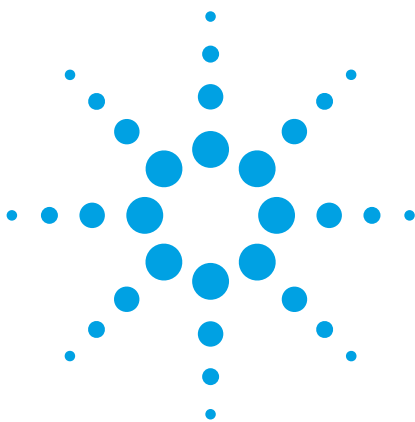




Agilent OpenLAB CDS ChemStation Edition for GC, LC, LC/MSD, CE, CE/MSD, and A/D Instruments

OpenLAB CDS ChemStation Edition C.01.02 OpenLAB Shared Services A.01.02

Functional Design Specification

General Description

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

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

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.



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

- Workstation (standalone)
- Workstation (stand-alone) with OpenLAB ECM
- Networked Workstation
- Networked Workstation with OpenLAB ECM
- Distributed System

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 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.

Agilent instruments supported on OpenLAB CDS ChemStation Edition include:

- Agilent 7890A gas chromatograph
- Agilent 7820A gas chromatograph
- Agilent 6890N, 6890 Plus and 6890A gas chromatographs
- Agilent 6850A gas chromatograph
- Agilent 35900E A/D Converter
- Agilent 1260 LC Series modules and systems for HPLC
- Agilent 1290 LC Series modules and systems for HPLC
- Agilent 1100/1200 LC Series modules and systems for HPLC
- Agilent 1100/1200 Series LC/MSD
- Agilent 1120 and 1220 Compact LC systems
- Agilent 7100 capillary electrophoresis systems

Agilent OpenLAB CDS EZChrom Edition supports a wide variety of instruments from other manufacturers.

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.
- 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.
- A distributed 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 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.

For any OpenLAB CDS ChemStation Edition configuration an Agilent OpenLAB Enterprise Content Management (ECM) Server can be added to provide a Microsoft SQL Server or Oracle database as the data repository for the system. Because Agilent OpenLAB ECM is tightly integrated with Agilent OpenLAB CDS ChemStation Edition for secure central data storage, Agilent OpenLAB ECM specifications are included in this document.

Agilent OpenLAB ECM adds:

- 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
- Advanced file organization and management including archiving and record retention controls
- Meta data extraction for keying and searching data
- Revision and audit trail features facilitating regulatory compliance

- A Software Development Kit for product integrations and feature extensibility

In addition, Add-on packages can be added to OpenLAB ECM to 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 break the system down and 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. 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.

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.

Instruments require immediate access to network communication so LAN adaptors should be configured to prevent Windows from powering off the adapter to save power.

TCP/IP networking in a LAN is required for all products. WAN's (wide area networks) are supported, but extra care needs to be taken to ensure the proper communication speed between the various host machines in the configuration.

When using virtual machines as OpenLAB CDS ChemStation Edition clients, 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. The virtual machine hardware and ESX configuration must also account for a potential communication bottleneck on an ESX host server.

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.

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 components necessary to support OpenLAB CDS ChemStation Edition on a domain are:

- Domain controller—broadcasts the domain name and negotiates access to machines.
- Domain name server (DNS)—maintains records of what hostnames belong to which IP on the network.
- Active directory—maintains the list of users and their access rights on the domain.

Note: OpenLAB CDS ChemStation Edition components may not be installed on a machine that is acting as a domain controller.

The domain components above host a variety of services and settings that must be configured appropriately to allow communication across machines. The following services and settings will need to be configured to fit your domain. In house IT is responsible for proper configuration of any custom domain solutions:

- Lookup zones and hostnames
- Group and security policies
- Subnet masks and Virtual LANS

Firewall Settings

If you are using a third party firewall on the network where OpenLAB CDS ChemStation Edition is installed, open these firewall ports to allow communication between the system components of OpenLAB CDS ChemStation Edition:

- Port 67 and 68: These ports are used for the receipt and response, respectively, of BootP server communications.
- Port 3389: This port is used by the OpenLAB CDS ChemStation Edition AIC.
- Port 3424: This port is used for the transfer of diagnostics information between system components, such as AICs and clients, and OpenLAB Shared Services.
- Port 6570 (default): This port is used for the active retrieval and release of product licenses.
- Port 6577: This port is used for the communications of all OpenLAB Shared Services relayed information. This includes instrument and run status, active trace data, and global configurations.
- Port 8080: This port is used to host the viewing page of current license grants and consumptions found in the OpenLAB Control Panel administration interface.
- Ports 8085-8090: These ports are used as an alternative to port 8080 if that port is in use by another page or process.
- Port 9000: This port is used for configuration of Agilent 7890 GCs.
- Ports 9001-9002: These ports are used by AICs to communicate with instruments and shared servers.
- Port 10000-10009: These ports are used for status and acquisition communication with Agilent 7890 GCs.
- Ports 27000-27009: These ports are used for communication of license availability.

Dynamic Ports: Dynamic ports are used for temporary communications between clients and instrument controllers. The ports used depend on the operating system in use and are configurable. Refer to the operating system documentation for more information.

The OpenLAB CDS installer will automatically open these ports on an enabled Windows firewall during installation.

Computer Hardware

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. Where interface cards are to be added, a PCI interface bus is required. 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.

The personal computer is interfaced to the analytical instruments through a LAN card, a GPIB internal card, a USB/GPIB interface, or a combination of a GPIB card and a LAN card. All cards plug directly into the computer's PCI interface. In addition, there are serially connected instruments, e.g., the ELSD is connected via RS232 directly to the workstation PC. Note that serially connected instruments are not supported on the Agilent Instrument Controller (AIC) or under VMware. 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.

