (XML) designed to store analytical results. Preservation of calculated results supports tracking of a revision history for data processing and enables reporting without reprocessing raw data.

Self-Assembled Result Sets

Results from more than one sequence can be combined into self-assembled result set for reprocessing, recalculation or reporting. In OpenLAB CDS ChemStation Edition, it is possible to create self-assembled result sets by combining selected or all data from multiple sequences and/or single runs in the navigation table in the Data Analysis view. The new self-assembled result set can then be created under a new name, reprocessed, stored and reported on as a single data set. These self-assembled result sets have a distinct appearance in the Data Analysis navigation pane, are clearly labeled with the new result set name in reports and are logged and tracked like native result sets. The appropriate use of self-assembled result sets in laboratories that must meet regulatory requirements should be governed by their applicable policies and procedures.

Software User Interface

OpenLAB CDS ChemStation Edition Views

The OpenLAB CDS ChemStation Edition user interface is organized into views that group software functionality according to typical analytical tasks. The following standard views are present in all software configurations:

- The Method and Run Control view for creating analysis methods, defining automation, performing and monitoring analyses
- The Data Analysis view for displaying, evaluating and calculating data
- The Review view for reviewing the data by applying report templates to existing results (requires Intelligent Reporting to be enabled)
- The Report Layout view for designing report templates

Additional views may be present if additional data evaluation modules have been added or for instrument configurations that support instrument diagnostics.

The Navigation Pane contains the Navigation Buttons, which allow rapid switching between the OpenLAB CDS ChemStation Edition views, and OpenLAB CDS ChemStation Edition Explorer pane which presents OpenLAB CDS ChemStation Edition files in tree structures similar to Windows Explorer™. The contents of the OpenLAB CDS ChemStation Edition Explorer are dependent on the selected view, giving the user access to the files used in each view.

Each view contains a set of standard user elements including menus and toolbars that unify the location and behavior of controls across the OpenLAB CDS ChemStation Edition. The toolbar provides rapid access to the common system parameter files such as methods and sequences and tools appropriate for the functions in the view. The right hand portion of each view is the workspace for the view. This workspace is tailored to the needs of each view and offers displays and controls appropriate to the tasks assigned to the view. The Navigation Pane can be hidden to increase the available workspace.

Method and Run Control View

The Method and Run Control view is intended for setting up and running data acquisitions. The workspace has a configuration switch to adjust the tools and displays for making individual runs or automated sequences of runs. Instrument status and control centers are shown on a schematic instrument diagram for GC, LC or CE instruments. The schematic instrument interface diagram for LC uses context-sensitive menus to allow rapid access to instrument parameters and an animated graphical overview of the status of each analysis as it proceeds.

Toolbars and panels can be configured to suit the operator's needs for:

- Controlling Runs and Sequences
- Monitoring Autosampler Injections
- Viewing and Managing a Sequence Queue
- Monitoring Detector Signals and Instrument Curves
- Viewing the Session Logbook

Screen layout tools allow selection of predefined arrangements of the workspace. Display windows and toolbars can be turned on and off to manage the workspace and reduce memory and Windows resource usage.

Data Analysis View

When a result set is opened in Data Analysis, the runs are displayed in a Navigation Table. The table displays information about each run and allows direct selection of runs and sets of runs for data analysis operations. Like the Navigation Pane, the Navigation Table can be hidden to increase available workspace.

Within the Data Analysis workspace, buttons allow switching between the Recalculation and the Reprocessing mode. Buttons allow selecting specific data analysis functionalities including integration, calibration, reporting, annotation, signal comparison and additional specialized modes if add-on software modules are installed. Each of these separate data analysis modes are supported with a mode-specific toolset.

Review View

The Review view is available if Intelligent Reporting has been selected during the configuration of an instrument. Using the Review view, users can select a combination of data files, and apply a report template to define the layout of the result display. Templates can apply to each individual run (Single Injection Report) or summarize the data set as a whole (Sequence Summary Report). In addition, it is possible to combine data from different sequences and/or single runs in the navigation table and create reports across the context of a sequence (Cross Sequence Report). The Review view is based on the ACAML results generated in the Data Analysis view, formatting and displaying results without modifying result values or generating new result revisions.

A selection of report templates is installed with the system and user-defined templates can be created for the specific requirements of each analysis. The toolbar provides functions for printing and exporting the generated reports to PDF, DOC and XLS formats.

Report Layout View

The Report Layout view allows you to define the layout of report templates. Two reporting layouts are available in OpenLAB CDS ChemStation Edition. You can either use Classic Reporting to define or update legacy report templates in the format used in earlier revisions of the OpenLAB CDS ChemStation Edition software. Alternatively you can employ Intelligent Reporting which uses templates defined in Microsoft .RDL format to generate reports from the ACAML data. The user chooses between the Classic Reporting Layout and the Intelligent Reporting Layout during the configuration of an instrument.

With Intelligent Reporting, report items are available organized by type in a tree structure. Items can be dragged from the list and dropped into the template to be arranged on a virtual page. Tabs allow switching between template definition and report preview.

Data Acquisition

During data acquisition, all signals acquired by the analytical instrument are converted from analog signals to digital signals in the detector. The digital signal is transmitted to OpenLAB CDS ChemStation Edition electronically and stored in the signal data file. For detectors without a digital interface to the OpenLAB CDS ChemStation Edition, an analog to digital convertor (A/D convertor) can supply the digital signal for storage.

Data Path and Transfer Settings

The data files associated with an analysis are stored in folders within a configured path on the system. The Paths tab in the OpenLAB CDS ChemStation Edition "Preferences" allows addition of folders for data, method or sequence template storage which can then be selected in the parameter screens as the analysis is setup. Storage locations can be on the local PC.

When the storage location is configured to central data storage, the "File Transfer Settings" tab in the OpenLAB CDS ChemStation Edition "Preferences" allows selection of the location on the server for data storage. Permitted locations are controlled from the central data storage content management tools. If operators have the appropriate permissions they can browse to and/or create new storage locations within the central data storage, or use predefined tokens for automatic path creation. With these tokens, the system automatically creates the required items if they do not already exist in the central repository. Alternatively, the path can be specified as Sequence Parameter. For more details on central data storage and tokens please refer to the chapter Central Data Storage below.

Analysis Control

The operator can start a single analysis or a sequence of analyses. If a sequence is running it may be paused to allow the current run to complete but the next run will not begin until the sequence is resumed. Both single runs and sequences can be stopped. Single runs will stop immediately, sequences will continue to the completion of the current injection unless the operator makes a second stop request. All analyses can be aborted which makes OpenLAB CDS ChemStation Edition cease all activities including data processing. Note that aborting serves as an emergency exit only and might leave the system in an undefined state.

Sequences can be added to a queue to run in the queued order. Queuing is covered in detail in the automation section.

Single injections can be named automatically using simple prefix-counters or pattern based naming. Users can combine any or all of the following elements:

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

For sequence data file naming three techniques are available:

- simple prefix counters,
- automatically generated by the ChemStation using a predefined naming scheme, or
- manually per sequence line.

Instrument Monitoring

The status of the instrument is continually monitored and updated on the instrument diagram. Unless the Classic instrument drivers are selected, there is a control in the system diagram tile for each module that open an instrument actuals display for the module. The live parameter display is different for each module but offers a selection of key operation condition measurements such as temperatures, flows and pressures reported from the instrument sensors. For GC the overall Instrument Actuals can be enabled from the View menu.

Color-coded status indicators display the overall status of each module and for the instrument as a whole. The following status modes are displayed according to the state of the instrument:

- Light Grey – Offline
- Dark Grey – Online in Standby Mode (lamps, pumps and temperature control off)
- Yellow – Not Ready
- Green – Ready but not running
- Magenta – Pre-run (waiting for injection), Injecting or Post-run
- Blue – Running
- Red – Error

Note: The color-coding applies to LC and CE only.

Analysis Monitoring

A color-coded status for the analysis is displayed using the same codes as described for the instrument. The currently loaded method and sequence are displayed. Indicators on the method and sequence icons indicate if the current parameters have been modified but not saved.

When an analysis is in progress, the elapsed time is displayed. When modules are minimized in the LC or CE dashboard, the status for the module is shown in the minimized representation.

One or more display windows may be used to monitor the data being acquired by the instrument in real time. The data are displayed in real measurement units such as mAU, Volts, degrees Celsius or bar. The windows may each show multiple overlaid chromatographic or electropherographic signals or instrument curves, which monitor the change of an instrument parameter, such as pressure, over time (depending on the capability of the instrument). The display default settings may be adjusted and are remembered by the system so users can set their own preferred settings as the instrument default. The window has zoom capability and the cursor may be used to display a specific signal's response at any point in time.

An online spectra monitor is available for OpenLAB CDS ChemStation Editions that support spectral evaluation. For UV detection it shows absorbance as a function of the wavelength in a continuously updated display. You can adjust both the displayed wavelength range and the absorbance scale. For MS detection the online spectra monitor displays the abundance as a function of the m/z range with the same means for adjustment.

The layout of the signal and status information windows, including the components of the schematic instrument interface diagram is saved automatically.

Analysis Logs

The transactions that occur during the analysis, including any errors and the instrument conditions at the start and the end of the analysis, are recorded in the system's logbook. The logbook records these events irrespective of whether they are displayed or not. The portion applying to an individual run is stored in the data file for the run.

The instrument conditions, such as flow, temperature, pressure and solvent composition for liquid chromatographs may be recorded and stored with each data file. These instrument parameters can be displayed and plotted to testify to the quality of each analysis. The exact nature of the parameters recorded depends both on the technique and the capabilities of the configured instrument.

Viewing Acquisition Methods

The Acquisition Method Viewer allows users to view the instrument parameters of a selected method in a read-only tabbed display. Optionally users may choose to view the method with the original configuration (the configuration of the original instrument the method was created with), or adapted to the current instrument configuration. Details of any adaptations of the method to the current instrument configuration are available as a list of changes for each tab.

Note: The viewer can not display instrument parameters from classic methods.

Data Processing During Analysis

During an analysis, the complete functionality of OpenLAB CDS ChemStation Edition can be used through the offline copy. While acquisition is running, the Data Analysis part of the online session of an instrument is not accessible, and data review has to be performed in the offline copy. Data for each completed run is available in offline data analysis.

A snapshot function is available for users who wish to start processing data before a run is complete. The snapshot is taken from the offline OpenLAB CDS ChemStation Edition session for the running instrument and creates a copy of the data being acquired that is immediately fully available for review and analysis. Additional snapshots can be taken with the previous snapshot being replaced by a copy of the current state of the data.

Data Analysis

The Data Analysis view provides functionality for displaying, evaluating and calculating data. With the Data Analysis navigation button in the Navigation Pane it is easily accessible from any OpenLAB CDS ChemStation Edition view. The Data Analysis view consists of at least three different Tasks. Additional tasks may be present if additional data evaluation modules have been added.

Opening Result Sets – Navigation Pane and Navigation Table

The data acquired is stored as individual data folders for single injections (also commonly called data files as each folder contains the complete data for one analysis). For sequence data, the results set stores the data in a hierarchy of folders. The OpenLAB CDS ChemStation Edition Navigation Pane displays all of the single run data folders at a given location as one icon representing a single sample vial. Sequence result sets are displayed as an icon representing three sample vials.

A data icon can open the data at the location it represents in a Navigation Table at the top of the Data Analysis workspace. This table then provides direct access to individual files or selections of files at the given location. Fly-overs indicate the path to data and methods. The Navigation Table has its own toolbar. The content of the navigation table is different for sequences and single runs:

Information shown	Single Run	Sequence
Overlay checkbox for automatic overlay	●	●
Status of run in storage	●	●
Type of data (data icon) (single run, sequence, result set, user-assembled or single run originating from sequence/result set/user-assembled)	●	●
Date and time	●	
Operator	●	
Sequence line number		●
Injection number		●
Vial number	●	●
Blank reference data file name (for signal-to-noise calculation)	●	●
Sample name	●	●
Acquisition method name	●	●
Sample type		●
Calibration level		●
Data analysis method last used	●	●
Sequence method last used		●
Sample information	●	●
Manual integration indicator	●	●
ISTD amount	●	●
Sample amount	●	●
Multiplier	●	●
Dilution	●	●
Data file name	●	●
ECM	●	

The context menus for the data icons in the navigation pane have an "Overlay" option which enables overlay of signals from runs that are not in the same result set. Automated continuous overlay can be selected to load one or more reference chromatograms from the current result set or another result set for visual comparison with each chromatogram selected for display.

One row, a selection of rows or all rows can be chosen as the source for the signal display. Within the file selection, one or all signals in each file can be selected for display. For maximum flexibility, checkboxes can be used to select files and signals from files in any combination desired. The selected signals can create a new display or be overlaid with the signals already displayed. The Signal/Review options allow restriction of the signals loaded for each file to those specified in the current method. In the Signal Task the overlaid signal display can be further optimized for review, for example by stacking chromatograms.

The context menus for the data icons have an "Add Data Files" option which enables adding runs from several sequences and /or single runs to the Navigation Table. This allows users to work with data from different sequences and/or single runs to compare them, recalculate them with a different or modified method, or create a new self-assembled result set.

Because result sets can contain hundreds of runs, the Navigation Table controls can be used to make the display manageable. The table controls can:

- Hide or show the table
- Adjust the vertical size of the table display window
- Sort the table by the contents of any column
- Filter the table based of a value selection in any column
- Build custom filters to display selections of table rows

Signal Task

With a signal or a selection of signals loaded, the Signal Task provides tools to display and compare one or more signals. These tools enable:

- Graphical vertical and horizontal alignment of signals to help visual comparison. Alignment can move, stretch or shrink each signal.
- Stack overlaid signals with a selected vertical and horizontal offset to generate a pseudo 3D display
- Signal inversion or mirroring to help visual comparison of two signals
- Subtraction of the last chromatogram or electropherogram in a set of chromatograms from all the others
- Graphical zoom and scroll functions
- Adjustment of display attributes including selection of tick marks, baselines, axes, retention/migration times, compound names and object titles (you can also select the font for the RT and compound labels, adjust the size and orientation of the display, select the display as overlaid or separated and select scaling factors)
- Graphical overlays of instrument parameter signals (depending on the capability of the instrument)
- Interactive addition of user-defined annotations, with the selection of font, size, text rotation and color (once defined, the annotations may be graphically moved, edited or deleted),
- Copying the display to the Windows clipboard in both metafile and bitmap format
- A pick mode function to display the values of individual data points in detector units
- Export of time/intensity digitized points to the Microsoft Windows clipboard.

Integration Task

The OpenLAB CDS ChemStation Edition integrator algorithm is a very sophisticated design tested against a very wide variety of chromatograms to provide the best possible ruggedness, reliability and ease-of-use. The Integration task displays integration results, allows interactive control of integration, and supports at least 1000 peaks in each chromatogram. A layered implementation allows activation of advanced features only when they are required to get accurate results. The following sections outline the key features and capabilities of OpenLAB CDS ChemStation Edition integration; detailed documentation of integration is available in the guide *Agilent OpenLAB CDS ChemStation Edition Reference to Operation Principles* (please refer to the chapter *Documentation* at the end of this document).

Initial Events – Integration Core Controls

The integration process is controlled by integration events. The most important events are initial slope sensitivity, peak width, baseline correction, area reject, and height reject. These values may be set by the operator or an auto-integration routine can set the values based on the calculated characteristics of the signal. A common set of parameters can be used for all signals or individual integration event tables can be defined for each chromatographic signal if multiple signals or more than one detector is used.

Parameters enable tangent skimming and set the conditions when integration switches to tangent skimming. Four selectable models can be used to calculate the baseline for the tangent skim:

- Exponential curve fitting
- New exponential skim
- Straight line skim
- Standard skim combining exponential and straight line calculations for the best fit

In the advanced baseline tracking mode, the integrator makes a second pass through the signal to establish more accurate baseline assignments for peak integration when the chromatographic baseline has significant slope.

Time-Based Integration Events

Integration event tools allow selection of time-based integration events and graphical selection of the time for each event selected. Events are collected in an events table which can be directly edited to change events and event times. The available events allow control of:

- Changes to initial events - Slope Sensitivity, Fixed Peak Width, Variable Peak Width, Tail Tangent Skim, Tangent Skim Mode, Area Reject, Height Reject
- Baseline placement - Baseline Now, Baseline Next Valley, Baseline at Valleys, Baseline Hold, Baseline Backwards, Split Peak
- Area summing over selected time ranges using Area Sum ON/OFF events
- Integration through Integration ON/OFF events
- Recognition of negative peaks
- Detections of shoulders on peaks that use second derivative or degree of curvature calculations
- Skimming a series of peaks riding on the tail of a larger peak using the Solvent Peak event
- Area Sum Slice - integrating contiguous time-slices of the chromatogram without any loss of time intervals. Area Sum Slice is used with Set Baseline from Range, Set Low Baseline from Range and Use Baseline from Range to accurately integrate complex chromatograms into several time-slices. The sophisticated baseline placement over a range uses a statistical algorithm with optional noise correction.

Manual Integration

When the integration algorithm is unable to establish the correct baseline or when adjusting the parameters might be too tedious, the Integration Task provides tools allowing the operator to draw baselines by clicking and dragging on the chromatogram. The tools allow:

- Drawing the baseline for a peak
- Drawing the baseline for a negative peak
- Drawing a baseline for a tangent skim
- Splitting a Peak
- Deleting a Peak

Additional tools allow: undo last manual integration, undo all manual integration, and immediate saving of the manual integration to the data.

As each baseline is drawn the integration results update automatically. Manual baselines are indicated in reports through the use of specific peak-type codes.

Manual integration events can be saved to the method or to the data. When different events are saved in both modes, both are applied. It is most appropriate to save manual integration to the data because it is defined in relation to the specific signal. Manual integration saved with the data is clearly marked with a symbol in the Navigation Table when the data is opened in Data Analysis. The manual integrations are saved permanently unless removed, and are reapplied after each reintegration.

With the Results Audit Trail enabled, all manual integration iterations are captured and documented. For more details on audit trails in OpenLAB CDS ChemStation Edition please refer to the chapter *Audit Trails and Logbooks*.

Peak Performance Calculations

An 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 a settings dialogs.