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 this manual applies to Hewlett-Packard computers and may not be optimized for other vendors' PCs. The standard configuration of the GPIB interface, for instance, may conflict with the memory configuration of a non-Hewlett-Packard computer. Additional accessory interface boards may cause conflicts of hardware related resources (I/O ports, interrupt settings, DMA channels). For a non-Hewlett-Packard computer, use the setup utility program supplied by the manufacturer to configure your computer and check the supplied documentation to eliminate resource conflicts in your PC's setup, especially regarding the configuration of the GPIB interface. 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.

Computer Hardware Requirements by Role

Requirements for All OpenLAB CDS Computers

In an OpenLAB CDS ChemStation Edition system, there are six primary computer roles, three related to the CDS and OpenLAB Shared Services, three additional if OpenLAB ECM is included as the data repository. Each role has a section below with the specific requirement for that role. All computers are expected to have a minimum 10/100 network adapter (100/1000 preferred) and access to a DVD ROM drive.

OpenLAB CDS ChemStation Edition, OpenLAB Shared Services servers, instrument controllers and client systems can be run on virtual machines that meet the requirements below. Use VMWare vSphere 4.0 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. The participation of a VMWare application expert is strongly recommended.

Microsoft .Net Framework 3.5 with Service Pack 1 software must be installed on any supported operating system prior to installing OpenLAB CDS ChemStation Edition components.

OpenLAB Shared Service Servers

OpenLAB Shared Services Servers are supported on Windows Server 2003 SP2 (32 bit) or Windows Server 2008 R2 (64 bit). The minimum processor is a 2 GHz single core but a 3 GHz dual core is preferred. Minimum physical memory (RAM) is 4 GB, 6 GB is recommended for 64 bit installations. Disk space minimum is 80 GB with 40 GB available.

Agilent OpenLAB Shared Services Servers manage information using a database. The database is installed and configured automatically during OpenLAB CDS ChemStation Edition workstation installation. When deploying networked system configurations, the database must be preinstalled to ensure acceptable performance of the system.

The following database software is supported for hosting OpenLAB Shared Services databases:

- SQL Server 2008 R2 Express (32-bit) : Installed with product
- SQL Server 2008 R2 Standard or Enterprise (32-bit)
- SQL Server 2008 R2 Standard or Enterprise (64-bit) (Windows Server 2008 R2 databases only)
- Oracle 11g R2 Standard and Enterprise Editions

Windows Installer 4.5 is required for SQL Installations on OpenLAB Shared Services Servers.

It is strongly recommended that you store database files and transaction logs (when applicable) on dedicated hard drives.

Agilent OpenLAB CDS ChemStation Edition supports the use of a central licensing server for the distribution and tracking of license entitlements. FlexNet Publisher v. 11.8 is supported for this purpose and is installed with the installation of OpenLAB Shared Services Server components.

OpenLAB CDS ChemStation Edition AICs

AICs can be built by installing the proper OpenLAB software on a server. Windows 2008 R2 is the only operating system supported. The minimum processor is a dual 2GHz quad core processor. Minimum physical memory (RAM) is 8 GB, 10 GB is recommended. Disk space minimum is 250 GB, with 50 GB available.

The Agilent product M8304AA comprises a HP ProLiant ML150 G6 R&D Server. This preconfigured AIC has dual 2 GHz quad core processors, 8 GB of RAM and two 500 GB hard drives.

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. LC/MSD and CE/MSD instruments are not supported on AICs and must be connected to dedicated workstations. 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.

There is no limit to the number of AICs allowed in an OpenLAB CDS ChemStation Edition distributed system.

OpenLAB CDS ChemStation Edition Workstations or Clients

Workstations or clients may be installed on computers running Windows XP SP3, Windows Vista SP1, or Windows 7 (32 or 64 bit). For Windows XP the minimum processor is a 1.5 GHz single core. For Windows Vista SP1 or Windows 7 (32 or 64 bit) the minimum processor is a 3.4 GHz single core.

The Workstation Standard Bundle PC shipped with the OpenLAB CDS ChemStation Edition Workstation PC bundle products is a Hewlett-Packard Z210 Xeon with an Intel® Xeon® Quad-Core Processor E3-1225 (3.10 GHz, 6 MB cache, 1333 MHz memory), 4GB RAM and 250GB storage.

Windows XP requires 1 GB physical (RAM) memory minimum with 4 GB recommended. With Windows Vista or Windows 7 (32 bit) the minimum is 2 GB and the recommended is 4 GB. Windows 7 (64 bit) requires 4GB RAM with 6 GB RAM recommended. Windows XP requires 100 GB of hard disk space. Windows Vista SP1 or Windows 7 (32 or 64 bit) require 160 GB of hard disk space.

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

OpenLAB ECM General Requirements

In order for OpenLAB CDS to use OpenLAB ECM as a file storage location, you will need Agilent OpenLAB ECM Server revision 3.3.2 SP1 or revision 3.4.1 and the Agilent OpenLAB ECM API v. 1.0.25.7 (Available as OpenLAB ECM 3.3.2 Hotfix03 or included with OpenLAB ECM 3.4.1).

OpenLAB ECM is accessed through a web client that requires Microsoft Internet Explorer. OpenLAB ECM Server revision 3.3.2 SP1 requires Microsoft Internet Explorer version 6 or version 7. To work with PDF documents Adobe Acrobat Reader 7, 8 or 9 is required. To work with Microsoft Office documents requires Microsoft Office 2003 or 2007. OpenLAB ECM Server revision 3.4.1 requires Microsoft Internet Explorer version 8. To work with PDF documents Adobe Acrobat Reader 9.0 (32 bit) is required. To work with Microsoft Office documents requires Microsoft Office 2003 or 2007 Adobe Acrobat Reader 9.0 (32 bit). To work with OpenLAB ECM and Microsoft Office Documents requires Microsoft Office 2007 or 2010.

OpenLAB ECM Database Server

For OpenLAB ECM 3.3.2 SP1 for an Oracle installation the database server can be Oracle 10g (10.2.0.4) Standard or Enterprise Edition. The SQL Server Version can SQL Server 2005 Standard or Enterprise SP3.

For OpenLAB ECM 3.4.1 for an Oracle installation the database server can be Oracle 11g (11.2.0.1) Standard or Enterprise Edition. The SQL Server Version can use SQL Server 2008 Standard or Enterprise R2.

OpenLAB ECM Server Hardware Requirements

There are several servers running in an OpenLAB ECM installation, a Web Server, a File Transfer Server, an Application Server, the Database Server, a Scheduler Server and some number of clients. Often, in smaller installations they are combined on a smaller number of physical servers, in larger installations, there may be more than one server of each type. The following table has the hardware specifications for each server, but a proper system design may adjust the allocation of resources and additional details are provided in product documentation.

OpenLAB ECM Server Type	Processor Min	Processor Recommended	Memory Minimum	Memory Preferred	Disk Space Minimum
Web	2 GHz	Dual Core or Dual Processor	1 GB	2 GB	20 GB
File Transfer	2 GHz	Dual Core or Dual Processor	2 GB	4 GB	120 GB
Application	2 GHz	Dual Core or Dual Processor	2 GB	4 GB or more	80 GB
Database	2 GHz	Dual Core or Dual Processor	2 GB	4 GB	100 GB
Scheduler	2 GHz		1 GB	2 GB (Win 7)	200 GB
Client	1.5 GHz		512 MB (Win XP)	1 GB (Win 7)	40 GB

Language Compatibility

The English version of OpenLAB CDS is validated on Windows English language version.

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.

IEEE-488 GP-IB Support Matrix

Instruments Supported on GP-IB (not on AICs)

- Agilent 6890 GC

82350A/B GP-IB Interface Cards

Analytical instruments can communicate with the Agilent OpenLAB CDS ChemStation Edition via GPIB using a GPIB board installed in the computer. Agilent 82350A or 82350B PCI high-performance GPIB interface cards can be used on Windows XP Professional systems. For

both cards a PCI slot is required on the PC.

The Agilent 82350 is a PCI GPIB interface card and no additional settings such as changing the I/O base address are required.

Please note that GPIB communication requires installation of the SICL I/O library version M.01.01.

Please ask your local Agilent Technologies representative for additional details.

USB/GP-IB Interface Support Matrix

Instruments supported on USB/GP-IB (USB port on PC is used, not on AICs)

Note: USB/GPIB interfaces are only supported with legacy LC instruments.

USB/GP-IB Interface

A USB/GPIB interface (82357A) allows you to directly connect from the USB port on your PC to GPIB instruments. The interface is small, portable, and flexible, uses industry standards and is easy to connect. The interface can be used on Windows XP Professional systems. The USB/GPIB cable is available as an option against the CE PC bundle (G1602BA Option 720) or as an internal support part (G1680-63200) from the Support Organization.

Please ask your local Agilent Technologies representative for additional details.

LAN-MIO Support Matrix

G1369A/B/C Agilent LAN Interface Cards

The firmware of the card must be revision A.01.05 or higher. For non-LC systems (35900E ADC, 6890 GC and 6850 GC) a minimum Firmware Revision of C.03.00 is required. Please refer to Service Note G1369-003.

J4100A JetDirect N Internal Printer Servers (MIO)

The firmware of the JetDirect card has to be revision K.08.32 or higher.

Note:

- The 6890N requires firmware revision N.05.04 or higher and LAN board firmware revision 04.7B3. LAN communication with the Agilent 6890A requires firmware revision A.03.08 or higher. This is available in an electronic chip format from Agilent Technologies. Please ask your local Agilent Technologies Representative for details.
- LAN communication with the Agilent 1100 Series requires a minimum firmware revision of A.06.02. The G1315C DAD-SL and G1365C MWD-SL detectors require a minimum firmware revision of B.01.02. A new LAN/RS-232 Firmware Update Tool 2.1 is available for updating firmware quickly and easily. Please ask your local Agilent Technologies representative for details.

Instruments / Modules Supported on LAN

- Agilent 1200/1100/1260 Series LC systems
- Agilent 1120/1220 Integrated LC systems
- Agilent 7890A GC
- Agilent 6890 GC
- Agilent 6850 GC
- Agilent 1200/1100 Series LC/MS systems
- Agilent 35900E A/D systems
- Agilent 1200 Chip Cube interface (G4240A for Ion Trap systems)
- Agilent Capillary Electrophoresis (CE) 7100
- Agilent Capillary Electrophoresis Mass Spectrometry (CE/MS) with CE 7100

G1369A/B/C LAN Interface Cards

LAN interface cards are used to connect analytical instruments to the LAN. Jet Direct or G1369A LAN cards are required. The minimum firmware required for LC systems used with the G1369A LAN card is Rev. A.01.05 or higher. For non-LC systems (35900E ADC, 6890 GC and 6850 GC) a minimum Firmware Revision of C.03.00 is required. Additional details are available in the Agilent G1369A LAN Interface manual.

Communication Protocols

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

The BootP protocol is used to configure the HP JetDirect or G1369LAN cards. The Boot strap protocol requires a BootP service (refer to the readme). The Agilent BootP Service Program uses the LAN communication parameters specified in the Configuration Editor to

establish communication. The Agilent BootP Service Program can be used for central administration and distribution of IP addresses and settings.

Fixed IP Addresses for Communication

IP addresses can be stored in the non-volatile RAM of the module's LAN card. Depending on the LAN card it is possible to assign a fixed IP address to the Agilent 1200/1100 Series modules, using either a handheld control module, a mode selecting a predefined address by DIP switch or Telnet to assign IP addresses. It is possible to assign a fixed IP address to the 6890N and 6850 using the front display.