Peak performance calculations as defined in US Pharmacopoeia (USP), European Pharmacopeia (EP) and Japanese Pharmacopeia (JP) include:

- Tailing factor (USP) or symmetry factor (EP, JP)
- Relative retention (EP) or separation factor(JP)
- Relative retention (USP) or selectivity
- Resolution (classic)
- Resolution (EP)
- Resolution (JP)
- Resolution (USP)
- USP efficiency or theoretical plates based on tangent method
- Efficiency (EP, JP) or theoretical plates based on half height method
- Relative Retention Time
- S/N ratio (EP, JP)
- Peak-to-valley ratio (USP,EP)

These values can be reported using Intelligent Reporting. The formulas and algorithms are detailed in the guide *OpenLAB CDS ChemStation Edition Reference to Operation Principles* (please refer to the chapter *Documentation* at the end of this document).

Calibration Task

The Agilent OpenLAB CDS ChemStation Edition Calibration Task in the Data Analysis displays:

- The signal or signals currently loaded
- The calibration table with a selection of calibration parameters configured from a comprehensive set
- A color coded bar highlights the retention time window of the compound selected in the table on the signal displays. The color indicates whether or not the selected peak is found in the current signals and whether a signal is a qualifier or the main signal for the compound (see below).
- The calibration curve for the selected compound

All the calibration task windows are linked so that changes in one are automatically reflected in all the others. This task allows graphical selection and modifications of the calibration data.

Quantification Settings

Quantification can be based on peak area and -height, and results can be selected for either response mode when the results are reported. Calibrations may be multi-level and may include multiple internal standard definitions.

Calibration histories are automatically saved and can be used to weight the recalibration calculations. The following calibration point weighting options are available:

- Equal – All calibration points have equal weight in the curve.
- Linear (Amnt) – A calibration point with the amount x has the weighting 1/x normalized to the smallest amount so that the largest weight factor is 1. Normalization is done by multiplying the weight with the smallest amount. For example the weight of a calibration point with the amount x is (1/x) * a, where a is the smallest amount of the calibrated compound prepared in the calibration standards. If the origin is included it is assigned the mean of the weightings of the other calibration points.
- Linear (Resp) – A calibration point with the response y has the weighting 1/y normalized to the smallest response so that the largest weight factor is 1. Normalization is done by multiplying the weight with the smallest response. For example the weight of a calibration point with the amount y is (1/y) * b, where b is the response corresponding to the smallest amount of the calibrated compound prepared in the calibration standards. If the origin is included it is assigned the mean of the weightings of the other calibration points.
- Quadratic (Amnt) – A calibration point with the amount x has the weighting 1/x2 normalized to the smallest amount so that the largest weight factor is 1. Normalization is done by multiplying the weight with the smallest amount. For example the weight of a calibration point with the amount x is (1/x2) * a2, where a is the smallest amount of the calibrated compound prepared in the calibration standards.
- Quadratic (Resp) — A calibration point with the response y has the weighting 1/y2 normalized to the smallest response so that the largest weight factor is 1. Normalization is done by multiplying the weight with the smallest response. For example the weight of a calibration point with the response y is (1/y2) * b2, where b is the response corresponding to the smallest amount of the calibrated compound prepared in the calibration standards.
- # Calibrations – A calibration point is weighted according to the number of recalibrations of the point. No normalization is done.

The origin treatment for multilevel calibration curves may be selected from:

- Ignored — the origin (0,0) is not used in the curve calculations,
- Included — the origin is used as one of the calibration points,
- Forced — the curve is forced through the origin, and
- Connected — the linear segment is constructed between the origin and lowest calibration level on the curve.

Compounds are identified based on a defined retention time and a retention time window. The size of the identification window can be set as a percent of retention time allowing for wider windows for later eluting peaks or as a fixed time window or a combination thereof. One or more reference peaks can be assigned in the calibration table. When a reference peak is located, the expected retention times for the other compounds are corrected based on the new reference peak retention time. Identification windows can be set independently for reference peaks.

Compound identification may be refined by defining individual retention time windows, parameter limits and qualifier peaks. Qualifier peaks are usually the same compound detected on a different signal with a predictable response ratio. They are used to check on peak identification by confirming the detected compound has the same relative response at a second wavelength as the compound in the calibration standard.

Each calibrated compound may have individual absolute limits for the amount, peak area, peak height, symmetry, efficiency in plates, resolution and k'. Results lying outside any defined limits are indicated on the analysis report. They may be used in conjunction with setting the type "Control" for samples during the automation setup. Control samples are checked against the defined limits to verify the performance of the system during automated analysis. OpenLAB CDS ChemStation Edition can calibrate methods with up to 1000 peaks and 2000 calibration points. This means, for example, with 1000 calibrated peaks only two calibration levels may be defined for each peak. With fewer peaks more levels may be defined in proportion to these limits (for example, 100 compounds could have 20 levels each).

The compound grouping capability allows the user to group calibrated peaks into a named group and report quantitative results for both the individual group members and the group itself. The group can be reported as the sum of the amounts for each group member, or a separate group calculation can be performed based on response factors calculated from the concentrations entered and the sum of the responses for the members of the group at each concentration.

In addition to the area summing available in the Integration Task, which sums all peaks in fixed time ranges, a peak sum table is available to define sum ranges for quantitation. Ranges are defined as rows in the table with a start and an end time. Each range can be named. An important feature of these sum ranges is that compounds defined in the calibration table are not included in the sum. This allows known peaks to be calculated based on standards and the other peaks in the same time range to be summed and calculated separately.

Calibration curves are constructed for each compound by using the concentrations entered for each compound at each calibration levels and the response measured for each compound when calibration standards are analyzed. The number of levels can be different for different compounds and the calibration standards can have different combinations of the compounds in the calibration table.

The algorithm used to generate the calibration curve may be selected for all the compounds or for each compound individually from:

- Piecewise - a point-to-point interpolation
- Linear - a linear regression fit of the data points
- Quadratic - a quadratic fit of the data points
- Cubic - a cubic fit of the data points
- Exponential - an exponential fit of the data points
- Logarithmic - a natural logarithmic fit of the data points
- Power - a power fit of the data points
- Average Resp/Amt - single response factor is calculated from the average of the inverted response factors.

Unknown peaks can be calculated using several approaches. They can be ignored, calculated using a fixed response factor entered into the calibration settings, or calculated using the calibration curve of one calibrated compound. The manual setup of the calibration table allows the use of response factors determined external to the system and the calculation of peaks relative to other peaks.

The calibration is saved to the method for application to sample analysis as defined in the report parameters for the method. Automation can identify the calibration standards and define the recalibration parameters so the calibration can be updated as needed during automated analysis. Recalibration standards can be averaged as the overall or weighted average of all the injections or replace the parameters in the calibration table. Recalibration can also update the expected retention times for the compounds in the calibration table.

Data Analysis Modes

The software comprises three data analysis modes: Recalculate mode, Last Result mode and Reprocess mode. The required functions associated with each mode are available in separate toolbars.

Recalculate Mode

The recalculation mode allows a quick recalculation of a sample or a set of samples with a different method.

In the Recalculate mode users can analyze runs as single runs without taking the sequence context into account or using the features of the sequence table. The mode offers a toolset to jump to the beginning or end of the navigation table, step on to the next or previous run, automatically step through the runs, stop automatic stepping, recalculate a run using a specific method, or clear the Navigation Table. Recalculation means analyzing on a run- per- run base. Only the runs shown in the Navigation Table are analyzed.

You can use recalculation in the following workflows, for example:

- You want to review the data files of a result set with a different method that is not currently in the result set, for example, a master method not used for acquisition, because your workflow employs separate acquisition and data analysis methods.
- You have edited a sequence method and want to review only specific runs using this method in order to check how well these parameters apply for different runs.

Last Result Mode

The "Last Result Mode" allows reproducing the last results for a sample or sample set regardless of the fact whether these results were created in a sequence context (acquisition, reprocessing) or not (Recalculate Mode).

In this mode, the data file method (DA.M) for each run is automatically loaded. DA.M is an exact copy of the method which was used for the last data analysis (during acquisition, reprocessing, or recalculation). So even if the sequence method has been changed in the meantime, you can reproduce the last result with the method originally used. In that way you can, for example, track changes done to the method in successive recalibration steps in a result set.

Using the Last Result Mode, it is 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 modify the data analysis parameters of the DA.M method and create a report. The changed DA.M method is automatically saved when the report is printed.

Reprocessing Mode

The reprocessing mode allows reprocessing of samples in the context of a sequence (e.g. for a bracketed calibration).

In this mode data is analyzed by reprocessing a complete sequence. In contrast to recalculation, all runs are reanalyzed in the sequence context: the calibration tables of the sequence methods are updated in the case of calibration runs, and changes to parameters in the sequence table, such as multipliers or amounts are taken into account. The result set includes all files needed for reprocessing: the data files, a copy of the sequence file, all the sequence methods and all the report templates originally employed with the acquisition. Thus, in order to reprocess a sequence users simply have to load a result set and start sequence reprocessing in the reprocessing mode.

Batch Review

Batch Review is an additional mode of data analysis that provides automation by allowing a fast and easy first-pass review of a batch of samples. The batch consists of all or a selection of runs from a sequence. You can check the calibration accuracy and the individual integrations before approving the results. All chromatogram-specific modified integration parameters can be saved for data traceability. Once data is accepted the entire batch can be reprocessed to generate reports with one keystroke. Batch review is disabled for systems connected to a central data storage.

OpenLAB Data Analysis

The new OpenLAB Data Analysis features intuitive operation, easy sample review and fast reprocessing of large sets of chromatographic data. It works with data from EZChrom and ChemStation Edition, allowing to use the same integration, calculation, calibration and reporting across the entire laboratory.

The OpenLAB Data Analysis offers extensive review capabilities for GC and LC data and provides all means for fully automated workflows. With enabling a very high level of automation from injection to the electronic results report, the software perfectly supports the workflow of chemical and petrochemical laboratories. The OpenLAB Data Analysis does not yet offer 3D capabilities to further analyze data generated by a Diode Array Detector (DAD) or Mass-Selective Detector (MSD).

OpenLAB Data Analysis can be used together with OpenLAB CDS ChemStation Edition and is a separate application running in its own window. It is supported on standalone workstations without central data storage only. 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. OpenLAB Data Analysis can be installed without OpenLAB CDS ChemStation Edition.

OpenLAB Data Analysis exclusively uses OpenLAB Intelligent Reporting. Users can create sample reports, sequence summary reports, and cross-sequence summary reports.

Access Control

Access control to OpenLAB Data Analysis can be enforced using OpenLAB Shared Services. Users and roles are managed with OpenLAB Control Panel. Two predefined roles are available at installation – DA Chemist and DA Technician. Each role may be edited to add or remove specific privileges or new roles may be created. Session locking protects data from unauthorized access. Roles and privileges limit user access to the required software functions (see the chapter Roles for a list of privileges).

The software does not yet provide further features for compliance with regulations like GLP or 21 CFR Part 11. There are no qualification services available.

Data and Method Compatibility

Users may focus on a single data analysis platform for OpenLAB CDS. Data acquired with OpenLAB CDS ChemStation Edition or EZChrom Edition can be reviewed and reprocessed. OpenLAB Data Analysis evaluates the raw data and the ACAML (=Agilent Common Analytical Markup Language) files generated by OpenLAB CDS A.01.01 or higher. To generate an ACAML file that can be used with OpenLAB Data Analysis, old ChemStation data must first be reprocessed with OpenLAB CDS A.01.01 or higher. For ChemStation data compatibility please also see chapter *Data, Method and Sequence Compatibility.*

OpenLAB Data Analysis includes both the EZChrom and ChemStation Integrator for backwards compatibility and flexibility to use the same integration across the laboratory.

The method compatibility is limited to identification – compounds can be imported from existing ChemStation and EZChrom methods. During processing, OpenLAB Data Analysis does not alter any ChemStation raw data or methods, but only writes new results to the ACAML results (see also chapter Data Model earlier in this document). The content of the ACAML results is displayed in the ChemStation in the Review view only. Therefore if OpenLAB CDS ChemStation Edition data was processed in OpenLAB Data Analysis, there is no impact on the results displayed in ChemStation Edition. Only in the Review view, there will be no results available until the data is reprocessed in ChemStation again.

User Interface

OpenLAB Data Analysis was designed for ease of use. It comes with a "flat" and intuitive user interface with Microsoft-style function ribbons providing fast access to the main functions.

OpenLAB Data Analysis separates the workflow into 3 different views. In the Data Selection View a data selection tree on the right allows fast access to data. The data selection tree shows the folder structure of the data path given in the OpenLAB Data Analysis project in OpenLAB Control Panel. The injections of the selected result set or single samples folder are shown in the Injection List window on the right. The injection list provides a preview of the details to help identifying the data of interest. Users can select data from multiple folders, load complete result sets, or selected single samples. Data selected for review and reprocessing is automatically loaded into the Data Processing View, where all data analysis tasks –integration, identification, calibration, quantitation and automatic report generation for single injections or sequences – can be performed. Processing methods can be developed and stored. In the Reporting View users may interactively create reports with a predefined report template or develop new report templates with the Report Template Editor (see chapter *Intelligent Reporting* for more details).

User may design their own layout and organize screens to meet the workflow-specific needs. Four predefined configurable layouts are available:

- Results – overview with chromatograms window, sample information window, injection results window
- Chromatograms – large chromatogram window to review and compare chromatograms
- Compounds – chromatogram window, zoomed peak details window, calibration curve window, injection results window
- Methods – chromatogram window, processing method window, injection results window

The size and position of the windows shown in the workspace can be changed. Windows can be tabbed, added or removed. Layout changes can be saved per user as custom layouts, complementing the predefined layouts. If needed, changes to pre-defined layouts can be reset to factory defaults.

Data Review

The data navigation and data viewing concept of OpenLAB Data Analysis are designed for fast and easy review with highest throughput. Users can work with both LC and GC data at the same time and use multiple methods and data sets in parallel. The capabilities include:

- Automatic scaling to a specific peak, ignore main peaks, or to the baseline. There is no need to zoom manually per sample.
- Very fast reprocessing: Most efficient data handling and optimal use of the PC hardware enable easy overlay and comparison of hundreds of signals without any visible impact on performance – 100 runs are just done in an instant.
- Peak Explorer: easily review and compare large amounts of data.

During routine work an unexpected occurrence of any kind may raise the need for further investigation, requiring careful inspection of many chromatograms. Likewise, in method development a lot of data requires fast evaluation techniques. Reviewing large numbers of samples and identifying possible trends is easily done using the new Peak Explorer. Artifacts such as missing or additional peaks, retention time shifts or integration problems are captured quickly.

Manual Integration

OpenLAB Data Analysis introduces a unique one-click peak integration tool. The manual integration tool of the OpenLAB Data Analysis enables manual correction of the integration with a single context sensitive tool, the integration wheel, replacing traditional toolbars. The integration wheel automatically provides the right toolset for integrating a particular peak. Peak integration adjustments are achieved by simply dragging and moving baseline points.

Reporting

OpenLAB CDS ChemStation Edition has two types of reporting; Classic Reporting which uses the reporting engine available in OpenLAB CDS ChemStation Edition revisions prior to the OpenLAB CDS ChemStation Edition, and Intelligent Reporting, an entirely new reporting engine introduced with OpenLAB CDS ChemStation Edition. Intelligent Reporting populates reports with analytical results stored in ACAML format using report templates defined in Microsoft's Report Definition Language (.RDL files).

Classic reporting enables the continued use of SOPs based on the Classic reports and the use of custom report templates developed for ChemStation revision A.xx.xx or B.xx.xx.

Intelligent Reporting can be enabled as a part of the instrument configuration. Classic Reporting is still available when Intelligent Reporting is enabled. However, with Intelligent Reporting enabled the Classic Report Layout editor is not available. Each method must select one reporting mode or the other, but both modes are fully supported in automated analysis and individual methods can be switched between the two modes. In addition, classic sequence summary reports can be combined with intelligent single injection reports and vice versa.

The OpenLAB Report Viewer opens report files directly from data files displayed in the Data Analysis Navigation table. Report files can be opened from the report menu or from the context menu for a selected file. Multiple files can be opened, each in a separate viewer, up to a user-defined maximum number. The labeling in the title bar of the report viewer can be configured to more easily identify report contents.

Quantitation Settings

The reporting modes share a set of Quantitation Settings which control the calculations performed to produce the quantitative results which will populate the report. The concentration can be calculated as:

- Percent – Response Percent $_X$ = (Response $_X$ / Sum of all Peak Responses) • 100
- ESTD – ESTD Amount $_X$ = (Response $_X$ • RF X)
- Norm% – Amount % $_X$ = (Amount $_X$ / Sum of all Amounts) • 100
- ISTD – ISTD Amount $_X$ = (Response $_X$ / Response IS) • RF $_X$ • Amount $_{IS}$
- ESTD% – ESTD Amount % $_X$ = (ESTD Amount $_X$ / Sample Amount) • 100
- ISTD% – ISTD Amount % $_X$ = (ISTD Amount $_X$ / Sample Amount) • 100

The response can be selected as peak area or peak height. This can be changed without requiring recalibration. The Internal Standard Amount and Sample Amount can be entered with the sample information at the time of analysis or, if the values are constant for the analysis method, as part of in the Quantitation Settings.

A Multiplier and a Dilution Factor can be specified; both will be multiplied with the calculated concentration. Like the amounts above they can either be entered at the time of analysis or as fixed values for the method in this dialog. A selection in this dialog determines whether or not the multiplier and dilution factor apply to the internal standards.

Classic Reporting

Report Style

The Reporting settings in the report specification dialog control the report content. The content is determined by the report style selected from a list of defined styles (report templates) and settings that apply to all styles.

Every standard report style contains common information sections:

- A header with the originating data file and the sample name.
- A footer with the instrument name, operator name, print time and page number in 'page x of y' format.
- A sample information block that includes sample name, vial number, method and sequence information, operator and instrument name and sample information text.
- A quantification results table containing a selection of values controlled by the report style and calculated according to the quantitation settings.

The built-in report styles are hard-coded into OpenLAB CDS ChemStation Edition and have special features that adapt to the configuration. For example, if central data storage is configured as the data storage for the OpenLAB CDS ChemStation Edition, the report will automatically include

- the location of the data in the storage, and
- the current result revision.

There are 15 built-in styles and they can add the following types of information:

- A cover page that can include user-defined fixed text
- Instrument modules with serial numbers and firmware revisions
- Instrument operating conditions at the start and end of the run
- The analytical column information for LC and LC/MSD systems
- The run logbook
- Calibration table and calibration graphics showing the location of each compound result on the corresponding calibration curve
- Spectra and peak purity analysis for each peak (3D LC)
- UV or MS Library search results
- Standard peak performance parameters
- Detailed peak performance calculations with graphics (calibrated compounds only)
- Signal to Noise calculations

Additional style settings provide the following content controls:

- Report results for all signals in a single table sorted by retention time (Sort by RT), or in a separate table for each signal (Sort by Signal).
- Repetition of the sample information block on every page
- To include the graphic for the chromatograms
- Add sample custom fields to sample info
- Add fraction table and tick marks (system must include a fraction collector)
- Add summed peaks table
- Add compound custom fields

The reporting of uncalibrated peaks can be selected between reporting these unknown peaks in the same table with the calibrated peak results, reporting them in a separate table, and not reporting them at all.

OpenLAB CDS ChemStation Edition for CE has an additional mobility report that uses the voltage signal and the electropherogram to compensate for the velocity of the compounds migrating through the detector cell.

Signal Plot Controls

The report can display one or more chromatograms with a series of controls for the format of the display.

The plot can be portrait or landscape on the page and in landscape can be set to span multiple pages (up to 10) to allow detailed views of long runs with large numbers of peaks. The vertical and horizontal size of the plot can be set as a percentage of the page size.

When multiple signals are present in the data file, any or all of the signals can be included in the plot window. The signals can be overlaid or displayed in separate windows.

Multiple signals can be normalized or plotted on a fixed scale. In either mode the range can be set for the time axis. When the signals are plotted in true scale, the response axis can be set. The display of the axes can be turned on or off.

Signals can be automatically annotated with integration baselines, peak tick marks, retention times, and compound names. The peak labels can be set not to be drawn overlapping on the signal. For the text labels the font, font style, font size, color, justification, and rotation can be set.

If OpenLAB CDS ChemStation Edition is connected to instruments that can record instrument parameters as a signal, such as temperature, flow and pressure, the user may also select to include these graphics on the plot with the detector signals.

Report Destinations

Reports may be output to any combination of the screen, a printer or to one or more files. If the screen is selected as the report destination, the report together with graphics will be displayed in the Report Viewer window. Reports in the preview window can be printed to the printer.

A report can be saved to a file in any selected subset or all of seven different formats. Each format has a unique file extension. The following formats are available:

- .TXT – The report text is printed as a UNICODE text file.
- .EMF – Each report graphic (signal or calibration curve) is saved in a Microsoft Windows enhanced metafile (.EMF). Each graphic in the report will create a separate file so several .EMF files may be created for a single report. The generated file format adheres to the Microsoft enhanced metafile format as defined in the Windows software development documentation. These files are compatible with the Aldus Placeable Metafile (APM) format used by a number of proprietary software packages.
- .DIF – The tabular report data is saved in Data Interchange Format (DIF). This format is accepted by spreadsheet programs such as Microsoft Excel. Independent from the report style selected, only the information contained in the report style Short will be saved. The results will be saved in more than one .DIF for a single report. See the explanation for .CSV files.
- .CSV – The report is in Comma Separated Values (.CSV) format. This is a very simple format for tabular data that is accepted by many spreadsheet programs and databases. Independent from the report style selected, only the information contained in the report style "Short" will be saved.

  There can be several .CSV files for a single report. For each report block, the first file, for example, REPORT00.CSV, contains the report header information. Subsequent files contain the tabular results. If the results are sorted by retention time, only one file is required for the complete table, for example, REPORT01.CSV. If the results are sorted by signal, a separate table is required for each signal. In this case, the files are named Report01.CSV through ReportNN.CSV, where NN is the number of the signal.
- .XLS – The report is exported to a Microsoft Excel spreadsheet in (.XLS) format. The .XLS will contain many worksheets. Each sheet contains a different portion of the information for the run taken directly from the registers in the OpenLAB CDS ChemStation Edition memory. The information in the sheet is very comprehensive but additional processing may be required to extract the needed elements.
- .HTML – Results are saved as gif files with an index.htm page for convenient viewing.
- .PDF – An Adobe PDF file version 1.4 is created using PDF-XChange 4.0 from Tracker Software Products LTD. The PDF functions are installed as a printer when the OpenLAB CDS is installed. The .PDF files are either created using a fixed name based on a specified prefix or automatically named using <result set name>_<data file name>. If results are sorted by signal more than one file may be created as explained above under .CSV.

Right clicking in the navigation table in the Data analysis view allows direct viewing of the reports written to files for the selected injection.

Specialized Reporting

Advanced reporting capabilities using the Classic Reporting include statistics on separation quality, reports that include trend analyses between samples and user-defined report layouts. These capabilities are fully functional but are largely obsoleted by the capabilities of Intelligent Reporting except for certain specific applications and situations where SOPs are built around Classic reports and the associated operating procedures.

The corresponding formulas and algorithms are detailed in the guide *OpenLAB CDS ChemStation Edition Reference to Operation Principles* (please refer to the chapter *Documentation* at the end of this document).

System Suitability Reports

System suitability reports enable users to report system performance parameters for individual analyses. There are three variations, or styles of these reports.

The Standard Performance report prints parameters for uncalibrated methods that include

- retention time
- capacity factor, k'
- peak area
- peak height
- symmetry
- true peak width at half height
- efficiency in plates
- resolution
- selectivity

For calibrated methods the compound name and amount replace the peak area, height and selectivity columns.

The report header includes the standard header and footer, sample information block, the analytical column parameters and optionally a plot of the chromatogram.

The Performance and Noise style adds an evaluation of the signal noise, in up to seven user-defined evaluation ranges, to the data from the performance report style. The noise parameters are reported as a signal-to-noise ratio for each peak or calibrated compound and a noise table for each signal. Each noise table includes noise calculated by the six times standard deviation, peak to peak and ASTM methods as well as the wander and drift.

The Extended Performance style adds plots of each individual calibrated peak showing graphically the peak start and stop times, half width and baseline. This style includes the following parameters in addition to the ones reported by the standard performance reports:

- area, height and amount
- skew
- excess
- USP tailing factor (equivalent to EP symmetry)
- time interval between data points and number of data points over the peak
- statistical moments (M0 to M4)
- peak width at half height calculated by the true, five sigma, tangent and tailing methods
- plate/column and plates/meter calculated by the peak width at half height, five sigma, tangent and statistical methods

Users may define their own noise evaluation ranges and acceptable limits for these performance criteria. Values lying outside the user-defined acceptable limits are indicated on the report.

Sequence Summary Reports

Sequence summary reports are produced at the end of a series of automated analyses. Their range of applications is from a brief summary of the samples analyzed to a detailed graphical repeatability or trend analysis of user-selectable parameters between different samples analyzed by the same method. The reports are built up from nine optional categories of information:

- a header page that may be user-defined
- the instrument configuration including revision numbers and analytical column or capillary specifications for LC, CE and LC/MSD systems
- the list of samples scheduled for analysis
- the logbook printout which states what was analyzed and documents the data acquisition and processing steps as well as any unexpected events
- a printout of the analytical methods
- individual sample reports
- statistics on calibration samples
- statistics on unknown samples
- a summary page that may be either a sample summary, one line of information per analysis, or a compound summary with a short compound summary table in addition to the sample summary.

The statistical reports may be selected as standard or extended styles. The Standard Style is text-based and includes the mean, standard deviation (SD), relative standard deviation (RSD) and standard error for the following parameters tabulated by compound:

- retention time
- area
- height
- peak width
- peak symmetry

The Extended Style includes graphical trend analyses based on a selection of parameters for statistical evaluation. The parameters that can be selected include

- retention time
- area
- height
- amount
- peak width at half height, by the sigma, tangent and tailing methods
- peak symmetry
- tailing factor
- capacity factor, k'
- theoretical plates by the peak width at half height, sigma, tangent and statistical methods
- resolution by the peak width at half height, sigma, tangent and statistical methods
- selectivity
- skew
- excess

Technique specific parameters for liquid chromatography include:

- peak purity evaluation factors (with the diode-array spectral evaluation module only)
- spectral library comparison factor (with the diode-array spectral evaluation module only)

The report includes a separate graphical trend analysis for each selected parameter. Sequence summary reports may be output to the printer, to file or both. The user may select to print or not print individual analysis reports together with the sequence summary.

Customized Reports

A customized reporting design view is included in OpenLAB CDS ChemStation Edition for users who want to define the exact content of their own reports. The user graphically defines a report layout which may include general sample information, signal, integration and quantitative analytical result information. The user may insert individual elements, such as text, tables and graphics. Inserted elements can be organized into sections and the relative position, size and orientation of each defined element can be adjusted graphically. The individual sections may be added, deleted, reordered and nested.

The user may define headers and footers to appear on every page, time stamps for the report and page numbering in the 'page x of y' format. The information included in the report may be any OpenLAB CDS ChemStation Edition- or user-defined parameter.

OpenLAB CDS ChemStation Edition macro programs can be linked to fields in the report enabling complex custom calculations or the addition of report elements beyond the capabilities of the report layout tools. Macros can also provide the logical control over sections of the report to show or hide them based on circumstances in the analysis.

Once the report has been designed it can be added to the report style list. These user-created report styles can be selected for methods in the same manner as the built-in report styles and are fully functional in automated analysis.

Intelligent Reporting

Agilent OpenLAB CDS Intelligent Reporting separates the processing and initial calculation of chromatographic signals from the reporting process. This allows new calculations and reports to be created without generating new result revisions because reports are based on stored result values rather than new values calculated from the raw data as the report is generated.

A key capability of Intelligent Reporting is the ability to build reports based on results across an entire sequence of injections as well as reporting results for each injection within a result set. Results from more than one sequence can be combined by combining data files from multiple sequences and/or single runs in the Navigation table in the Review view and reporting on them with a cross-sequence report template. For database-based reporting, OpenLAB ECM Intelligent Reporter can be added to an OpenLAB ECM based system. Using OpenLAB ECM Intelligent Reporter results are stored to a result database and reports can span all result sets residing in the same result database. Server-based Intelligent Reporting requires the Agilent OpenLAB ECM Intelligent Reporter software suite (G4635AA OpenLAB ECM Intelligent Reporter Server and G4636AA OpenLAB ECM Intelligent Reporter Client).

Analytical Result File Format - Agilent Common Analytical Markup Language (ACAML)

The Agilent Common Analytical Markup Language (ACAML) schema is a document format based on the XML (eXtensible Markup Language) standard using a patented schema. The approach is to define a technique- and application-independent unified language and schema. ACAML can be used to describe analytical data in a generic way, without any special aspects (e.g., result-centric viewpoint) starting from a single instrument or method up to a complex scenario with multiple instruments, methods, users and hundreds or thousands of samples. ACAML provides a common standard that allows seamless exchange of information between various platforms and applications. The current revision of ACAML only supports chromatography data (LC, GC) and does not support CE or the MS specific data generated by MS detection.

The ACAML schema is strong-typed to support standardized data-exchange and resist uncontrolled growth of self-defined types, which complicate automated data processing. The schema definition makes sure that each instance document is well defined and the referential integrity between all objects is guaranteed. No additional applications (like a special ACAML validator) are required to handle and validate ACAML instance-documents. The schema definition of the latest revision ACAML can be found on the OpenLAB CDS Support DVD supplied as a part of the OpenLAB CDS software DVD set.

Creating Intelligent Report Templates

Reports can be single injection reports which will repeat for each injection in the selected data set, single sequence reports which include results for each injection within one sequence in a single report, or cross-sequence summaries which can include results from multiple sequences (or single runs) within a single report. Standard Intelligent Reporting for the OpenLAB CDS ChemStation Edition can report at the injection or single signal level.

Intelligent Report templates are based on the Report Definition Language (RDL), a standardized XML format provided by Microsoft. To create new report templates, you can use the Report Template Editor (RTE) which is the report template toolset in the Report Layout view when Intelligent Reporting is enabled (by default in OpenLAB CDS ChemStation Edition).

RTE provides an easy-to-use interface that helps you create report templates using drag-and-drop predefined report elements. Elements or individual items are arranged in a WYSIWYG workspace with extensive configurable properties. RTE offers additional functions that are not available in the standard RDL report editors provided by Microsoft, such as Microsoft SQL Server Report Builder or Microsoft Visual Studio.

These functions are:

- Display of scalable chromatograms and spectra (UV and MS)
- Usage of custom variables and aggregators (custom calculator)

However, the Microsoft editors also offer functions that are not available in RTE, but are rarely used for CDS reporting. Templates created in RTE can be further modified with the standard editors to introduce e.g. toggle items for interactive report preview, free design of result matrices, charts with interactive tool tips or web publishing of lab wide reports. Note that with RTE, you cannot edit templates that have been modified with Microsoft SQL server Report Builder or Visual Studio.

Microsoft SQL server Report Builder and Visual Studio requires advanced knowledge of template development concepts and tools. For more information, please refer to the *OpenLAB Report Template Designer Concepts Guide* (see chapter *Documentation*). This manual also contains detailed descriptions of the Agilent report templates that are delivered with OpenLAB ECM Intelligent Reporter. These templates are specifically designed for usage in Visual Studio and contain some advanced features for interactive result preview that are not available in RTE.

Intelligent Report Items

Fields can be selected and placed into the template for all result values generated by OpenLAB CDS ChemStation Edition during an acquisition and the subsequent data processing operations. You can select and arrange the data fields in the report template according to your requirements, limited only by the structure relationships of the individual values.

The available data fields are arranged in the following categories:

- Sequence
- Sample
- Injection
- Signal
- Compound
- Peak
- Calibration Curve
- Instrument
- Project

A detailed description of the individual fields and their meaning and application is provided in *OpenLAB Report Template Designer Concepts Guide*.

A tree of report items is provided; each of the report items may be dropped into the report template, positioned, sized and configured. The items may be individual elements like a chromatogram graphic display, items with a defined repeat such as a spectrum for each peak, or preconfigured report sections. Each of these report items is commonly referred to as a snippet. The large list of individual elements is organized into the following categories:

- Chromatograms
- Tables
- Matrices
- Sequences
- Samples
- Calibration Curves
- Spectra
- Fields
- Special Objects
- Charts
- Method Information
- Instrument Information

For each item and for many individual elements within each item configuring the properties allows control of included data (peaks, compounds, signals, injections) as appropriate for the item. The data can be sorted, grouped or the element repeated based on unique values for one or more selected fields. Display styles and formats can be set for each item.

When items have other specific properties such as scaling for graphic displays, legends for charts, or fields for peak labeling, additional property tabs are available with the property dialog for the item.

Intelligent Reporting supports all calibration curve types, including log/log (OpenLAB Data Analysis only), quadratic, log, exponential and other curve types. For disabled calibration points markers are printed (OpenLAB Data Analysis only).

Individual report items may be locked to protect their definition in the report template. The privilege to lock and unlock items 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 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.

Custom table report items can be created using the .NET Software Developers Kit (SDK). It can render data from any data source. Intelligent Reporting also supports external code references. This allows to extend reporting with custom .NET code (dll's), create own complex calculations and read data from external files.

Intelligent Report Calculations

In the Report Template Editor, you can assign expressions to modify or create the contents of the report. Expressions can create or modify labels such as setting case for text, calculate values such as an impurity as a percent of a compound amount, or generate new values such as pass/fail indications based on a compound amount or any other calculation result. Expressions can be used for filtering data. As a result even complex filters can be done without IF expressions.

You can store the values, calculations and statistical calculations as variables or arrays (aggregators) and access these variables or aggregated arrays from subsequent report items in the template. The Expression Editor helps create valid expressions by providing direct field selection to make sure fields names are correct, function selection to offer properly formatted function calls and syntax checking for the complete expression. All expressions are based on Microsoft Visual Basic.

Keyed variables and aggregating functions can be used to collect and transfer the values from tables into subsequent tables for advanced calculations.

Items can be placed in any arrangement unless there is a relationship between an item and one or more following items. This means tables or graphs can be placed side by side. The templates are read and calculated from left to right and top to bottom, so any calculation variable above or to the left of the current element will be available to the current item.

Conditional formatting is selected through the properties dialog and allows users to configure the font color, style and weight, and background color based on the value of a data field. For example, the compound amount might be reported on a red background if the amount exceeds or falls below a certain value. Table columns can be formatted using conditional formatting based on expression results. Expressions may include custom variables and parameters.

Previewing Intelligent Reports

When you develop a new report template in the Report Layout view, OpenLAB CDS ChemStation Edition has a default dataset that will be used to populate item displays and the report preview. Since reports are often highly specific to the structure and labeling of the data in the report set, data can be selected in the Data Analysis or the Review view and will be automatically propagated to the Report Layout view. The selected data becomes the dataset used to populate the report previews, allowing interactive report development with accurate result content.

Once templates are saved, example reports can be printed, saved as PDF files or exported directly to Microsoft Excel XLS files from the Report Layout view using the preview data sent from the Data Analysis or Review view. For more accurate or complete testing, saved templates can be accessed from the Review view and applied to any dataset available in OpenLAB CDS ChemStation Edition. As in the Report Layout view, reports can be printed, saved as PDF or exported as XLS. In addition, 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 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. Document maps are converted to PDF bookmarks when exporting a report to PDF format.

Cross-Sequence Reporting

Intelligent Reporting in OpenLAB CDS ChemStation Edition is not limited to the result within a single sequence. The navigation table in the Review view allows combining data from multiple sequences and/or single runs. A cross-sequence template applied to data from different sequences and/or single runs will allow statistical calculations across the boundaries of a sequence. In addition, it is possible to create self-assembled result sets in the Data Analysis view; Data from multiple sequences and/or single runs can be combined in the navigation table. All or some of the data can be selected and a new self-assembled result set can be created (for more detail, see the section on *Self-Assembled Result Sets*).