Additional Hardware Required for LAN Instrument Control

An industry standard LAN PC card is shipped with all Agilent OpenLAB CDS ChemStation Edition 32-Bit PC bundles. An instrument LAN card can also be ordered from Agilent Technologies as an option to the instrument or as an individual part. Please ask your Agilent Technologies representative for details. Industry standard LAN cabling using twisted pair or coaxial cabling:

- Twisted pair –10/100 baseT twisted pair cabling with RJ45 connectors can be used together with an Agilent G2402A 8-port 10/100 auto sensing switch for the ability to connect one or more instrument 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 1200/1100 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 maximum data rate.

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. Recommended black and white printers are the HP LaserJet family using PCL 5e or 6. For lower performance applications it is possible to use the HP DeskJet family. Please note that the HP DeskJet printer family is not recommended for high throughput applications. Recommended color printers are the HP LaserJet 2500TN, OfficeJet Pro K550DTWN or an HP DeskJet family printer.

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.

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 they have been assigned.

OpenLAB Control Panel functions are divided into views selected through buttons in the lower left panel 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 is installed.

OpenLAB Control Panel Instrument View

The Navigation Panel

All instruments connected to the system are displayed in tree in the Navigation panel 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 panel for the individual instrument in the panel 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 distributed systems, the AIC for the instrument is selected from a list of AICs 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. For many instruments, two generations of drivers are available; RC.Net and Classic. It is generally advised to use the new RC.Net drivers where possible. 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 panel, 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

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 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 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 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 panel on the left allows users to select a given section. Corresponding tools and workspace appear for each selection.

The items available in the navigation table 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 this 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.

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
- 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.

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. More information on roles is provided in the roles section of this document.

Groups

Groups defined by the authentication provider can be imported and added to the access list for the OpenLAB CDS. 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. More information on roles is provided in the roles section of this document.

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 and the group may be selected for a role or the privileges selected individually.

The table below lists each role and the checkmarks indicate the privileges assigned by the role.

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
Administration									
Manage Printers	✓	✓							
Edit Activity Log Properties	✓	✓							
Purge Activity Log	✓	✓							
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	✓		✓						

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
Project Management									
View Project or Project Group (not editable)	✓			✓		✓	✓	✓	✓
Manage Project or Project Group	✓			✓					
Manage Project or Project Group Access	✓			✓					
E-Signature									
E-Signature Sign Data Files	✓			✓					
E-Signature Revoke	✓			✓					
OpenLAB CDS ChemStation Edition Control									
Run Acquisition	✓						✓	✓	✓
OpenLAB CDS ChemStation Edition Data									
Delete Data	✓					✓	✓		
Manual Integration	✓					✓	✓	✓	
Save Data to ECM	✓					✓	✓	✓	✓
OpenLAB CDS ChemStation Edition Instrument									
Modify Instrument Configuration	✓						✓		
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	✓					✓	✓	✓	

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
OpenLAB CDS ChemStation Method (cont'd)									
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	✓						✓	✓	
OpenLAB CDS ChemStation Edition Security									
Break Session Lock	✓					✓	✓		
Command Line	✓					✓	✓		
Manage Transfer Queue	✓					✓	✓		
Modify ECM Transfer Preferences	✓						✓		
OpenLAB CDS ChemStation Edition Sequence									
Delete Sequence	✓					✓	✓	✓	
Edit Sequence Summary	✓						✓	✓	✓
Reprocess	✓						✓	✓	
Save Sequence	✓						✓	✓	
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	✓						✓	✓	
Enable Full Menu	✓					✓	✓	✓	

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:

- Agilent Informatics Software Portal
- Agilent Support
- Agilent's Website

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. An .ICO file can be selected to associate an icon with each link.

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 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 WorkStation 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 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-day Startup License for the system. The expiration period starts with the first launch 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.

Licenses are specific to the computer they are installed on but may be returned and reissued for a different computer when a hardware change is required. The license can be returned and reissued twice.

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. A detailed list of the log files on each instrument controller can be generated. All or selected files can be marked on the list and the marked files can be written to a file allowing diagnostic information to be collected easily.

A list of MAC addresses with their associated IP addresses can be created and managed by the instrument controller.

Diagnostics

Version

The version section displays the software version and build.

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, during a support call for documentation.

The OpenLAB Shared Services Server can be pinged to determine its ability to respond on the network. A service mode, restricted to Agilent access the Agilent OpenLAB Diagnostics Dashboard. The dashboard can modify the local or remote log configuration and create local diagnostic reports.

Log Files

A report can be created and exported for the OpenLAB Shared Services Server or for the whole system. 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 Controller Report: listing e.g., the instruments on an instrument controller
- Instrument Report: listing the configured instruments
- Project Report: listing projects (only if OpenLAB ECM Intelligent Reporter is installed)
- Roles Report: listing roles and their privileges
- System Report: listing instruments, user and groups and their roles and roles and privileges
- User and Group Report: listing instruments, user and groups and their roles

The create report tool opens the report as a PDF, the export XML tool allows reports to be saved as an XML export file.

System Maintenance

OpenLAB Shared Services includes an additional tool, the OpenLAB Server Utility which 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, quantification 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 (M8301-90011).

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 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 audit trails, require an OpenLAB ECM server 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 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 ECM for storage

OpenLAB CDS ChemStation Edition can be set to open the data transfer queue when the OpenLAB CDS ChemStation Edition opens to make sure data transfer issues are noticed.

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

The audit trails for methods 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. 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.

Configuration Profiles

Each OpenLAB CDS ChemStation Edition workstation can be set to access the OpenLAB Shared Services Server without OpenLAB ECM or to enable data transfer to OpenLAB ECM.

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 (M8301-90021).

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 data from multiple sequences and/or single runs in the navigation table in the data Analysis view, selecting those data that are to be part of the self-assembled result set. 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 panel, 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
- 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 or verification procedures. An OpenLAB CDS ChemStation Edition Companion view is available for routine GC analyses when it is desirable to have instrument operators run samples from an easy-to-use, preconfigured table.