Automating Intelligent Reporting

If Intelligent Reporting is selected in the report specification for the method, an Intelligent Report template can be selected to set the layout for the report for each injection. A second template can be selected for calibration injections to allow calibration injections to be reported using a different report layout. The report destination can be a printer, the screen and/or a file.

When reporting to a file the format can be PDF, XLS, TXT and/or DOC. The file will be written to the current data file folder using a fixed name or an automatically generated name. The automatic naming can be configured by combining current injection value tokens, spaces and text. The tokens available for file naming represent:

- Current Date
- Current Time
- Sequence Name
- Result Set (name)
- Sample Name
- LIMS ID
- Injection Date and Time
- Data File Name
- Sample Location

An option can be checked to copy the report file to a selected location. The location can be entered into the field or a button will select browsing to a location. A new folder can be created for the files. Note however that if copying the report to a network share, if access to the network share is interrupted, the report is not going to be copied to the remote location.

In the sequence output parameters, an Intelligent Report format can be selected to print a report at the completion of sequence acquisition and data processing. Typically this would be a single sequence report and can be as simple as a summary of the injections in the sequence or a fully defined report with sections calculating and presenting the injections according to their purpose. The sections can be defined as needed but might include sections like system suitability precision statistics, percent difference between check standards and calibration standards, statistics for replicate sample injections, etc. When reporting the sequence summary report to a file the format can be PDF, XLS, TXT and/or DOC. The file will be written to the current sequence data folder using a fixed name or an automatically generated name. The automatic naming can be configured by combining current sequence value tokens, spaces and text. The tokens available for file naming represent:

- Current Date
- Current Time
- Sequence Name
- Result Set (name)
- LIMS ID

If OpenLAB Data Store or OpenLAB ECM is installed, the sequence summary report can be optionally copied to the central data storage system separately.

As it can be difficult to reproduce reports from old result sets since the applicable report templates may have be modified or removed from the system, OpenLAB CDS ChemStation Edition saves all intelligent report templates used with a result set into the result set to preserve them with the data and results.

Data Utilities and Compatibilities

AIA File Support

OpenLAB CDS ChemStation Edition can import and export data files in the ANDI (Analytical Data Interchange) chromatography format of the Analytical Instrument Association (AIA), revision 1.0, copyright 1992. Data import is supported at compliance level one (sample information and signal data) and data export at compliance level two (sample information, signal data and integration results).

For LC/MS data, the AIA export dialog can select the signals and time ranges for the export. A batch export utility allows the automated export of AIA format signals for all signals in all injections with the resulting AIA files created in a selected destination directory.

Export CSV or DIF

Tabular information in the memory of OpenLAB CDS ChemStation Edition can be exported in either CSV or DIF format. A selection dialog allows selection of the export source from the following list:

- Integration Results
- Calibration Table
- Signal
- Spectrum
- Calibration Curve
- Active Graphic Window
- Table

For the selected item a window lists the items that will be exported for the selected source. The file path and name can be specified or selected. The ASCII character used as the field delimiter can be defined. A checkbox enables export to the clipboard to allow pasting into another application.

Dynamic Data Exchange

OpenLAB CDS ChemStation Edition includes commands and functions to support the Dynamic Data Exchange (DDE) standard of the Microsoft Windows platform as both a DDE client and a DDE server. The command set includes commands to establish and terminate connections, transfer information in both directions and execute remote functions.

Data, Method and Sequence Compatibility

All files (data files, methods, sequences, log files etc.) created on previous ChemStation Rev. A.xx.xx or B.xx.xx can be loaded and used in OpenLAB CDS ChemStation Edition. Files from earlier revisions are converted to a new structure when they are saved in OpenLAB CDS ChemStation Edition. The new structure is not backwards compatible, so files saved in OpenLAB CDS ChemStation Edition can't be returned for use with older ChemStation Rev. A.xx.xx or B.xx.xx systems. The system will warn users to save files with a new name when performing the one-time conversion from an earlier revision. It is always recommended to convert a copy of the original files or to save the converted files to a new name to preserve the original.

Converted methods may contain new parameters not available in earlier revisions of the OpenLAB CDS ChemStation Edition. These parameters will contain default values after the conversion, so it is always recommended to review the content of converted methods before using them for new data acquisition.

Data from OpenLAB CDS ChemStation Editions prior to Rev. B.02.01 was not in the new result set format (also referred to as sequence container). This data can be opened and processed as single sample data and sequences can be reprocessed in the Method and Run Control view following legacy processing procedures. However, a conversion utility allows the separate elements needed to process sequences in earlier revisions to be processed into an OpenLAB CDS ChemStation Edition result set. The utility prompts for a sequence file (.S) a method file (.M), a source folder containing sequence data files and a destination folder for the completed result set. The source data folder must contain the data files specified by the sequence file, the batch file (.B) for the sequence, and the sequence log file. When the conversion is complete the data can be processed using all of OpenLAB CDS ChemStation Edition views and tools.

XML Interface

XML (eXtensible Markup Language) is a protocol for structuring data in a defined text format. The XML file contains data with embedded structural information. XML has become a de facto standard for exchanging data between different systems, particularly for writing defined data into and out of databases.

To connect OpenLAB CDS ChemStation Edition to a Laboratory Information Management System (LIMS) or Knowledge Management System (KMS) OpenLAB CDS ChemStation Edition offers an interface based on the standardized XML format.

The interface allows the manual import of a sample work list in XML format into the OpenLAB CDS ChemStation Edition sequence table. This process can be automated using the OpenLAB CDS ChemStation Edition macro language.

The OpenLAB CDS ChemStation Edition XML interface enables manual or fully automated export of sample and result information. The XML schema files provided with the software allow an easy adaptation of the interface for a specific LIMS or knowledge management system. More information is available in the *Agilent OpenLAB CDS ChemStation Edition XML Connectivity Guide* (see chapter *Documentation*).

Customization

Custom Fields

Per sample and per compound custom fields are available and can be used to enter, store and export information for classic as well as intelligent reporting which is not defined by standard OpenLAB CDS ChemStation Edition operation. The fields are specified in the method, so fields can be different for each method. Each field has a selectable type as numeric, text or date/time. Fields have a user-defined name and an optional default value. Up to 10 per sample custom fields can be defined and up to 10 per compound fields.

Field values are entered with the sample information, either in the sample information dialog for single injections or in the sequence table for automated analysis. Custom fields can be marked as mandatory. When a field is mandatory, the operator must supply a value for the field before he is allowed to begin acquisition.

Data entered into custom fields are available for both classic and Intelligent Reports. Intelligent Reports can use custom field values in calculations and logical operations.

OpenLAB CDS ChemStation Edition Macro Programming Language

OpenLAB CDS ChemStation Edition can be customized using its powerful built-in command language. Commands may be typed in and executed through a command line or written to a file to create a macro program. The OpenLAB CDS ChemStation Edition macro language is a fully formed BASIC-like language where commands are in the form of a keyword with a defined set of parameters.

Macros may define variables, create and populate tables or data objects in the OpenLAB CDS ChemStation Edition memory, and access memory constructs created by the normal OpenLAB CDS ChemStation Edition functions. Macros can define user interface elements such as prompts, dialog boxes, menus and toolbars. Logic commands can build conditional or looping constructs, perform physical I/O including file handling or printing with nested and recursive calls.

Macros have access to instrument operations, instrument parameters and operating system commands, and can execute other applications supporting command line control.

Macros can be invoked from the command line, from defined user interface controls, and from defined parameters in the method. A defined hook subsystem allows macros to be automatically loaded when OpenLAB CDS ChemStation Edition starts and hooked into specific connection points within the OpenLAB CDS ChemStation Edition execution. Hooks allow very intimate access to OpenLAB CDS ChemStation Edition while carefully protecting the OpenLAB CDS ChemStation Edition automation engine from disruption by malformed user code.

More information on customization is available in the *Macro Programming Guide* within the Agilent OpenLAB CDS ChemStation Edition online help. The *Macro Programming Guide for RC .NET Drivers in OpenLAB CDS ChemStation Edition* details instrument commands and is provided with the OpenLAB documentation on the software DVD.

Automation

Sequence Overview

Automated analysis is based on a tabular sample work list specifying a sequence of injections, the method for the analysis and all associated sample parameters such as sample name, sample type, calculation factors, and optional parameters. This automation table is stored as a sequence template and may be reused to run subsequent sets of analyses. This sequence template, all methods used for analysis of the sequence, all data generated from instrument data acquisition, all results calculated during data analysis and all intelligent report templates comprise the result set.

The result set is a folder with a unique name generated from a user-selected naming pattern that can contain a combination of date, time, operator, instrument, acquisition PC, and/or sequence name along with spaces and fixed text.

OpenLAB CDS ChemStation Edition sequences can assign a different method to the injections on each line in the sequence table. A configurable equilibration delay waits for the specified time when a new method is loaded to allow for column equilibration before beginning analyses with the new method.

The acquisition can automatically name data files or combine a user-defined prefix of up to fifteen characters with sequential file numbering. The user may select to run full analyses or data acquisition only.

At the completion of the sequence, or if the sequence terminates with an error, OpenLAB CDS ChemStation Edition may execute one of a selection of technique-specific shutdown commands or a user-defined shutdown macro to complete a series of specific commands.

OpenLAB CDS ChemStation Edition provides three different toolsets for creating and submitting sequences to the sequence queue, all of which are outlined in the subsequent chapters. More details are given in the *OpenLAB CDS ChemStation Edition Concepts and Workflows Guide* (see chapter *Documentation*).

Analysis and Processing Controls in the Sequence Table

The sequence table opens as a spreadsheet-like user interface that allows users to specify vial position, sample name, analysis method and number of injections for each sample row. Users can insert or add multiple empty lines, or delete selected lines. The sequence table supports Excel-like editing as well as copy to and paste from Excel. The user can jump between individual cells in the table and copy, cut or paste individual cells or entire rows or series of rows in order to build sequences efficiently and quickly. A recent change can be revoked or reinstated with an “Undo”/“Redo” action or the whole table can be cleared in a single step using “Clear”.

An advanced sequence table toolset enables an even smarter and faster setup of the entire sequence table. The “Insert/FillDown Wizard” allows users to fill the complete Sequence Table, or selected parts of the Sequence Table, with similar data. The data is taken from the selected sequence lines and applied to the inserted or appended lines. The simplest mode is to just repeat a given line n times. A more sophisticated mode provides means to insert lines based on a given pattern. The parameters in the “Insert/FillDown” Wizard are organized in three groups:

- New Sequence Lines enables users to insert multiple copies of the selected sequence lines after the selected lines, after a specified number of samples of sample type “Sample” or append multiple copies of the selected sequence lines at the end of the table.
- The Sample location can be defined to increment, increment by a certain pattern (for wellplates), increment for sample type “Sample” only (locations of type “Calibration”, “Control Sample” or “Blank” will retain their values), repeat the location, or leave the sample location empty.
- The Sample Name for new or appended lines is automatically populated based on the sample name given in the selected line with several options: detect and increment a given counter in the sample name, append and increment a counter to the sample name, increment the sample names of type “Sample” only, repeat the sample name given in the selected sequence line, or specify no sample names. Users may choose to retain the same name for identical sample location.

The sequence table can be filtered to only display a defined subset of sequence lines. Conditions for filtering are defined in the "Filter options" and include sample type, method name, calibration level, sample location and sample name. For Sample name and method name the filter can be applied to the precise name or a string that must be contained.

Selecting the sample type controls the data processing invoked for the sample. When the type is Sample the injections are treated as unknown samples and are evaluated and reported according to the method specification. Calibration samples are used to update the calibration table of the method. Calibration update options are described below; sophisticated update controls support a variety of calibration and recalibration scenarios. Control samples are evaluated against the limits set for each compound. If the results lie outside the specified range for any peak value the execution of the sequence will be halted.

For each calibration injection the calibration level is selected and the calibration update is set to replace or average. Replace uses the current injection to calculate a new response factor for each compound. Setting the update to average uses previous calibration information together with the values from the current injection to calculate new response factors based on the average. The average is the average of all calibration injections. Setting a recalibration interval activates cyclic recalibration where the standard is injected after the defined number of unknown samples has been injected. When calibration update is set to bracketing, an interval is set and each interval of unknown samples is bracketed by standard injections. For each bracket interval, the samples are quantitated based on the average response of the standards immediately before and after the unknown samples in the bracket interval. If response factors have been entered into the calibration manually, the update can be set to Delta% to enable an update of the response factor based on the percent difference between subsequent calibration standard injections.

The sequence table has columns for two factors, the "Multiplier" and the "Dilution Factor" which will be multiplied with the calculated amount for each sample. The sample amount can be supplied and if amount % calculations are selected the amount calculated for an unknown will be calculated as a percent of the sample amount value supplied. If one or more internal standards are used for the analysis, the ISTD amount columns can be used to specify the internal standard concentrations for each sample. The software supports up to 8 ISTDs.

The Sample Info field can be used to add a much larger text description to a sample than allowed in the sample name field. Another text label can be added in the LIMS ID column. The LIMS ID is typically used to supply a unique identifier for results exported to other systems. LIMS ID2 and LIMS ID3 are populated with values imported from a LIMS and can be turned user-editable using the command line.

Depending on the configured instruments and modules, additional fields will appear. For example if an Agilent LC system includes a fraction collector the "Fract. Start" column will appear in the sequence table. Or if dual injection is enabled for GC, the injection source column will appear and allow for a choice between front and back injection. Another example is "Target Mass" which is only available if a CE/MS or LC/MS is installed.

For dual-simultaneous injection sequences, employing more than one injector, the table view can be toggled between execution order (alternate locations) or separated by injection location. For samplers with barcode reader support the sample names can be read from the barcodes and put into the "Sample Name" field of the current or multiple selected sequence lines.

The "Sequence Preview" shows the sequence exactly as it will be executed, with all repeat calibrations, control samples and blanks included in the correct order of sequence. The "Column Configuration" allows users to permanently customize the view by selecting the columns to display in the Sequence Table. If needed, all changes can be reset to the original state.

Starting Sequences

As soon as starting a sequence (submitting it to the queue) the sequence template is converted to the order shown in the sequence preview – a run-by-run list. The generated sequence file will be stored in the result set. Sequences may be paused to run single injection priority samples by another method, then restarted without disrupting the automation. Samples can be added to the sequence table while the sequence is executing. Adding a new sequence line to a running sequence will result in different data file names for the added samples to help distinguish these runs from others.

Graphical Sample Entry

In addition to the table-based sequence setup OpenLAB CDS ChemStation Edition offers an intuitive graphical sample entry workflow. The user interface consists of three elements:

- Sampler Panel - graphical representation of the sampling system in use for container allocation.
- Container Panel – visual display of the selected sample container and the loaded samples. It is used for graphical sample range selection.
- Sample List Table – tabular list of samples gathered from the "Container Panel" for sequence creation.

Based on the selected sample container in the "Sampler Panel" users can easily create new sample entries in the graphical user interface. They simply click on the locations in the container visualization of the "Container Panel" that they want to add a samples to. The newly defined sample locations will be color coded where the color corresponding to the selected sample type. The sample entries automatically appear in the "Sample List Table" underneath. Users can save commonly used parameters for similar samples in sample templates. These templates can be applied to samples of the same nature when graphically adding them to the sample list.

For all autosamplers that physically allow rearranging of plates, users can even drag entire plates to other positions or drawers in the user interface. The vial locations are automatically adjusted in the sample list. The container configuration can be saved with the sequence template, or exported to PDF.

Similar to the sequence table the sample list table offers functions that help editing the sample list, such as Copy/Paste, Append or Filldown. Sequences can be submitted to the end of the queue or to be run as soon as possible.

Users may also use the sample list table to edit new sample lists as well as existing sample lists that were already submitted to the queue. This includes loading the currently active sample list from the queue, making edits and resubmitting to the queue.

Sample Container Types

Sample containers refer to instrument trays or plates that hold the samples/vials. Sample containers have different dimensions and different vial capacity depending on the instrument. Sample container types describe the physical properties of a specific tray or plate in an XML format. Custom sample container types can be centrally managed and shared across the lab with OpenLAB Shared Services by importing an XML file containing the sample container type definition in OpenLAB Control Panel. All CDS clients connected to the same Shared Services Server will have common Sample Containers definitions.

Easy Sequence

Easy Sequence is a user interface for quick and easy setup of sequences from templates. With Easy Sequence, multiple sequences can be submitted to the sequence queue to be run on the data system. In addition, a calibration setup provides an easy to use drag-and-drop interface to specify calibration types and sample positions.

Partial Sequence

The partial sequence functionality allows users to see the order of execution of the sequence and also select individual sample entries to rerun or re-evaluate. When re-evaluating data already acquired, users can specify whether reprocessing uses the original sample quantification data or new data entered in the sequence's sample table.

Queuing Sequences

Multiple and different classic or Easy Sequences as well single injections can be added to the queue. The Queue Planner allows additional sequences to be inserted into the queue or appended to the end of queue. The order of queued sequences can be changed. Pauses can be queued between sequences to allow defined points for user interaction. Any sequence in the queue can be removed or modified for any injections scheduled following the current injection. Priority change or deletion of queue entries is protected by user privileges. (See chapter *OpenLAB Control Panel Administration*).

Printing Sequences

Both the sequence and partial sequence tables may be printed.

Central Data Storage

Agilent provides two systems for central data storage:

- OpenLAB Data Store is available as a single server solution providing centralized data management for small to medium laboratories with up to 30 instruments. It provides the necessary security in support of regulatory compliance.
- OpenLAB ECM is available as a single server or multi- server, distributed solution for comprehensive data management needs for laboratories with a few instruments to 100s of instruments. It also provides the necessary security in support of regulatory compliance.

Both systems are web-based electronic libraries that allow users to safely archive and catalog any electronic file. Users may store and index analytical raw data, reports, and all other types of documents. The stored files can be shared with other users. Any electronic file type, such as Microsoft Office documents, Adobe PDF documents, images, and molecular drawings, as well as raw data and reports generated by ChemStation can be stored.

Either of these central data storage systems allows you to easily collect, organize, search, and review all of your ChemStation data. They automatically extract searchable metadata from files, and provide powerful search capabilities. ECM additionally provides embedded viewers for many file types.

The interface to the central data storage system is opened via Microsoft Internet Explorer, also referred to as the web client.

In this document, the terms „central data storage" or "central repository" refer to instances of either OpenLAB ECM or OpenLAB Data Store. As the interface and workflows for both systems are very similar, the specific product names are only used in places where there is a difference in associated concepts or procedures.

OpenLAB CDS ChemStation Edition data are stored in the central data storage as compressed files: single runs as *.D.SSIzip, result sets as *.SC.SSIzip sequence templates as *.S.SSIzip, methods as *.M.SSIzip. Compression is carried out automatically when the data are uploaded to the central data storage. When the data are later downloaded from the central data storage to the ChemStation, they are unzipped into the ChemStation Explorer.

OpenLAB ECM is available in the following installation scenarios:

- Workstation
- Networked Workstation
- Distributed System

OpenLAB Data Store supports the following installation scenarios:

- Secure ChemStation Workstation
- Networked Workstation
- Distributed System

ChemStation File Types in the Central Data Storage

OpenLAB CDS ChemStation Edition provides an interface to the central data storage, which enable users to store analytical data and reports in a secure location. From ChemStation, users can log in to the central data storage and store all kinds of ChemStation files in the central data repository:

- Methods (*.m)
- Sequence templates (*.s)
- Data files (*.d)
- Report templates for Intelligent Reporting (*.rdl)
- Reports (*.pdf, *.xls, *.doc, or *.txt)
- Library files (*.uvl)
- Column databases (*.mdb)
- Easy Sequence templates (*.est)
- Classic report templates (*.frp)

The storage of ChemStation data can be either automatic (that is, at the end of a single run or sequence) or manual. The data can later be downloaded to ChemStation for review or reprocessing at any time. Furthermore, OpenLAB CDS ChemStation Edition in combination with central data storage offers features that enable users to comply with 21 CFR Part 11 and similar regulations for electronic records and electronic signatures. Please refer to the chapter *Good Laboratory Practice* below for more details.

File Management in ECM

ECM provides a four-tier data storage model with a structure of Location, Cabinet, Drawer, Folder; this hierarchy imitates the familiar concept of multi-drawer filing cabinets in a room, with each drawer containing multiple files. The Location, Cabinet, Drawer and Folder names comprise the path name of the storage location, the data being stored in the Folder.

For convenience, the OpenLAB CDS ChemStation Edition provides pre-defined tokens for the Location, Cabinet, Drawer, and Folder for automatic path creation. With these tokens, the system automatically creates the required items if they do not already exist in the central repository. The following tokens are available:

- Instrument name,
- Operator name,
- Instrument number, or
- Computer name.

File Management in Data Store

OpenLAB Data Store provides a multi-level storage model. The number of levels is not limited, and data can be stored in any folder level. The OpenLAB CDS ChemStation Edition provides the same pre-defined tokens for all elements of the Remote Data Path as for OpenLAB ECM.

Workflows and File Handling

When the data is uploaded to the central data storage, local copies of the files still remain in the OpenLAB CDS ChemStation Edition file system. If an item is loaded from the central data storage back into OpenLAB CDS ChemStation Edition, it is automatically loaded into its original location. Local copies of data stored in the central data storage can be automatically cleaned on the local subsystem during shutdown of the OpenLAB CDS ChemStation Edition. Only data that was successfully stored to the central data repository is removed.

Different options are available regarding the automatic upload of single runs and result sets. This is in contrast to downloading stored data from the central repository to the local file system, which always requires a manual load action. Methods, sequence templates and report templates always require a manual upload to the central data storage as well as a manual download to local file system for use with OpenLAB CDS ChemStation Edition.

The automatic upload is determined by the "Transfer Settings" defined in the "File Transfer Settings" tab of the OpenLAB CDS ChemStation Edition "Preferences". The following options are available for data upload:

- *After Acquisition* – Use this option to automatically store data in the central data storage directly after the acquisition has finished. The raw data is initially stored locally. After completing the acquisition, the data is automatically uploaded to the central repository.
- *After Reprocessing* – Use this option to automatically store data in the central data storage directly after the reprocessing has finished. This applies to data that has been previously stored in the central repository. A new version of the data is created in the central storage for the reprocessed or changed data.
- *After any Data Modification* – Use this option to automatically store data in the central data storage after the review and update of single runs or individual data files in a result set. A new version of the data is created in the central storage for the changed data.
- *Import after Reprocessing* – Use this option to upload locally stored data to the central data repository for the first time. This applies to locally saved data that was not yet stored in the central data storage. It is reprocessed and then automatically imported into the central repository as the initial version.

All commands for interactive up- or download of files are combined into a single menu in OpenLAB CDS ChemStation Edition that is only available when central data storage is configured – the ECM or Data Store menu. Depending on the current view, users can load different files defined by the context. In the Data Analysis view, users can load single run data or sequence data. These data are automatically set to the status checked out in the central data storage system. The checked out status of a data file is visible to another user and prevents him from inadvertently altering a data file that has been downloaded to another ChemStation. In the Method and Run Control view, users can load methods and sequence templates. These items are only retrieved from the central repository, but they are not automatically checked out. For Intelligent Reporting, report templates can be downloaded from the central data storage in the Report Layout view.

It is sometimes necessary to modify a master method, sequence template or report template. Unlike data files, the methods, sequence templates, and report templates are not automatically checked out of the central data storage system. In order to prevent other users from modifying the same item it should be checked out manually; the "Open As Checked Out" command marks the item as checked out in the central data storage system. An item checked out by another user is marked with a red icon. It can still be loaded in OpenLAB CDS ChemStation Edition as a copy but it cannot be saved back to the central data storage before the other user has uploaded his version. A check-out can also be undone without creating a new version if no change was made to the checked-out item.

The following chapter is a summary of the different workflows in OpenLAB CDS ChemStation Edition that involve the central data storage. For a more detailed description please refer to the *Agilent OpenLAB CDS ChemStation Edition with Central Data Storage User's Guide* (see chapter *Documentation*).

Updating the local master methods, sequence templates or report templates

If one or more master method, sequence template, or report template was updated in the central data storage system (i.e. a new version is created), it is possible to update the local copy of all modified methods and templates. From the ECM or Data Store menu the changed files can be updated in a single step per category using the “Update Master Methods”, “Update Sequence Templates” or “Update Report Templates” commands. Each command reveals a table with all items that have previously been uploaded to the central data storage with version information for local and server copy. Users may choose in a single step to locally update all those items with a higher version number in the central repository.

Centrally stored data in the ChemStation Explorer

Data, methods, sequence templates and report templates that are centrally stored in a data repository have a distinct appearance the ChemStation Explorer. A particular icon makes them easy to distinguish from data that is only stored locally. The color coding of the icon indicates the current status of the item:

- Green – the item is stored in the central data repository and has not been changed locally.
- Yellow – the item is stored in the central data repository and has been modified locally.

Good Laboratory Practice

OpenLAB CDS ChemStation Edition is developed to internationally recognized design and development standards and has a number of features specifically to help users document that their analyses meet current regulations and quality standards including, but not limited to the Food and Drug Administration's (FDA) rules 21 CFR 210 (Good Manufacturing Practice for Drugs), 21 CFR 211 (current Good Manufacturing Practice for finished pharmaceuticals), 21 CFR 58 (Good Laboratory Practice). These features help users validate and specify methods, verify that methods are fit for their intended use, verify system performance and operation and ensure the traceability, integrity and security of the data.

OpenLAB CDS provides the following software functionalities which enables compliance with of 21 CFR Part 11 and similar rules:

- Mandatory login with connection to the central data storage system
- Configurable session locking
- Configurable ChemStation user roles and privileges
- Full data traceability through audit trails for methods, sequences and results
- Full data versioning

For those specifically concerned with 21-CFR Part 11 or the European Medicine Agency's (EMEA) Guidelines to Good Manufacturing Practice (GMPs) - Annex 11 (EU Annex 11) compliance please consult the technical notes *Integration of Agilent OpenLAB CDS ChemStation Edition with OpenLAB Data Store - Compliance with 21 CFR Part 11* or *Integration of Agilent OpenLAB CDS ChemStation Edition with OpenLAB ECM - Compliance with 21 CFR Part 11* (for publication numbers see chapter *Documentation*).

Development Process

The Agilent Certificate of Validation shipped with each software package documents the software development and testing steps executed as part of the development cycle. The development process is registered to the ISO 9001 quality standard.

OpenLAB CDS Validation

Agilent offers validation services for the OpenLAB CDS family of software products and for a wide variety of Agilent instruments and those from other manufacturers. These services utilize detailed protocols developed by Agilent and are delivered by certified support personnel. For more information please refer to the document *Agilent Compliance Services Portfolio:Enterprise Edition* (see chapter *Documentation*).

Software Verification

An automated Software Verification Tool is installed with each software component of the OpenLAB CDS ChemStation Edition. This utility has a reference file providing an index of the files required for a proper installation. The utility checks the reference list against the files installed, their locations and revisions, including operating system files with specific dependencies.

This test is typically performed at installation and can be performed at any time to verify the file level integrity of the software installed on each computer in the installation. Test reports can be printed or saved to files.

The Agilent Software Verification Tool for OpenLAB CDS can be used to verify a successful installation of a new version or patch. This does not replace the Installation Qualification (IQ) service, which is delivered by an authorized Agilent service provider.

System Verification

In the Data Analysis view of OpenLAB CDS ChemStation Edition users can launch the "Verification" dialog from the View menu to start the system verification utility. The system verification tests automatically verify the correct operation of the data evaluation software by comparing results generated when a test is executed against pre-recorded known values. A selection of tests is provided with the software to enable testing of specific data analysis calculations. New verification tests can be defined, allowing users to utilize their own data files and methods to create the test.

System Access Controls

Earlier sections of this document describe in detail the user authentication and system access controls. The options provided accommodate a wide variety of operational policies.

Method Specification and Use

The method is the primary instantiation of the analysis procedure in the OpenLAB CDS ChemStation Edition. The method is specifically designed to support accurate, complete and secure maintenance of system operating parameters.

The complete instrument and data analysis specification is stored in one location. Core parameter files are in a proprietary, binary format to prevent editing outside the control of OpenLAB CDS ChemStation Edition.

The method change history log automatically records how and when a method was changed. Users can be required to add a reason for the change to the change history log. The change history log is stored as part of the method. The change history log may be viewed and printed.

The acquisition method is saved with the data file to record the settings at the time of the analysis. The result set contains both the shared method applied sequentially to each analysis and a separate copy for each injection containing the exact settings for that specific injection.

The method is saved to each injection a second time at the completion of all the analytical steps. This preserves the data processing settings and allows exact reconstruction of the reported data at a later date.

Data Traceability, Integrity and Security

Data security is achieved in the PC environment through operating system security features. Proper configuration and requirements for operational security are detailed in the software installation manuals and the OpenLAB CDS administration manuals. The identity used to log into the PC does not have access to the data storage locations, if the data are stored remotely in OpenLAB Data Store or OpenLAB ECM, and data is created and stored under the authority of the application software.

The operational traceability is provided through a hierarchical set of software logs. Events are stored in one or more logs according to their role in the operation so a coherent history is available for each data element.

An instrument logbook records instrument and operator activities at all times. This log contains operational and instrument based events, independent of active analysis, and lists the beginning and end of each single run or sequence but not the detailed activities within the analyses.

For automated analyses, a sequence logbook records the start and end of each individual analysis, and error messages generated within the scope of the sequence. A selection of instrument measured instrument parameters is recorded at the beginning and end of each analysis to track the instrument operation as the analyses are performed. After acquisition and the initial automated data processing, data analysis operations are logged in detail, with the operation performed, the operator performing the actions and the date and time stamp.

The actual instrument conditions, such as pressure, flow, and temperature, which occurred during each analysis, are also recorded if the configured instrument supports this capability. This data can be subsequently displayed graphically with the chromatogram to show the actual instrument conditions during that particular analysis. These graphics may be included on each report.

Audit Trails and Logbooks

In order to enable compliance with 21 CRF Part 11 and similar regulations, OpenLAB CDS ChemStation Edition offers several audit trails and logbooks to document all activities associated with methods, sequences, results, reports, or any files stored in the central repository. These audit trails and logbooks track all changes that are made to any file, including data acquisition, re- analysis, and long- term archiving. The audit trails are stored and archived together with the sample or method data.

Once enabled the Audit Trails cannot be disabled.

Method Audit Trail

Each method has a Method Audit Trail. By default, this Method Audit Trail contains only the comments that users must provide each time when saving a method. As there is no control over the provided text, there is no guarantee that the method changes are reproducible.

To fulfil the requirements for audit trails as mandated by 21 CFR Part 11 and similar regulations, OpenLAB CDS ChemStation Edition makes it possible to generate a more detailed Method Audit Trail. If the function is activated, the Method Audit Trail contains not only the user comments, but also each individual changed parameter with its old and new value. All changeable data analysis parameters are tracked. This means that you can reproduce exactly which value has been changed to what, when, and by whom.

Depending on the instrument driver, the Method Audit Trail may also contain an entry for each changed instrument setting. This feature is supported, for example, by Agilent LC System RC.Net drivers and Agilent GC 7890 System drivers.

The Method Audit Trail can be enabled for the current method or for all methods.

Results Audit Trail

If activated, the Results Audit Trail is added to the existing Data File Logbook. By default, each Data File Logbook will only contain the acquisition parameters and reprocessing information for the corresponding sample. The Results Audit Trail additionally tracks the changes of all data analysis parameters for this sample. The Results Audit Trail is enabled for an individual OpenLAB CDS ChemStation Edition session or an entire workstation or AIC.

Sequence Audit Trail

The Sequence Audit Trail is automatically enabled with the Results Audit Trail. The Sequence Audit Trail is started with the acquisition or re-processing of a sequence and is added to the Sequence Logbook. The sequence logbook itself contains a record of each method run and error conditions that occurred during the acquisition or reprocessing of the sequence.

When it is activated, the Sequence Audit Trail is generated for all sequences that are created with unique folder creation switched on. It is created whenever a non-template sequence is changed for the first time and, once created, is continuously updated for each change. It is saved along with the sequence, and tracks all changes to:

- any table cells of the sequence table
- insertion and deletion of sequence lines
- the values in the „Sequence Parameters" of the sequence
- values in sequence-related custom fields

For each change, the application logs:

- date and time of the creation of the audit trail entry
- the user who was logged on when the audit trail entry was generated
- a system- generated description of the change that resulted in the audit trail entry
- a user- generated comment

The latest Sequence Audit Trail entry is added to the top of the list. The list can be displayed and printed.

Report History

During data review OpenLAB CDS ChemStation Edition single injection reports can be created in multiple ways – display the report on the screen, send it to a printer, or save the report as a generic pdf-file (report.pdf). These interactive report outputs may easily be lost or overwritten, especially when several reports are printed one after the other.

To keep track of all steps, OpenLAB CDS ChemStation Edition automatically stores all reports that have been generated in a "Report History". The "Report History" contains all reports created for the current data file and can be exported or printed. The Report History is only available if the system is configured with central data storage.

Audit Trail of Central Data Storage

The Audit Trail of the central data storage system is a record showing who accessed the system and when, and what operations he or she performed during a given period of time. The Audit Trail contains file-related, system administration, folder administration, and (for ECM) scheduler-related entries. For example, administrators can see when a file was added and who added it. For each operation, the central data storage system asks the user for a reason. This reason is also shown in the Audit Trail. For automatic uploads there are default reasons given by the system.

In OpenLAB Data Store the Audit Trail is always enabled, while in OpenLAB ECM it has be enabled manually during account creation.

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 central data storage is configured, 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 central repository as a new revision. Once the data are stored in the central data storage, each operation that modifies the data will result in a new revision once the data are uploaded again.

A transaction log is maintained in OpenLAB Data Store or OpenLAB ECM respectively 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.

Instrument Control

The instrument control capabilities of OpenLAB CDS ChemStation Edition may be expanded through the purchase of additional instrument driver licenses to allow for multiple instruments or mixed technique configurations. The instrument control capabilities are documented in the following sections, each relating to a specific technique.

Agilent OpenLAB CDS drivers are based on the RC.NET architecture. Information in this document refers to this driver type, unless otherwise noted. Native "classic" drivers for legacy modules of the 1100 and 1200 HPLC series are still provided with OpenLAB CDS ChemStation Edition. These classic drivers cannot be run in the same instrument with RC.NET drivers. In addition for some instrument classes "Classic Plus" drivers are available with OpenLAB CDS ChemStation Edition (ELSD, CTC and Single Quad MS). The Classic Plus driver types can be combined with RC.NET drivers via their CIC ports.

The supported instruments and firmware are further detailed in the *Agilent OpenLAB Chromatography Data System Supported Instruments and Firmware Guide* (see chapter *Documentation*).

OpenLAB CDS ChemStation Edition for GC

Instruments

The Agilent OpenLAB CDS ChemStation Edition for GC combines instrument control, data acquisition, and data analysis software for the Agilent 7890, 7820, 6890, and 6850 Series gas chromatographs (GC), and the Agilent 490 Micro GC.

The Agilent OpenLAB CDS ChemStation Edition is interfaced to the GC via LAN and collects full range digital data from detectors. Depending on the detector type, data can be acquired at rates up to 200 Hz from the Agilent 6890 and Agilent 6850 Series, and up to 500 Hz from the 7890 Series GC.

When interfaced to an Agilent gas chromatograph, the Agilent OpenLAB CDS ChemStation Edition can control GC parameters for heated zones, oven temperatures, detectors, inlets, cryogenic cooling, signals, electronic pressure and flow control, and cool on-column temperature programming. In addition to GC control the following features are noted:

- Graphical user interface for easy access to all method parameters for 78xx and 68xx GCs
- Method resolution to verify and alert the operator of potential problems if a method was created on a different GC system or if the instrument configuration has changed.
- Method Resolution Audit Trail to track the history of method resolution occurrences and related actions
- Signal Events (Switching between front and back detectors, zero signal, and delay signal collection)
- Calibration of capillary columns to properly specify length and diameter for pressure and flow calculations.
- Method transfer from the 6890 to the 7890 GC.

The Agilent OpenLAB CDS ChemStation Edition can display graphically the oven temperature, inlet temperature, inlet pressure, auxiliary channel pressure and column flow programs. The Agilent OpenLAB CDS ChemStation Edition also can control, through a timetable, a maximum of eight valves or relays.