The Navigation Pane contains the Navigation Buttons, which allow rapid switching between the OpenLAB CDS ChemStation Edition views, and OpenLAB CDS ChemStation Edition Explorer panel 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 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
- 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 Panel, 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 run 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 and XLS formats.

Report Layout View

The Report Layout view allows you to define the layout of report templates. 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 or 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 an OpenLAB ECM server, the File Transfer Settings tab in the OpenLAB CDS ChemStation Edition Preferences allows selection of the location on the server for data storage. The OpenLAB ECM drawer and folder can be selected from the path (OpenLAB ECM location and cabinet). Permitted locations are controlled from the OpenLAB ECM content management tools. If the operator has the appropriate permissions they can browse to and/or create new storage locations within OpenLAB ECM.

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.

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.

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

Analysis Monitoring

A color-coded status for the analysis is displayed using the same codes as 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 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 or bar. The windows may each show multiple overlaid chromatographic/electropherographic signals or instrument parameters, such as pressure. 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 spectra evaluation. 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.

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.

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

Opening Result Sets – Navigation Panel 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 Panel 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.

The context menus for the data icons 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 preferences allow restriction of the signals loaded for each file to those specified in the current method.

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 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 the last chromatogram/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 and compound names (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 document Agilent OpenLAB CDS ChemStation Edition Reference to Operation Principles (M8301-90021).

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
- 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

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.

Calibration Task – Quantification Settings

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 retention time window of the compound selected in the table on the signal displays. The color indicates whether or not the select 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 mode windows are linked so that changes in one are automatically reflected in all the others. This mode allows graphical selection and modifications of the calibration data.

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 (Amt) — A calibration point with the amount x has the weighting $1/x^2$ 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 $(1/x^2) * a^2$, 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 $1/y^2$ 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 $(1/y^2) * b^2$, 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 point 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 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 response factor 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 true 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.

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.

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 – $\text{Response PercentX} = (\text{ResponseX} / \text{Sum of all Peak Responses}) * 100$
- ESTD – $\text{ESTD AmountX} = (\text{ResponseX} * \text{RFX})$
- Norm% - $\text{Amount \%X} = (\text{AmountX} / \text{Sum of all Amounts}) * 100$
- ISTD – $(\text{ResponseX} / \text{ResponseIS}) * \text{RFX} * \text{AmountIS}$
- ESTD% - $\text{ESTD Amount \%X} = (\text{ESTD AmountX} / \text{Sample Amount}) * 100$
- ISTD% - $\text{ISTD Amount \%X} = (\text{ISTD AmountX} / \text{Sample Amount}) * 100$

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 they can be entered in the Quantitation Settings.

A Multiplier and a Dilution Factor can be entered; both will be multiplied with the calculated concentration. Like the amounts above they can either be entered at the time of analysis or entered 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 report styles settings in the report specification dialog control the report content. The content is the product of 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 OpenLAB OpenLAB ECM is configured as the data storage for the OpenLAB CDS ChemStation Edition, the report will automatically include the location of the data in OpenLAB ECM 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/MS Library search results
- Peak performance calculations with graphics
- Signal to Noise

Additional style settings provide the following content controls:

- Quantitative Result Sorted By: RT reports results for all signals in a single table sorted by retention time, Signal reports results in a separate table for each 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 tic marks (system must include a fraction collector)
- 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 Preview window. Only one report can appear in the window at a time, in automated operation each new report replaces the previous one. Reports in the preview window can be printed to the printer.

A report can be saved to a file in any 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.

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 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 statistic methods
- resolution by the peak width at half height, sigma, tangent and statistic 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, G4636AA OpenLAB ECM Intelligent Reporter Client, and G4648AA OpenLAB ECM Intelligent Reporter Designer).

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 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

All Intelligent Report templates are based on the Report Definition Language (RDL), a standardized XML format provided by Microsoft. To create report templates, you can either use the Report Template Editor (RTE) which is the report template toolset in the Report Layout view when Intelligent Reporting is enabled, or Microsoft SQL Server Business Intelligence Development Studio (BI Studio).

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. Note that with RTE, you cannot edit templates that have been created with BI Studio.

BI Studio provides a complete range of report template creation functions, and requires advanced knowledge of template development concepts and tools. For more information, please refer to the OpenLAB Report Template Designer Guide (G4635-90007) included on the OpenLAB CDS ChemStation Edition C.01.02 installation media. This manual also contains detailed descriptions of the Agilent BI Studio report templates that are delivered with OpenLAB ECM Intelligent Reporter. These templates are specifically designed for usage in BI Studio and contain some advanced features that are not available in RTE. In BI Studio, you can edit any report template, whether it was created with RTE or with BI Studio.

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 OpenLAB CDS ChemStation Edition can report at the injection or single signal level.

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 Guide (G4635-90007).

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

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 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.

You can store the values, calculations and statistical calculations as variables and access these variables 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.

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.

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 and/or XLS. 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.

As it can be difficult to reproduce reports from old result sets since the applicable report templates may have been 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 LCMS 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 manual import of 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 (M8301-90100).

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 not defined by standard OpenLAB CDS ChemStation Edition operation. The fields are defined in the method, so fields can be defined differently 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 field is mandatory, the operator must supply a value for the field before they are 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 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 including 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 allows 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 Interface Guide for the RC .NET Module Driver in OpenLAB CDS ChemStation Edition C.01.02 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 execute one of a selection of technique specific shutdown commands or a user-defined shutdown macro to complete a series of specific commands.

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. 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 values, 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 an internal standard is used for the analysis, the ISTD amount column can be used to specify the internal standard concentration for each sample.

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 1200/1100 LC system includes a fraction collector the “Fract. Start” column will appear in the sequence table.

The user can configure the columns to be displayed in the sequence table as well as the individual column widths. 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 sequence table can easily be created or modified using the fill-down wizard functions. This wizard can insert, append or fill-down and supports the core columns in the sequence table.