Sampling Systems

The Agilent 7693A, Agilent 7650A and Agilent 7683 Series automatic liquid samplers allow for complete automation of sample introduction in single front, single rear or dual-injector configurations.

Dual-injector configurations allow individual or synchronous injections for the Agilent 7890 and 6890 Series GCs with the Agilent 7693A and Agilent 7683 Series automatic liquid samplers. Each automatic sampler allows a 3-vial turret, 8-vial turret, or 150-vial access if a sample tray is fitted. One Agilent 7650A automatic liquid sampler (50 vial capacity turret) at a time is operable on a compatible GC, in front or back inlet.

The 6850 GC also supports the G2880A 22/27 positions tray.

The Agilent OpenLAB CDS ChemStation Edition allows random sample access and priority sample injection.

The Agilent OpenLAB CDS ChemStation Edition allows the user to optionally display a Sampling Diagram window containing a graphical display of the vial tray, indicating which samples have already run, which sample is currently running, and which samples will be run for the 7890 and 68xx GCs.

For the analysis of volatile analytes the Agilent 7697A or G1888 Headspace Samplers and the Agilent 78xx and 68xx GCs can be used in combination with the Agilent Integrated Headspace Software for control and programming of the sampler.

The 7693A ALS and Tray with the Easy Sample Prep software, an add-on software to OpenLAB CDS ChemStation Edition, enables an easy way to build and run GC sample preparation programs.

The Agilent PAL Samplers can combine liquid, headspace, and SPME injection into one instrument, so users can switch from one application to another on the same GC workstation. The following injectors are available:

- Agilent G6501B and G6502B GC Sampler 80 cm for Liquid Injection
- Agilent G6509B GC Sampler 120 cm for Liquid Injection

The following CTC Combi-PAL and CTC GC-PAL injectors are supported in addition by the Agilent OpenLAB CDS ChemStation Edition: G6500-CTC , G6501-CTC, G6502-CTC and G6509-CTC.

Barcode Reading

The 7693A ALS 150 vial tray with optional bar code reading and heating can be used to help build automation sequences and verify that the identity of the injected sample matches the name in the sequence table at injection time.

Sample names can be read from barcodes and automatically filled in:

- *During sequence* – the sequence is started with blank sample names in the sequence table. Before each injection, the barcode on a sample vial is read and the respective sample name is written into the Sample Name field of the report.
- *Before starting a sequence* – Users may fill in the sample name from the barcode label on the vial directly into the sequence table by highlighting the sample name column and selecting the barcode icon. The software automatically writes the barcode to each sample name field in the sequence table unattended.

Manage Rules and Alerts

OpenLAB CDS ChemStation Edition enables users to manage certain rules and alerts for autosampler devices on a system-wide level. There are two types of events that can invoke configurable actions:

Configurable pre-injection error handling (missing vial for a tray; plunger error for injector)

- Skip the vial
- Pause the sequence or single run
- Stop sequence or run

Configurable action after pressing GC stop button

- Stop only the current run and generate a report, then continue to the next line in the sequence.
- Abort sequence (previous behavior)

Retention Time Locking Software

Retention Time Locking is a useful tool in method transfer between instruments with the same column type and carrier gas. RTL software in Agilent OpenLAB CDS ChemStation Edition assists with the process of determining and using RTL calibrations.

RTL software also provides the capability to search retention timetables. Searching unknowns is based primarily on retention times and may also include element information (selective detectors) to narrow search results further. The RTL libraries can be created, edited, imported and exported.

OpenLAB CDS ChemStation Edition for LC

OpenLAB CDS ChemStation Edition for LC controls and acquires data from the Agilent 1100 and Agilent 1200 Infinity Series modules and systems for LC with the optionally built-in diode array detector (DAD) and the 35900E dual channel interfaces. All the sampling, pumping and detector options of the Agilent 1200/1100 Series LC modules can be controlled.

The majority of instruments are controlled via LAN. Some modules require a USB (e.g. G4301A SFC Module) or RS232 (G4218A ELSD, Agilent 218 / SD1 PrepLC) connection.

Sampling Systems

The injection systems may be manual or automated with an autosampler, well-plate autosampler or multisampler. All automatic injectors may be programmed for different injection volumes; the speed of injection and the injector wash procedure. The user may also specify a complete injector program for sample dilution, standard addition or sample derivatization. The commands available for the injector program include draw, eject, mix, wait, inject, sampler valve and column switch control. These can be defined in conjunction with the sample, a vial/well-plate offset from the sample, a numbered vial/well, waste and air.

The Agilent bar code reader (G2256A) is available for selected autosampler configurations. It can be used to help build automation sequences and verify the identity of the injected sample matches the name in the sequence table at injection time. In LC configurations it can also be used to mix liquid samples as a step in an injection program.

The following list summarizes the different types of Agilent 1100 and Agilent 1200 Infinity Series injection systems that are supported by OpenLAB CDS ChemStation Edition:

- 1290 Infinity II and 1260 Infinity Multisamplers
- 1290 Infinity Autosampler
- 1100 Series, 1260 Infinity Standard Autosamplers
- 1100 Series, 1200 Series and 1260 Infinity High Performance Autosamplers and Micro Autosamplers
- 1260 Infinity Dual-Loop Autosampler
- 1100 Series and 1260 Infinity Preparative Autosamplers
- 1290 Infinity LC Injector HTS and HTC
- 1100 Series Well-plate Autosamplers
- 1260 Infinity Manual Injectors
- 1290 Infinity Flexible Cube

For a detailed and current list of all supported sampling systems please refer to the *Agilent OpenLAB Chromatography Data System Supported Instruments and Firmware Guide* (see chapter *Documentation*) and the driver release notes delivered with each new version of the Agilent instrument drivers (included on the driver DVD).

Solvent Delivery Systems

All the solvent delivery systems have a set of initial parameters, including pressure limits, initial flow and composition, that are complemented by a time-table for programming changes in flow, composition and pressure limits. These parameters can be viewed graphically. Users can define a post-run time for column equilibration.

OpenLAB CDS ChemStation Edition supports an extensive list of Agilent 1100 and Agilent 1200 Infinity Series solvent delivery systems, including:

- 1100 Series and 1260 Infinity Isocratic Pumps
- 1100 Series, 1260 Infinity, 1290 Infinity and 1290 Infinity II Quaternary Pumps
- 1260 Infinity, 1290 Infinity and 1290 Infinity II Binary Pumps
- 1260 Infinity Capillary Pumps
- 1260 Infinity Nanoflow Pumps

For a detailed and current list of all supported solvent delivery systems please refer to the *Agilent OpenLAB Chromatography Data System Supported Instruments and Firmware Guide* (see chapter *Documentation*).

Column Compartments

The following Agilent 1200 Infinity Series column compartments are supported:

- 1260 Infinity Thermostatted Column Compartment
- 1200 Series Thermostatted Column Compartment SL
- 1290 Infinity and 1290 Infinity II Thermostatted Column Compartments

Depending on the type of column compartment different temperatures may be set. For example, the 1290 Infinity II Multicolumn Thermostat facilitates precise column thermostatting over a temperature range from 20 °C below ambient up to 110 °C. Please refer to the instrument specifications for details. The temperature is programmable during the run through a timetable. Column switching valves are programmable from the software.

Some Column Compartments, such as the 1290 Infinity Thermostatted Column Compartment can be clustered for maximum flexibility for multi-method applications such as automated method development.

Valves

The Agilent OpenLAB CDS ChemStation Edition supports external valves as well as quick change valves installed into the column compartment. All Agilent Quick-Change Valves are fully controlled by OpenLAB CDS ChemStation Edition. Valve switching and position monitoring are integrated conveniently with the graphical user interface regardless of where the valve drive is mounted.

For a detailed and current list of all supported valves please refer to the *Agilent OpenLAB Chromatography Data System Supported Instruments and Firmware Guide* (see chapter *Documentation*).

Detectors

OpenLAB CDS ChemStation Edition supports a very long list of Agilent 1100 Series and Agilent 1200 Infinity Series detectors, including:

- 1100 Series, 1200 Series, 1260 Infinity, 1290 Infinity and 1290 Infinity II Diode Array Detectors (DAD)
- 1100 Series, 1200 Series, and 1260 Infinity Multiple Wavelength Detectors (MWD)
- 1100 Series, 1200 Series, 1260 Infinity, 1290 Infinity and 1290 Infinity II Variable Wavelength Detectors (VWD)
- 1100 Series and 1260 Infinity Fluorescence Detectors (FLD)
- 1260 Infinity Refractive Index Detectors (RID)
- 1260 Infinity, 1290 Infinity and 1290 Infinity II Evaporative Light Scattering Detectors (ELSD)

For a detailed and current list of all supported detectors please refer to the *Agilent OpenLAB Chromatography Data System Supported Instruments and Firmware Guide* (see chapter *Documentation*).

UV Detection

The Agilent OpenLAB CDS ChemStation Edition software can simultaneously acquire multiple chromatographic and reference signals each with an independent bandwidth. The data and spectra acquisition rate and the maximum number of signals depend on the capabilities of the individual detector in use. Spectral data from all DADs may be acquired in a peak-controlled or full acquisition mode. All Detectors may have the initial parameters changed during a run by a time-based program.

Agilent 1100 Series and 1200 Infinity Series DADs, MWDs and VWDs support up to 240 Hz data acquisition (with or without spectral data) to a maximum of 8 signals, complemented by additional instrument curves. The VWD may be programmed with a single detection wavelength, the Infinity II VWD supports the use of two wavelengths in parallel. The flow cells and UV lamps utilize RFID tags to capture and store lamp and cell information. The improved Temperature Management System provides ambient rejection and stable cell temperature. Users can program a baseline adjustment (balance) or wavelength (signal) change in the timetable. For DADs additionally the threshold, peak detector peakwidth and spectral acquisition mode can be changed during a run. Initial parameters that may be set include signal wavelengths and reference wavelengths, spectral acquisition mode (if applicable), signal sampling rate and an automatic baseline reset (autobalance). The VWD can perform wavelength scans during the course of an analysis.

Special Detection

The Agilent 1100 Series and Agilent 1200 Infinity Series FLDs may be programmed for single wavelength or simultaneous multiple wavelength detection and spectra acquisition. Up to four signals at different excitation or different emission wavelengths may be obtained. Within a timetable initial excitation or emission wavelengths, response time, PMT Gain and baseline behavior as well as spectral parameters may be changed. Excitation or emission spectra can be watched online and stored fully or peak-controlled. For a single compound trapped in the flow cell, complete information on excitation and emission spectra is available in a single task with the fluorescence scan and can be watched as an isoplot or as 3D-graphics. Spectral data from capable FLDs may be acquired in a peak-controlled or full acquisition mode.

The optical unit temperature of the Agilent 1200 Infinity Series RID maintains a steady optical unit temperature of 5°C above ambient and up to 55°C. The signal acquisition rate may be set to a maximum of 37 Hz. During the course of an analysis the RID can be programmed with a timetable to change polarity and peakwidth of the acquired chromatographic signal.

The Agilent 1200 Infinity Series ELSDs deliver evaporation down to 10 °C providing maximum sensitivity for compounds with significant volatility below 30 °C and up to 120 °C. The available temperature range varies by product. The instrument provides a data sampling rate of up to 80 Hz. Initial parameters include a digital filter, which can be set to optimize signal-to-noise ratio and peak shape, gain and signal offset. Initial parameters including the temperature can be changed during a run using a time table.

For most current information and more details on the instrument capabilities please refer to the corresponding user manuals and data sheets.

Fraction Collectors (LC Purification Systems)

All different versions of the Agilent 1100 Series and Agilent 1200 Infinity Series fraction collectors can be fully controlled from Agilent OpenLAB CDS ChemStation Edition. Fraction data can be reviewed in the fraction task of the data analysis screen. The maximum number of fraction collectors connected to one LC Purification System is limited to 3 (with the possibility for one additional recovery fraction collector). Depending on the system configuration up to two LC Purification Systems can be controlled from a single OpenLAB CDS ChemStation Edition system (without purification related software add on). Optional add-on software, e.g. Easy Access (G2725AA) or the OpenLAB CDS Automated Purification Software (M8368AA, M8369AA) provides advanced functionalities for the standalone OpenLAB CDS ChemStation Edition workstation.

Clusters

A cluster allows combining several modules into one logical unit. Such a cluster is shown as a single instrument module in the OpenLAB CDS ChemStation Edition – for example, a pump valve cluster for the selection of multiple solvents with a pump, a thermostatted column compartment cluster for varying columns and temperatures, a preparative pump cluster, allowing the combination of two isocratic pumps to form one logical binary pump, or a Detector cluster, such as the Agilent 1200 Infinity Series HDR DAD solution, which combines the signals from two diode array detectors for high dynamic range detection.

For most current information and more details on the instrument capabilities please refer to the corresponding user manuals and data sheets, as well as the driver release notes delivered with each new version of the Agilent instrument drivers (included on the driver DVD).

A/D Convertors

35900E series A/D

The Agilent 35900E dual channel interface allows the system to acquire data from detectors that are not directly interfaced for data acquisition, such as a third party detector. One or two analog signals per instrument may be configured; if only one is used the other is available for use with another instrument. Data rates up to 100 Hz per signal may be defined. The user may also define the units for acquisition and their relationship to the voltage signal (units/volt).

The Agilent 35900E interfaces offer external event control through digital TTL (transistor-transistor logic) signals, each of which are given specific state (high and low) names, that may be time-programmed before, during and after an analysis. The Agilent 35900E can be configured for up to eight signals for each independent channel.

For most current information and more details on the instrument capabilities please refer to the corresponding user manuals and data sheets.

Universal Interface Box

The Agilent 1200 Infinity Series Universal Interface Box and Universal Interface Box II are multipurpose accessories for the Agilent 1200 Infinity Series that extend instrument communication capability to high quality analog and digital output and input. It provides a general connection interface for existing and upcoming Agilent sensors (e.g. pH-, temperature-, leak- sensors) and other accessory equipment. Peak-based fraction collection with external detectors and mass-based fraction collection with Agilent MS detectors rely on the Universal Interface Box II.

Extended LC Systems and Workflow Solutions

OpenLAB CDS ChemStation Edition supports a broad list of LC solutions including:

- the Method Development Solution,
- the Analytical SFC System,
- the Bio-Inert LC System,
- the 2D LC Solutions, and
- the Automated Purification System.

Some solutions require additional software add-ons. Please refer to the eFamilarization for additional information.

Agilent 1290 Infinity Intelligent System Emulation Technology (ISET)

The "Agilent 1290 Intelligent System Emulation Technology" (ISET) enables the 1290 Infinity and Infinity II LC to execute other HPLC and UHPLC methods and deliver nearly the same chromatographic results without any change of the instrument or the original method. This technology is based on two components: the high performance 1290 Infinity technology, and the ISET emulation algorithm.

OpenLAB CDS ChemStation Edition for LC supports ISET for instrument- to- instrument method transferability. ISET can emulate the following instruments:

- Agilent 1100 and 1200 Series
- Agilent 1260 Infinity LC
- Agilent 1220 Infinity LC
- Agilent 1120 Compact LC
- Agilent 1290 Infinity LC (can be emulated by the 1290 Infinity II LC)
- Waters Alliance
- Generic emulation of other HPLC devices

For more information please refer to the *Agilent 1290 Infinity with ISET user manual* (see chapter *Documentation*).

3rd Party Instrument Control

Support for Waters Acquity and Alliance

Waters Corp. and Agilent Technologies are cooperating on a technical level in order to achieve reliable instrument control of the Waters LC and LC/MS hardware in OpenLAB CDS ChemStation Edition. The Waters Acquity Driver for OpenLAB CDS, was developed by Agilent and incorporates a core Waters driver component developed, tested and officially released by Waters. This Waters core component handles the complete instrument communication and ensures full control of the Waters Acquity, LAN-based e-Alliance and LAN-based UV detectors according to Waters' own requirements for these instruments.

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

- Waters Acquity Sample Manager (SM)
- Waters Acquity Binary Solvent Manager (BSM)
- Waters Acquity Column Manager (CM)
- Waters Acquity Sample Manager FTN (FTN)
- Waters Acquity Quaternary Solvent Manager (QSM)
- Waters Acquity Column Manager (CM-A)
- Waters Acquity H-Class Column Manager AUX
- Waters Acquity and Acquity H-Class Sample Organizer
- Waters Acquity and Acquity H-Class TUV Detector (TUV)
- Waters Acquity and Acquity H-Class PDA Detector (PDA)
- Waters Acquity and Acquity H-Class PDA eLambda Detector (PDA)
- Waters Acquity and Acquity H-Class Fluorescence Detector (FLR)
- Waters Acquity and Acquity H-Class ELSD Detector (ELS)

The Waters Alliance/e-Alliance LC driver supports the following Waters Alliance modules in OpenLAB CDS ChemStation Edition:

- the Waters Alliance 2690
- the Waters Alliance 2695
- the Waters 2695e "e-Alliance"
- the Waters PDA 2996
- Waters PDA 2998
- the Waters UV 2487 Dual Wavelength Detector
- the Waters UV 2489 Dual Wavelength Detector.

Depending on the instrument type the Waters Acquity and Alliance instruments require GPIB or Ethernet LAN-based communication for instrument control. OpenLAB CDS ChemStation Edition provides both, LAN-based communication, using TCP/IP or, for control of instruments that don't support LAN, the GPIB communication protocol. The GPIB communication requires a GPIB board installed in the computer or an external USB/GPIB interface directly connecting from the PC's USB port to the GPIB instrument. The following GPIB interfaces are supported:

- National Instruments 488.2 PCI-GPIB, or
- National Instruments GPIB-USB-HS.

For more details please refer to the user manuals (see chapter *Documentation*).

OpenLAB CDS ChemStation Edition for CE

OpenLAB CDS ChemStation Edition for CE controls and acquires data from the Agilent 7100 capillary electrophoresis (CE) system with a built-in diode array detector (DAD), optionally connected to a 6100 Series Single Quadrupole MS.

The open-platform approach allows flexible integration with Agilent MS or 3rd-party detectors, extending usability for enhanced sensitivity and specificity.

OpenLAB CDS ChemStation Edition for CE provides different acquisitions modes:

- Capillary Electrophoresis (CE) Mode
- Capillary electrochromatography (CEC) Mode
- Capillary Electrophoresis plus pressure mode (CEp)
- Capillary Electrophoresis with SQ MS (CEMS)
- Capillary Electrophoresis with SQ MS plus pressure mode (CEMSp)

Methods in CE are dependent on CE mode selected. Therefore they are stored in distinct locations specific to the mode.

Vial Table

OpenLAB CDS ChemStation Edition for CE provides the "Vial Table" for associating vials in the vial tray with samples or task specific system vials such as inlet and outlet vials, flush vial, clean tubes vial, and the waste. System vials belong to the system configuration and are reserved by symbolic names in the vial table. The Vial Table is linked to the Sequence Table. When a sequence is loaded, the information from the Sequence Table is copied into the Vial Table.

When a method or a sequence is loaded, a consistency check is made between the vial allocations in the Vial Table and those in the method or sequence. Conflict resolution tables allow for a convenient correction of conflicts between methods and vial table, or sequence and vial table.

CE Data Evaluation

Some data analysis functionality is specific to the use of the OpenLAB CDS ChemStation Edition for CE. Below is a brief summary. For more details please refer to the *Agilent OpenLAB CDS ChemStation Edition Reference to Operation Principles* (Please refer to the chapter *Documentation*).

Integration Parameters

In capillary electrophoresis peaks are often asymmetrical. For the purpose of integration some CE-specific parameters called "peak top types" are available. The integrator offers the following types:

- Highest Point – for triangular shaped peaks and varying concentrations,
- Parabolic Interpolation – for tailing, unseparated peaks,
- Center of Gravity – for triangular shaped peaks at similar concentrations,
- Gauss Fit – for symmetric peaks.

Migration Time - based Calibrations

For Standard Calibration Mode the setting "Calculate with Corrected Areas" enables a correction to the peak area based on the migration time. In this mode, the area is divided by the migration time which can improve reproducibility in quantitative analysis when migration times are unstable.

In addition to the Standard Calibration, there are three capillary electrophoresis specific, migration time based calibrations that can be applied to a single selectable signal:

- Protein Molecular Weight Calibration – Calibration based on molecular weight and a reference peak: $\log (MW) = k_1 \cdot (t_{ref}/t) + k_0$
- DNA Base-Pair Calibration – Calibration based on the number of base pairs: $\log(\#BP) = k_1 \cdot (1/t) + k_0$
- Capillary Isoelectric Focusing Calibration (cIEF) – Calibration based on the isoelectric points (pI) of proteins: $pI = k_1 \cdot t + k_0$

Migration time- based calibrations and recalibrations can be included in a sequence, but only for explicit calibrations and cyclic recalibrations; bracketed recalibration is not possible. There is no SequenceSummary report with migration time- based calibrations.

Calibration using Mobility Correction

An unstable Electro Osmotic Flow (EOF) results in a rather high standard deviation of migration times. OpenLAB CDS ChemStation Edition for CE provides mobility correction to significantly reduce the effect of run- to- run migration time shifts. The migration time of a mobility reference peak is used for increasing the migration time reproducibility. The EOF marker or internal standard can also be used as the mobility reference peak. The EOF marker is a neutral marker which corresponds to the velocity of the EOF.

There are two mobility correction types available:

- *Effective Mobility Correction* – Effective Mobility Correction uses the effective mobilities of all peaks and requires the availability of an EOF marker and the voltage ramp data together with the electropherogram.
- *Relative Mobility Correction* – Relative Mobility Correction requires no EOF marker and can operate in the absence of voltage data assuming a constant voltage for all measurements.

Reporting

OpenLAB CDS ChemStation Edition for CE has an additional mobility report that uses the voltage signal and the electropherogram to compensate for the velocity of the compounds migrating through the detector cell.

CE/MS Control and Data Evaluation

Most capabilities provided by adding 3D MS instrument control and data evaluation to the OpenLAB CDS ChemStation Edition for CE are the same as for LC/MS. They are described in detail in the chapter *OpenLAB CDS ChemStation Edition for LC/MSD Systems*.

Background Subtraction (BSB) can be applied by subtracting the recently selected mass spectrum from each point in the current electropherogram. The resulting data is saved in the same directory and with the same name as the original data file; however, the file extension is changed to .BSB.

Some features that are available in the LC/MS software are either not available or not applicable to CE/MS applications but are used in LC. The function peak matching is not applicable for CE-MS and is therefore not active.

OpenLAB CDS ChemStation Edition Value Line

OpenLAB CDS ChemStation Edition Value Line (VL) is a version of OpenLAB CDS ChemStation Edition designed for use with the Agilent 7820 GC and 1220 Infinity LC. Additionally it provides control and data processing for the 490 Micro GC, and the 1260 Infinity Quaternary LC, 1260 Infinity Quaternary VL LC, and 1260 Infinity Isocratic systems. OpenLAB CDS ChemStation Edition VL has the following limitations and characteristics:

- Supported only with standalone Workstation configuration, no central data storage.
- Limited to single instrument configurations.
- Offers full functionality of OpenLAB CDS ChemStation Edition software.
- Allows control of the 1120 and 1220 Infinity LC with all modules except modular pumps.
- Allows control of the 7820 GC and 490 Micro GC.
- Does not support GC software add-ons (e.g., Headspace).
- No control of any Binary LC, Bio-inert LC, Preparative LC or SFC Systems, nor High Performance Autosamplers or ELSD Detectors
- OpenLAB CDS ChemStation Edition Value Line for LC does not support LC/MS configurations.
- OpenLAB CDS ChemStation Edition Value Line is restricted to the RC.NET drivers. It does not include classic drivers or classic configurations.

OpenLAB CDS 3D UV Add-on

Using OpenLAB CDS 3D UV Add-on, UV-visible spectra acquired using a diode-array detector may be graphically selected from a chromatogram signal for visual inspection and comparison or may be used for peak purity determinations, wavelength optimization and component identification through spectral libraries. The spectral library functionality can be extended to automatic identification of components in up to four user-defined spectral libraries based on peak or target compound identification.

Interactive Spectral Processing

Users may graphically select spectra from a chromatographic signal for visual inspection and printing. The spectra are displayed in a separate spectral window and may be overlaid for comparisons. The user can select spectra in the following modes:

- individual spectrum,
- peak apex spectrum,
- average spectrum over a graphically defined retention time range,
- range of spectra,
- all spectra over a peak

The user may also select how the spectra are processed when they are extracted. The available options include:

- setting the subtracted reference spectrum or spectra,
- limiting the extracted wavelength range,
- customizing the spectral and reference display,
- setting the spectral processing. Options include setting a smoothing and splining factor, logarithmic processing and derivative order.

Peak Purity Determinations

Peak purity may be determined interactively on a peak by peak basis, for all peaks from a certain data file, or automatically at the end of each analysis as part of the method. Users may optimize peak purity processing for accuracy or performance by setting preferences relating to:

- the number of spectra used over a peak,
- the wavelength range used for the purity determination,
- the reference spectra,
- the purity threshold,
- spectral processing including logarithmic, smoothing and splining factors and derivative order.

The purity components are calculated and displayed. These include

- a normalized display of the used spectra for visual inspection of the differences,
- the signals,
- signal-based ratiogram,
- similarity and threshold curves.

Similarity curves give the most detailed information about a peak's purity. User-selected or average spectra are compared with all the other spectra acquired during the peak's elution and the resulting spectral comparison factors are plotted as the similarity curve. For a perfectly pure peak the similarity curve will be a straight line corresponding to a theoretically pure compound. Impurities will cause a deviation from this ideal line. The similarity curves are plotted with reference to the theoretically pure line and the user-defined purity threshold. The similarity curve gives the best indication of any impurities that occurred in the peak as it eluted. The deviation of the similarity curve from the ideal theoretically pure value is influenced by both compound impurities and spectral noise.

The user-defined purity threshold may be replaced by a system calculated threshold curve based on the signal-to-noise ratio of the peak in question. The noise sample may be user selected and, if truly representative of the spectral noise when the peak eluted, compensates for any deviation of the similarity curve, from the theoretically pure value, attributable to spectral noise.

If details are not clear in the display, the content of the Spectra, Signals and Purity window can be zoomed.

For more information, see the *Understanding Your Spectra Module Guide* (see chapter *Documentation*).

Wavelength Optimization using the Iso-absorbance Plot

UV-visible spectra, acquired continuously during an analysis, can be used to determine the optimum signal wavelengths and bandwidths for routine detection by a signal-based method. The iso-absorbance plot displays the acquired spectra as a color-contoured map of wavelength against retention time together with areas for the display of both signals and spectra defined by the position of the cross-hairs on the iso-absorbance plot.

The iso-absorbance map can be used in four modes:

- The Quick view mode allows users to view and compare spectra and signals by moving a crosshair over the area of the contour map. Spectra and signals are continuously extracted and updated in the display areas. The extracted spectra and signals may be frozen in the display areas for comparison purposes.
- The Zoom mode allows users to zoom into areas of interest on the iso-absorbance map.
- The Signals mode allows users to extract a particular signal, with a graphically determined bandwidth, into the chromatographic window for routine data processing such as integration and quantification.
- The Spectral mode allows users to extract spectra into the spectral window for further processing.

The iso-absorbance plot is typically used during method development to explore a sample's response at different UV-visible wavelengths in order to determine the optimal detection wavelengths and bandwidths through experimentation with the integration and quantification processes. Users can define the contour color schemes and retention time and wavelength ranges for display.

Three Dimensional Plot

UV-visible spectra acquired continuously during an analysis, can be displayed as a three-dimensional plot. The display may be graphically adjusted by the users in the time, intensity and wavelength domains. The resolution of the plot is selectable.

- The orientation of the plot can be adjusted graphically. The orientation of the display is not restricted in any dimension.
- The plot may be printed.
- The color scheme used in the plot may be selected from a number of choices.

Spectral Libraries

Spectral libraries allow users to positively identify compounds by comparing the spectra of peaks in the sample to libraries of spectra derived from analytical standards.

OpenLAB CDS ChemStation Edition allows users to use libraries both interactively and automatically. OpenLAB CDS ChemStation Edition can manage an unlimited number of spectral libraries each with up to as many entries as there is available system memory (typically hundreds of entries). Libraries may be loaded and searched by selecting individual spectra from a chromatogram and searching the library for the best matches. The library search may be constrained by specifying a search template that allows the user to define a retention time window and include the informational data associated with each library entry. For example, the applicable retention time can be constrained to ± 5 % of the library retention time and the entry names must start with the letter 'B'. The search results may be displayed on the screen and printed.

Users may build their own libraries by analyzing known substances under defined analytical conditions, creating a new library and entering the individual spectra and the information fields to describe the entry into the library. Library entries may be added, deleted, edited, viewed or printed. Details of each spectrum in a library including absorbance and wavelength data may be examined.

Automated Spectral Library Search Reports

Automated spectral library search reports allow users to automatically identify and quantify unknown samples based on the positive identification from up to four separate spectral libraries. Search criteria may be specified for each library separately through a library search template that allows users to constrain the search both in the retention time and library entry identification parameters.

One of three search modes may be selected:

- *Standard search mode* identifies each integrated peak in the chromatogram from the library.
- *Target analysis from the calibration table* limits the library search to those library entries identically named in the calibration table. Identification may be further constrained through the use of the library template to restrict other search criteria such as the retention time window. After positive identification, quantification proceeds according to the data in the calibration table.
- *Target analysis from the library* uses the library entries to identify peaks in the chromatogram that are within the RT window specified for the particular library entry. This mode differs from the standard search mode in that it excludes peaks whose retention times are not covered by library entry time windows.

Consequently it is typically faster than the Standard search, especially if there are many more peaks in the sample than there are entries in the library. After positive identification, quantification proceeds according to the data in the calibration table.

The calculation of the peak purity factor may be included as part of the library search. Report styles can be selected to produce simple library search reports or a combination of library search and standard performance reports described above.

Spectral Data Import and Export

The OpenLAB CDS ChemStation Edition spectral module can import spectra stored in Agilent's .WAV format files and industry standard JCAMP spectrum files.

The OpenLAB CDS ChemStation Edition data file is compatible with Agilent's ChemStation for UV-visible spectroscopy running in the Windows environment. Both DAD- and UV/visible spectra may be exchanged between the two systems either as OpenLAB CDS ChemStation Edition register files or through the Windows clipboard.

OpenLAB CDS ChemStation Edition for LC/MSD Systems

OpenLAB CDS ChemStation Edition for LC/MSD provides control, data acquisition, and data evaluation capabilities for Agilent 1100 Series and Agilent 1200 Infinity Series Single Quadrupole (SQ) LC/MSD systems. To control an LC/MSD System a "3D UV Add-on" License and a "LC 3D MS Add-on" License are required in addition to the OpenLAB CDS ChemStation Edition Workstation and the "Instrument Driver License for Agilent LC". Together, these software components provide integrated control with a common graphical user interface for all of the Agilent 1100 Series and Agilent 1200 Infinity Series LC modules and systems, including the Agilent 1200 Infinity Series DAD as well as the Agilent 6100 Series Single Quadrupole LC/MSD. Agilent CE/MS configurations are also supported. In addition to the Agilent 1100 Series and Agilent 1200 Infinity Series families of modules and systems, the Agilent 35900E A/D interface can be controlled as part of LC/MSD systems. OpenLAB CDS ChemStation Edition for LC/MSD supports a single Agilent 1100 Series and Agilent 1200 Infinity Series LC system connected to an Agilent 6100 Series Single Quadrupole MSD system.

LC/MS System Control

The software provides digital control of the LC/MSD API ion source and ion optics, dynamic ramping of ion optics element voltages, and control for spraying and drying gases. Method-specific LC/MSD parameters include spectral acquisition mode (scan/SIM), signal sampling rate, LC/MSD tune file, ionization mode (APCI, APPI or API-ES mode) and polarity (positive or negative ion detection). Within a LC/MSD method, LC/MSD-timed events include mass range, SIM ion groups, mass analyzer stepsize, fragmentor voltage, electron multiplier gain, MS on/off, and API ion source parameters. Fragmentor voltage settings may be dynamically ramped within a scan to optimize response for various m/z values. LC/MSD operating parameters such as fragmentor voltage, drying gas temperature, and EMV gain can be acquired and saved with a data file. These instrument parameters can be displayed and plotted as a record of the exact values associated with the acquired data.

In addition to the standard OpenLAB CDS ChemStation Edition automation capabilities for single run methods and multiple method sequences, an FIA (Flow Injection Analysis) Series automation mode is available through software selection. In this mode the Agilent 6100 Series Single Quadrupole LC/MSD system can be programmed to make multiple injections from a single or multiple sample vials storing all data in a single datafile. Up to two LC/MSD method parameters can be programmatically varied with each injection. The FIA mode requires an Agilent 1100 Series or Agilent 1200 Infinity Series LC Autosampler.

The system includes the ability to do ultrafast scanning and includes autotune for fast scanning. Also included is support of the Agilent Analog Output Accessory which provides up to 4 SIM or TIC signals directly to a customer LIMS system.

The system can monitor up to 16 *m/z* values for the purposes of triggering an output signal for mass based fraction collection.

For most current information and more details on the instrument capabilities please refer to the corresponding user manuals and data sheets.

LC/MSD Tuning

OpenLAB CDS ChemStation Edition for LC/MSD includes a LC/MSD Tune view in which users of the Agilent 6100 Series Single Quadrupole LC/MSD may select to either automatically, or manually tune the instrument. The Agilent 6100 Series Single Quadrupole LC/MSD integrated calibrant delivery system is software-controlled, and together with the software autotune provides fully automated tuning of the LC/MSD for API-electrospray (API-ES), atmospheric pressure chemical ionization (APCI) and atmospheric pressure photo ionization (APPI) modes of operation. An extensive set of manual tune capabilities is also provided for users who wish to manually tune the LC/MSD.

Diagnostics/Early Maintenance Feedback

The Agilent 1200/1100 Series LC/MSD software extends the diagnosis view of the existing OpenLAB CDS ChemStation Edition for LC to include tests for the Agilent 1200/1100 Series LC/MSD. The diagnosis view is designed to help users identify instrument malfunctions starting from a particular symptom.

Maintenance and repair procedures for the Agilent 1200/1100 Series LC/MSD can be called directly within the diagnosis view from the Agilent 1200/1100 Series LC/MSD Maintenance and Repair CD-ROM. The procedures include parts and materials breakdowns and clear animated step-by-step graphics and multimedia clips for each repair procedure.

Early Maintenance Feedback (EMF) automatically notifies the user when maintenance is required for key system components such as rough pumps, calibrant delivery system, spray chamber, and electron multiplier.

LC/MSD Data Evaluation

The OpenLAB CDS ChemStation Edition for LC/MSD includes all of the data evaluation capabilities of the Agilent 3D ChemStation for LC, including data evaluation for UV-visible spectra acquired from a supported diode-array detector (DAD). In addition, the OpenLAB CDS ChemStation Edition for LC/MSD includes capabilities for evaluation of mass spectral data acquired from the Agilent 6100 Series Single Quadrupole LC/MSD module.

Both UV-visible and LC/MSD data can be viewed, compared, and printed. Chromatograms from the separate detectors may be simultaneously displayed, aligned, and resized to correlate peaks from one chromatogram to the other. Mass spectra and UV/visible spectra can be simultaneously reviewed using a common spectral toolset. Reports can include either UV-visible or mass spectral data, or both. For data involving multiply charged ions, add-on software is available to deconvolute the spectra and calculate the molecular weight.

Interactive Data Processing

The data from the mass selective detector may be displayed in a number of ways. The total ion chromatogram (TIC) is the summation of all mass signals (m/z values) over the entire acquired data range. An extracted ion chromatogram (EIC) displays the signals of individual ions (m/z values) or a range of m/z values. A Base Peak Chromatogram (BPC) which produces a chromatogram showing the abundance of the most abundant ion in each spectrum can be displayed.

The mass selective detector signals (TIC and /or EICs) may be displayed along with those from other LC detectors. The software permits peak alignment for chromatograms from different detectors connected in series. Full, comparative mass and UV-visible spectra manipulation are available including selection of spectra by:

- individual spectrum,
- peak apex spectrum,
- average spectrum over a graphically defined retention time range
- range of spectra,
- all spectra over a peak.