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.

Printing Sequences

Both the sequence and partial sequence tables may be printed.

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

Easy Sequences can be added to the queue. Additional Easy Sequences are added to the end of queue, and the order in which the Easy Sequences are run can be changed.

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.

Data Analysis: Reprocessing Mode

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

Data Analysis: Recalculation Mode

The recalculation mode allows a quick recalculation of a sample or a set of samples with a different method. The required functions associated with each mode are available in separate toolbars.

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.

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, 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.

For those specifically concerned with 21-CFR Part 11 compliance please consult the document Integration of Agilent OpenLAB CDS

ChemStation Edition with OpenLAB ECM - Compliance with 21 CFR Part 11 (5991-1472EN).

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. It is documented together with onsite revalidation protocols in the Validation CD-ROM.

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.

Installation Qualification

An automated Installation Qualification (IQ) utility 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.

Operational Qualification / Performance Verification (OQ/PV)

The 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.

The Verification view is only available for LC, LC/MS, CE and CE/MS.

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 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.

Secure Data Storage and Result Revisions

With file-based data storage alone, the current results and the logs are properly preserved but the complete revision history is not recorded. When OpenLAB ECM is configured as the central repository, the complete revision history is preserved. At the completion of a set of operations, the result set is zipped into an SSIZip and saved to the OpenLAB ECM as a new revision. Once the data are stored in OpenLAB ECM, each operation that modifies the data will result in a new revision once the data are uploaded again to OpenLAB ECM.

A transaction log is maintained in OpenLAB ECM 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.

The supported instruments and firmware are detailed in the Agilent OpenLAB Chromatography Data System Supported Instruments and Firmware Guide (M8300-90011).

Agilent OpenLAB CDS ChemStation Edition for GC

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 gas chromatographs and the Agilent 35900E A/D converter.

The Agilent OpenLAB CDS ChemStation Edition is interfaced to the GC via LAN or GPIB 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 7890A 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 (Agilent 7890, 6890 and 6850 Series only) will 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.
- Improved GC Driver with setpoint and actuals
- Signal Events(Switching between front and back detectors, zero signal, and delay signal collection)
- Capillary columns can be calibrated 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 for the 78xx and 68xx GCs. The Agilent OpenLAB CDS ChemStation Edition also can control, through a timetable, a maximum of eight valves or relays.

Sampling

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

Dual-injector configurations (Agilent 7890 A, and 6890 Series GCs) allow individual or synchronous injections. Each automatic sampler allows a 3-vial turret, 8-vial turret, or 150-vial access if a sample tray is fitted (7890A and 6890 Series only). 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.

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

The Agilent OpenLAB CDS ChemStation Edition can acquire a third and fourth signal from external detectors in a single run by adding the 35900E A/D converter.

Retention Time Locking Software

Retention Time Locking is a useful technique developed by Agilent Technologies to match analyte retention times between and among Agilent GC systems. RTL is essentially based on void time matching through an empirically determined pressure-retention time calibration curve. RTL calibration curves are specific to the analyte chosen (pick one analyte in your standard, the best choice is a peak well separated from other peaks and in the middle portion of the chromatogram), type of column used (stationary phase type, phase ratio, and column dimensions), carrier gas type, and oven temperature program used in the method. Once the calibration has been done for an initial ("original") method, the method and its associated RTL calibration can be transferred to another instrument with the same column type and carrier gas type. RTL software in Agilent OpenLAB CDS ChemStation Edition assists with the process of determining and using RTL calibrations.

To lock a new system to the original system, carrier gas head pressure is adjusted using the RTL calibration curve. The retention time of a target compound (same one used to generate the RTL calibration) can be locked onto the desired retention time value. All other analyte retention times will then also match those of the original.

RTL software also provides the capability to search retention timetables. Searching unknowns is based primarily on retention times and may also include element information (such as one might get from selective detectors) to narrow search results further. Users can create, edit, import and export RTL libraries.

Agilent OpenLAB CDS ChemStation Edition for LC

OpenLAB CDS ChemStation Edition for LC and additional LC instrument module controls and acquires data from the Agilent 1200/1100 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.

Sampling Systems

The injection systems may be manual or automated with an autosampler or well-plate autosampler. 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 Agilent 1200/1100 injection systems are supported:

- 1100 Autosampler (G1313A)
- 1100 Series Micro Autosampler (G1389A)
- 1200 Series Standard Autosampler (G1329A, thermostatable with illumination)
- 1260 Standard Autosampler (G1329B)
- Thermostatted standard autosampler (G1327A)
- 1260 SFC standard autosampler (G4303A)
- 1100 Well-plate Autosampler (G1367A)
- 1200 Series High Performance Autosampler (G1367B)
- 1200 Series High Performance Autosampler SL (G1367C, high pressure compatible with illumination)
- 1200 Series High Performance Autosampler SL Plus (G1367D)
- 1260 High Performance Autosampler (G1367E)
- Thermostatted well-plate autosampler (G1368A)
- Micro well-plate autosampler (G1377A with illumination)
- Thermostatted micro well-plate sampler (G1378A)
- Preparative autosampler (G2260A with illumination)

- Thermostatted preparative sampler (G2261A)
- Agilent sample capacity extension (G2257A) for the Agilent 1100 Series well-plate sampler G1367A and microwell-plate sampler G1377A
- Agilent dual loop autosampler (G2258A with illumination)
- Agilent thermostat option (G1330A /B)
- Agilent fraction collectors (G1364A /B/ C/D)
- Agilent 1200/1100 Series barcode reader (G2256A) for the sample capacity extension (G2257A)
- Agilent G1367D High Performance Autosampler SL Plus
- 1260 High Performance Autosampler (G1367E)
- 1260 SFC standard autosampler (G4303A)
- 1290 Infinity Autosampler (G4226A)
- 1260 bio-inert high perform. autosampler (G5667A)

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 postrun time for column equilibration.

The following Agilent 1200/1100 solvent delivery systems are supported:

- Binary pump (G1312A)
- Binary pump SL (G1312B)
- 1260 Binary Pump VL (G1312C)
- 1290 Infinity Binary Pump (G4220A)
- 1290 Infinity Binary Pump VL (G4220B)
- 1260 Series SFC Binary Pump (G4302A)
- Isocratic pump (G1310A)
- 1260 Isocratic Pump (G1310B)
- Quaternary pump (G1354A / G1311A)
- 1260 Quaternary Pump (G1311B)
- 1260 Quaternary Pump VL (G1311C)
- 1260 Infinity bio-inert quaternary pump (G5611A)
- Preparative pump (G1361A /G1391A with gradient extension)
- Capillary pump (G1376A pump only / G1382A with degasser)
- Agilent 1200/1100 nanoflow pump (G2226A pump only, G2225A with degasser)

Column Compartments

The following Agilent 1200 column compartments are supported:

- 1260 Thermostatted Column Compartment (G1316A)
- 1200 Thermostatted Column Compartment SL (G1316B)
- 1290 Thermostatted Column Compartment (G1316C)

The Agilent 1200 Series thermostatted column compartment SL (G1316B) can be set between 10 °C and 100 °C and provides post column cooling capability. The Agilent 1100 Series thermostatted column compartment can be set between 10 °C below ambient and 80 °C. The temperature is programmable during the run through a timetable. Column switching valves are programmable from the software.

Valves

The Agilent OpenLAB CDS ChemStation Edition supports external valves as well as thermostatted valves built into the column compartment.

The following external Agilent valves are supported:

- Agilent 1200/1100 Series 6-position/7-port valve (G1156A)
- Agilent 1200 Series 2-position/10-port valve (G1157A)
- Agilent 1200 Series 2-position/6-port (standard) valve (G1158A)
- Agilent 1200 Series 2 position/6-port Valve 600bar (G1158B)
- Agilent 1200 Series 6-position selection valve (G1159A)
- Agilent 1200 Series 12-position/13-port selection valve (G1160A)
- Agilent 1200/1100 Series 2-position/6-port (micro) valve (G1162A)
- Agilent 1100 Series 2-position/10-port (micro) valve (G1163A)

The following thermostatted valves built into the column compartment are supported:

- 2-position/6-port valve option (G1316B# 055) up to 600bar
- 2-position/6-port micro valve option (G1316B # 056) up to 600bar
- 2-position/10-port valve option (G1316B # 057) up to 600bar
- 2-position/6-port valve option (G1316A# 055)
- 2-position/6-port micro valve option (G1316A # 056)
- 2-position/10-port valve option (G1316A # 057)

The maximum number of external valves connected to one Agilent 1200/1100 Series HPLC system is limited to 5 or less, depending on the system configuration. For details please contact your Agilent representative.

Detectors

The following Agilent 1200/1100 detectors are supported:

- 1100 Diode-array Detector (G1315A)
- 1200 Diode-array Detector (G1315B)
- 1260 Diode Array Detector VL+ (G1315C)
- 1260 Diode Array Detector VL (G1315D)
- 1290 Infinity Diode-Array Detector (G4212A)
- 1260 Diode Array Detector (G4212B)
- 1100 Multi-Wavelength Detector (G1365A)
- 1200 Multi-Wavelength Detector (G1365B)
- 1260 Multiple Wavelength Detector (G1365C)
- 1260 Multiple Wavelength Detector VL (G1365D)
- 1100 Variable Wavelength Detector (G1314A)
- 1260 Variable Wavelength Detector VL (G1314B)
- 1260 Variable Wavelength Detector VL+ (G1314C)
- 1200 Series Variable Wavelength Detector (G1314D)
- 1290 Variable Wavelength Detector (G1314E)
- 1260 Variable Wavelength Detector (G1314F)
- 1200 Series Fluorescence Detector (G1321A)
- 1260 Fluorescence Detector (G1321B)
- 1260 Refractive Index Detector (G1362A)
- 1260 Evap. Light-scattering Detector (G4218A)

Spectral data from all diode array detectors may be acquired in a peak-controlled or full acquisition mode.

The Agilent 1200 Series diode array detector (DAD-SL), G1315C, and the Agilent 1200 Series multiple wavelength detector (MWD-SL), G1365C, support 80 Hz full spectral data acquisition. The G1315C and G1365C support up to 80 Hz data acquisition, and G1315D and G1365D support up to 20 Hz data acquisition of up to 8 signals, additional instrument curves and offer data buffering on a built-in Compact Flash Card to provide 'data never lost' insurance. The cells and UV lamp utilize RFID tags to capture and store lamp and cell information. The improved Temperature Management System provides ambient rejection and stable cell temperature.

The Agilent OpenLAB CDS ChemStation Edition software can simultaneously acquire five chromatographic and reference signals each with an independent bandwidth from the Agilent 1100 Series diode-array detector (G1315A or G1315B).

The detectors have a graphical test for signal intensity and wavelength calibration. All DADs may have the initial parameters changed during a run by a time-based program. Users can program wavelength and spectral acquisition mode changes in the time table.

Initial parameters that may be set for the DADs include signal wavelengths and reference wavelengths, spectral acquisition mode, signal sampling rate and autobalance.

The Agilent 1200/1100 Series variable wavelength detector (VWD) may be programmed with a single detection wavelength. Data acquisition rates may be programmed for peak widths from <0.12 up to 8.00 seconds. The VWD can be programmed with a timetable to change the wavelength and perform wavelength scans during the course of an analysis.

The Agilent 1200 Series multiple wavelength detector (MWD-SL), G1365C, can simultaneously acquire up to 8 signals at an 80 Hz data acquisition rate. Data Buffering is possible on a built-in Compact Flash Card providing 'data never lost' insurance. The cells and UV lamp utilize RFID tags to capture and store lamp and cell information. The improved Temperature Management System provides ambient rejection and stable cell temperature.