The user may also select how the spectra are processed when they are displayed. The available options include:

- background subtracted spectra,
- limiting the m/z range,
- smoothing,
- normalization,
- continuous curves or histogram mode.

If NIST library search software is installed, spectra can be “piped” to NIST and library searched.

Quantification

All of the standard OpenLAB CDS ChemStation Edition quantification capabilities are available for use with mass spectral data. TIC or EIC signals can be used for quantification. Support for co-eluting labeled Internal Standards as well as Qualifier Ion Ratios is built into the software.

Peak Purity

The OpenLAB CDS ChemStation Edition for LC/MSD includes all the UV-visible peak purity data evaluation capabilities of the Agilent diode-array detector (DAD) spectral evaluation module. Capability for peak purity determination using LC/MSD mass spectral data is also included. Peak purity may be determined interactively on either a peak by peak basis, for all the peaks from a certain data file, or automatically at the end of an analysis as part of the method.

The user can select to interactively evaluate peak purity for data sets that include both DAD spectral data and LC/MSD spectral data in either a single or dual mode. In single mode, the software configures the purity user interface for evaluation of data from either one of the two data types at a time. The user can toggle between the data types if desired. The dual mode user interface permits simultaneous evaluation of spectral purity using both DAD and LC/MSD data.

In interactive operation, the LC/MSD peak purity function examines the most significant ions across a user-selected chromatographic peak to determine if more than one compound is present. The software automatically overlays extracted ion chromatograms for the selected peak, with each extracted ion chromatogram displayed in a separate color. A table of the number of components located and the two most significant ions used to resolve each component is displayed. The next/previous peak or the next/previous impure peak can be selected by simple mouse actions. A purity report that includes peak purity assessment for all peaks in a chromatogram can also be specified and displayed/printed.

Iso-abundance Plot and Three Dimensional Plot

In addition to iso-absorbance and three dimensional plots for UV-visible spectral data, the OpenLAB CDS ChemStation Edition for LC/MSD also provides equivalent capabilities for mass spectral data.

The MS iso-abundance plot displays acquired mass spectra as a color-contoured map of m/z against retention time together with areas for display of m/z signals and mass spectra defined by the position of cross-hairs on the iso-abundance plot. In the iso-abundance plot, a color scale is used to represent signal intensity. Users can define the contour color schemes and retention time and m/z ranges for the display.

Acquired mass spectra can also be displayed as a three dimensional plot of m/z against retention time and abundance. The display can be graphically adjusted by the user in the time, m/z, and intensity domains. The resolution of the plot is selectable, and the orientation of the plot can be adjusted graphically. The plot may be printed, and the color scheme adjusted.

OpenLAB CDS ChemStation Edition for A/D

The OpenLAB CDS ChemStation Edition for A/D with additional A/D interface acquisition module controls and acquires data from the Agilent 35900E dual channel interface. This enables OpenLAB CDS ChemStation Edition to acquire data from instruments that are not capable of being directly connected for data acquisition through the standard LAN interface (in some cases also GP-IB or RS-232) using the RC.NET interface standard. Instead, the instruments are connected via the 35900E dual channel interface for analog data acquisition. One or two analog signals per instrument may be configured; if only one is used the other is available independently for use with another instrument. Data may be acquired at up to 100 Hz per signal. The user may also define the units for acquisition and their relationship to the voltage signal (units/volt). The Agilent 35900E interfaces offer external event control through digital TTL (transistor-transistor logic) signals, each of which are given specific state (high and low) names, which may be time-programmed before, during and after an analysis. The Agilent 35900E can be configured for up to eight TTL signals for each independent channel.

In addition to controlling a complete instrument via an A/D converter, OpenLAB CDS ChemStation Edition for LC can be configured to control a device (e.g. a non-Agilent detector) connected via the Agilent 35900E dual channel interface.

OpenLAB CDS ChemStation Edition Data Analysis Only

The Data Analysis Only product enables users to review and reprocess LC, GC, CE, LC/MS and CE/MS ChemStation data. The product is a pure data analysis product and cannot be extended with any instrument drivers. The capabilities of the software are described in the data analysis section earlier in this document.

Secure Workstation for OpenLAB CDS ChemStation Edition

The Secure Workstation for OpenLAB CDS ChemStation Edition is a combination of two existing products (OpenLAB CDS ChemStation Edition and OpenLAB Data Store) running on the same computer for 2 instruments maximum.

The Secure Workstation for OpenLAB CDS ChemStation Edition provides secure central data storage for standalone workstations and cannot be installed in a networked configuration. An alternative option to multiple OpenLAB CDS ChemStation Edition standalone workstations with secure data storage in the same laboratory, is a networked environment with a central Data Store server.

Compatible Software Modules

The following table gives and overview of the compatible add-on software modules for OpenLAB CDS ChemStation Edition.

Product Number	Product Name	Product Description	Workstation	Networked Workstation	With Central Data Storage	Distributed System
M8363AA	LC/MS Deconvolution & Bioanalysis Software	Adds LC/MS Deconvolution / Bioanalysis capabilities	•	•	•	•
M8365AA	LC Dissolution Software	Adds support for the dissolution workflow (sample analysis and data evaluation)	•	•	•	
M8350AA	Match Compare Software	Add-on to automate the task of comparing quality control chromatograms of samples including flavors, fragrances, paints, and peptide digests	•			
M8351AA	Match Compare Software Upgrade	Upgrade from Varian Software	•			
G1968	Active Splitter Add-on Software	Software to control the Active Flow Splitter for LC/MS	•	•	•	
G2081AA	RTL Pesticide Library	RTL Library for Pesticides	•	•		
G2196AA	Method Scouting Wizard Software	Method Development Software	•	•	•	•
G2198AA	2D-LC Acquisition Software	Add-on software to enable two-dimensional Chromatography with the Agilent 1290 Infinity 2D-LC Solution	•	•	•	
G2725AA	Easy Access LC/MS Software	Simple Production User Interface for LC/MS	•	•		
G2725CA	Walkup Software	Simple Production User Interface for LC and LC/MS	•	•		
G2887BA	SIMDIS Data Analysis Software	Data Analysis Software for Simulated Distillation	•	•		
G2924AA	Integrated Headspace Control Software	Headspace Control Software	•	•	•	•
G3382AA	Control for PAL Autosampler (includes license for the CTC Control software)	CTC PAL Control Software	•	•	•	•
G3772AA	MassHunter Analytical Studio Reviewer	Adds MassHunter Analytical Studio Reviewer for review large amounts of LC/MS data	•	•	•	
G4600AA	GC and GC/MS User Manuals & Tools	Installs GC and GC/MS User Manuals and Tools	•	•	•	
G6586AA	Agilent LTM I Control Software	Adds control of the LTM Series I for 7890/6890 GC	•	•		
G7300AA	Easy SamplePrep Software	GC Sample Preparation Software	•	•	•	•

Product Number	Product Name	Product Description	Workstation	Networked Workstation	With Central Data Storage	Distributed System
G7318AA	7697A Headspace Control Software	Headspace Control Software for 7697A Headspace Sampler	•	•	•	•
G7818A	Cirrus GPC Software for ChemStation	GPC Analysis and Data Analysis Software	•	•		
M8368AA, M8369AA	OpenLAB CDS Automated Purification Software	Facilitates automated transfer of purification methodologies from analytical to preparative scale	•	•		
M8550A	Agilent Lab Advisor for LC & CE – Advanced Software	Advanced Lab Advisor Software for LC & CE	•	•	•	•
M8555A	Agilent Lab Advisor for LC & CE – Basic Software	Basic Lab Advisor Software for LC & CE	•	•	•	•
G3335AA	MassHunter Software	Automatic Translation of Data into MassHunter format and optional automated processing and reporting by MassHunter Qualitative Analysis	•	•		

Note: Please contact your local Agilent Technologies representative for additional details.

eFamilarization

The powerful new eFamiliarization for OpenLAB CDS helps users to easily learn the new functionality at their own pace, whenever they want. The modules walk users through detailed steps of using the OpenLAB CDS software. The on-demand eLearning materials give users a new experience where they not only learn the concepts, but are learning through task-based software simulation. This allows users to get the experience of using OpenLAB CDS software even without an installation of the software.

eFamilarization is available in English, Japanese and Chinese, and is continuously updated to cover new software functionality introduced by new releases.

In addition to learning materials, OpenLAB eFamiliarization includes useful tools like the new “Familiarization Calculator” which allows to quickly determine applicable familiarization topics for upgrade customers in order to customize their familiarization to be as time effective as possible.

Documentation

In this chapter you will find a brief summary of all relevant documentation that is available for OpenLAB CDS ChemStation Edition and how to find it. The documentation includes:

- User documentation covering installation, administration and usage,
- eFamiliarization facilitating an easy learning experience for basic operation, and
- Technical notes with further not covered by the documentation above.

User documentation is provided as PDF files on the software disks (see chapter *Documentation and Manuals on the OpenLAB CDS ChemStation Edition DVD Set* for more details) and as electronic help files installed with the software. The documentation set can be divided into the following broad categories:

- Installing OpenLAB CDS ChemStation Edition software,
- Using OpenLAB CDS ChemStation Edition software,
- Understanding the principles of how the software works
- Customizing OpenLAB CDS ChemStation Edition,
- Interfacing OpenLAB CDS ChemStation Edition with LIMS

Further documentation is available on the Agilent Website:

- Information specific to Central Data Storage (OpenLAB Data Store & OpenLAB ECM)
- Technical Notes
- Hardware Manuals

Accessing OpenLAB CDS Documentation and Manuals

All OpenLAB CDS Documentation is accessible 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.

Installation

The OpenLAB CDS ChemStation Edition software product comes with a series of installation manuals that includes:

1. Hardware, software and network requirements:
    - OpenLAB CDS Hardware and Software Requirements
    - OpenLAB CDS Network Requirements Guide
    - OpenLAB CDS Supported Instruments and Firmware Guide
2. Upgrade preparation:
    - OpenLAB CDS ChemStation Edition Upgrade Preparation
    - Impact Analysis for OpenLAB CDS ChemStation Edition (available on request)
3. Installation manuals specific to the purchased configuration:
    - OpenLAB CDS WorkStation Installation and Configuration Guide
    - OpenLAB CDS Networked Workstation Installation Guide
    - OpenLAB CDS Networked and Distributed System Installation and Configuration
    - OpenLAB CDS Software License Installation Guide,
    - Creating OpenLAB Shared Services Databases on Oracle Systems
4. Instrument installation:
    - OpenLAB CDS ChemStation Edition Instrument Configuration Guide
    - OpenLAB CDS Supported Instruments and Firmware Guide

Learning and Using

OpenLAB CDS ChemStation Edition includes comprehensive, Windows-style, context sensitive and indexed online help. The detailed explanations are backed up by graphics where appropriate, and may be copied to the Windows clipboard for incorporation in the users own documentation, or printed.

The OpenLAB CDS eFamilarization facilitates easy learning of the main aspects of OpenLAB CDS ChemStation Edition at a user's own pace. See above, chapter *eFamilarization* for more details.

Understanding OpenLAB CDS ChemStation Edition

A pair of manuals, *OpenLAB CDS ChemStation Edition Concepts and Workflows*, and *OpenLAB CDS ChemStation Edition Reference to Operation Principles*, provide detailed information about the functionality of the software and way in which the functions are implemented. The Concepts and Workflows manual explains the layout of the software and the way functions combine into workflows, the Reference to Operation Principles manual provides the details of the algorithms and calculations. When OpenLAB CDS ChemStation Edition is connected to OpenLAB ECM, the *OpenLAB CDS ChemStation Edition with Central Data Storage Concepts Guide* provides additional concepts relating to the combined functionality.

The *OpenLAB CDS Report Template Editor Concept Guide* is dedicated to detailed information on creating Intelligent Report templates.

The *Understanding Your Spectra Module Guide* describes the concepts behind the spectra module and complements the information given in the Concepts and Workflows and Reference to Operation Principles Guides. It covers the principles of spectral analysis, spectral libraries and peak purity determination.

Customization

Sophisticated users who wish to customize the operation of the OpenLAB CDS ChemStation Edition, or who want to build in additional features, may do so by writing macros using the command set. The *Commands Help* file and the *Macro Programming Guide* are accessed directly from the OpenLAB CDS ChemStation Edition Help menu. The Macro Programming Guide provides an explanation of key programming concepts and a reference to variables and data structures in the memory of the OpenLAB CDS ChemStation Edition. The Command help file is the programmer's function reference. It includes syntax and parameter explanations with example macros illustrating the use of many of the commands. As this information is in the online help, the users can copy the examples and command syntax directly into their own macro source files.

For instrument control programs, a manual, *Macro Programming Guide for RC .NET Drivers in OpenLAB CDS ChemStation Edition*, provides a detailed syntax reference for the instrument control commands.

Interfacing

The *OpenLAB CDS ChemStation Edition XML Connectivity Guide* includes installation and reference information for implementing an XML interface between the Agilent OpenLAB CDS ChemStation Edition and a LIMS (Laboratory Information Management System). The guide contains examples of the XML files and the schemas used to generate them.

Data Store and ECM

OpenLAB Data Store comes with a series of manuals covering hardware, software and network requirements, installation, maintenance and administration:

Publication Number	Title
M8620-90117	OpenLAB Data Store Hardware and Software Requirements
M8620-90012	OpenLAB Data Store Installation Guide
M8620-90116	OpenLAB Data Store Maintenance Guide
M8620-90115	OpenLAB Data Store Guide for Administrators

The following OpenLAB ECM references are available:

Publication Number	Title
5991-5512EN	OpenLAB ECM Hardware and Software Requirements

Note: For many manuals there are also localized versions available.

Technical Notes and other Publications

- Agilent Original Bundle PC (5990-7990EN)
- Virtualizing Agilent OpenLAB CDS ChemStation Edition with VMware (5991-3637EN)
- Integration of Agilent OpenLAB CDS ChemStation Edition with OpenLAB Data Store - Compliance with 21 CFR Part 11 (5991-1470EN)
- Integration of Agilent OpenLAB CDS ChemStation Edition with OpenLAB ECM - Compliance with 21 CFR Part 11 (5991-1472EN)
- Agilent Compliance Services Portfolio: Enterprise Edition (5989-4440EN)

Hardware Manuals referenced in this document

- Agilent 1290 Infinity with ISET user manual (G4220-90310)
- OpenLAB CDS Waters ACQUITY Drivers Installation and User's Guide (M8505-90000)
- OpenLAB CDS Waters Alliance HPLC Instrument Control Add-On Installation, Upgrade and Migration Guide (M8239-90001)

Documentation and Manuals on the OpenLAB CDS ChemStation Edition DVD Set

The following manuals and documents are included on the OpenLAB CDS DVD set:

Publication			
M8300-90015	OpenLAB CDS Supported Instruments and Firmware Guide	CDS_SupportedInstFirmware.pdf	1
M8301-90055	OpenLAB CDS Network Requirements	CDS_network-requirements.pdf	1
M8301-90046	OpenLAB CDS Hardware and Software Requirements	CDS_hw-sw-requirements.pdf	1
M8301-90007	OpenLAB CDS WorkStation Installation and Configuration Guide	CDS_WS-InstallationGuide.pdf	1
M8305-90006	OpenLAB CDS Networked and Distributed System Installation and Configuration	CDS_NWSDS-Installation.pdf	1
M8301-90113	Creating OpenLAB Shared Services Databases on Oracle Systems	CDS_oracle12.pdf	1
M8301-90063	Agilent IO Libraries Suite for OpenLAB CDS	CDS_IO-Libraries.pdf	3
M8304-90002	OpenLAB CDS ChemStation Edition AIC (M8304AA) Setup Guide	CDS_CS_AIC-SetupGuide.pdf	2
M8301-90033	OpenLAB CDS ChemStation Edition Upgrade Preparation Guide	CDS_CS-Upgrade.pdf	2
M8301-90162	Reusing Data from ChemStation B.04.03 SP1 and SP2 in OpenLAB CDS ChemStation Edition	CDS_CS-data-Migration.pdf	2
M8301-90073	OpenLAB CDS Software License Installation Guide	CDS_LicenseInstallationGuide.pdf	1
M8305-90013	OpenLAB CDS Guide for Administrators	CDS_admin.pdf	1
M8300-90006	OpenLAB CDS ChemStation Edition Instrument Configuration Guide	CDS_CS-InstrumentConfig.pdf	2
M8301-90100	OpenLAB CDS ChemStation Edition XML Connectivity Guide	CDS_CS_XML.pdf	2
n/a	ACAML 1.5	ACAML.15.xsd	6
M8305-90020	OpenLAB CDS Report Template Editor Concept Guide	RTEConceptsGuide.pdf	6
M8301-90016	OpenLAB CDS ChemStation Edition Concepts and Workflows	CDS_CS-concepts.pdf	2
M8301-90025	OpenLAB CDS ChemStation Edition Reference to Operation Principles	CDS_CS-references.pdf	2
M8301-90170	OpenLAB CDS ChemStation Edition Understanding Your Spectra Module	CS-LC3D_SpectraModule.pdf	2
n/a	Macro Programming Guide For RC .NET Drivers in OpenLAB CDS ChemStation Edition	Macro Programming Guide RC.Net.pdf	2
M8301-90084	OpenLAB CDS ChemStation Edition with Central Data Storage User's Guide	CDS_CS-with-DataStorage.pdf	2
M8313-90001	Secure Workstation for OpenLAB CDS ChemStation Edition Installation Guide	SecureWS_install.pdf	1
M8313-90011	Secure Workstation for OpenLAB CDS ChemStation Edition User's Guide	SecureWS_using.pdf	2
M8313-90021	Secure Workstation for OpenLAB CDS ChemStation Edition Maintenance Guide	SecureWS_maintenance.pdf	2
M8201-90507	Declaration of Software Validation OpenLAB CDS	CDS_DeclarationSoftwareValidation.pdf	1
M8313-90501	Declaration of Software Validation Secure Workstation for OpenLAB CDS ChemStation Edition	CDS_DeclarationSoftwareValidation-SecureWS.pdf	1

Note: For many manuals there are also localized versions available.

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

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