The Agilent 1200/1100 Series multiple wavelength detector (MWD) (G1365A or G1365B) can simultaneously acquire up to five chromatographic signals each with independent reference wavelengths and bandwidths. The signal acquisition rate may be set for peak widths between 0.1 and 16 seconds. During the course of an analysis the MWD can be programmed with a timetable to change

wavelengths, bandwidths and peak-widths for all five wavelengths.

The optical unit temperature of the Agilent 1200/1100 Series refractive index detector (RID) can be set between 20 and 55°C. The signal acquisition rate may be adjusted for peak widths from <0.12 up to 8 seconds. During the course of an analysis the RID can be programmed with a timetable to change polarity and peakwidth of the acquired chromatographic signal. For diagnostic and troubleshooting purposes, it is possible to store Diode Signal 1, Diode Signal 2, Optical Unit Temperature, Polarity and the Balance Signal in addition to the chromatographic signal.

The Agilent 1100 Series fluorescence detector (FLD) 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 and analyzed as described for DAD spectra. 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 iso-plot or as 3D-graphics.

The Agilent 35900E dual channel interface allows the system to acquire data from detectors that are not interfaced for data acquisition through GP-IB or LAN, 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.

Fraction Collectors

All different versions of the Agilent 1200/1100 Series fraction collectors (G1364A, G1364B, G1364C, G1364D) 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 Agilent 1100 Series Purification system is limited to 3 (with the possibility for one additional recovery fraction collector). Depending on the system configuration up to two Purification systems can be controlled from single OpenLAB CDS ChemStation Edition system (without purification related software add on). Optional add-on software, e.g. Easy Access (G2725AA) provides advanced functionalities for the stand-alone OpenLAB CDS ChemStation Edition workstation.

Compact

The following Agilent 1200/1100 Compact systems are supported:

- 1120 Compact LC HW only (G4286A)
- 1220 LC Isocratic System (G4286B)
- 1120 Compact LC HW only (G4287A)
- 1220 LC System (G4287B)
- 1120 Compact LC HW only (G4288A)
- 1220 LC Gradient System (G4288B)
- 1220 LC Gradient System VL (G4288C)
- 1120 Compact LC HW only (G4289A)
- 1220 LC System (G4289B)
- 1220 LC System VL (G4289C)
- 1120 Compact LC HW only (G4290A)
- 1220 LC Gradient System (G4290B)
- 1220 LC Gradient System VL (G4290C)
- 1220 LC System (G4291B)
- 1220 LC System VL (G4292B)
- 1220 LC System (G4293B)
- 1220 LC System VL (G4293C)

Agilent 1200/1100 Series Instrument Verification

OpenLAB CDS ChemStation Edition for LC includes an instrument operational qualification and performance verification (OQ/PV) view in which users of the Agilent 1200/1100 Series of modules and systems may select a series of semi- or fully-automated tests to test the operational suitability of the LC instrument.

To perform instrument verification it is first necessary to purchase the relevant service from Agilent Technologies. The required method and sequence files will be installed at the time of service delivery by an authorized Agilent service provider.

Agilent 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 1200/1100 Series LC/MSD systems. To control an LC/MSD System, in addition to the OpenLAB CDS ChemStation Edition Workstation (M8301AA) and Instrument Driver for Agilent LC (M8500AA), a 3D UV Add-on (M8360AA) and LC 3D MS Add-on (M8362AA) are required. Together, these software components provide integrated control with a common graphical user interface for all of the Agilent 1200/1100 Series LC modules and systems, including the Agilent 1200 Series DAD as well as the Agilent 1200 Series LC/MSD. In addition to the Agilent 1200 Series family 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 1200/1100 Series LC/MSD system.

LC/MSD 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, which requires the Agilent 1200/1100 Series LC autosampler, the Agilent 1200/1100 Series 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 system includes the ability to do fast scanning of up to 5250 amu/sec and includes autotune for fast scanning. Also included is support of the Agilent Analog Output Accessory which provides up to 12 SIM signals directly to a customer LIMS system.

LC/MSD Tuning

OpenLAB CDS ChemStation Edition for LC/MSD includes a LC/MSD tune view in which users of the Agilent 1200/1100 Series LC/MSD may select to either automatically, or manually tune the instrument. The Agilent 1200/1100 Series LC/MSD integrated calibrant delivery system is software-controlled, and together with the software autotune provides fully automated tuning of the Agilent 1200/1100 Series 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 Agilent 1200/1100 Series LC/MSD.

Agilent 1200/ 1100 Series LC/MSD Instrument Verification

Computer-aided operational qualification and performance verification (OQ/PV) tests and procedures can be used to verify that system performance is acceptable on an ongoing basis. Early maintenance feedback (EMF) tracks the status of system maintenance items and provides notification when a preventive maintenance procedure is due. On-line diagnostics enable system troubleshooting using integrated tests. System logbooks provide date- and time-stamped records of runs, errors, and maintenance events.

To perform instrument verification it is first necessary to purchase the relevant service from Agilent Technologies. The required method and sequence files will be installed at the time of service delivery by an authorized Agilent service provider. Please contact your local Agilent Technologies representative for more details.

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 LC/MSD OpenLAB CDS ChemStation Edition 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 1100 Series 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.

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.

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

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.

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 LC/MSD OpenLAB CDS ChemStation Edition 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.

Agilent 1200 Chip Cube Interface (G4240A)

The Agilent 1200 Chip Cube interface is designed for LC systems using an Agilent Ion Trap MSD as detector and Bruker Software for Data Analysis. OpenLAB CDS ChemStation Edition provides software support for this interface.

Agilent OpenLAB CDS ChemStation Edition for A/D

The OpenLAB CDS ChemStation Edition for A/D and additional A/D interface acquisition module controls and acquires data from the Agilent 35900E dual channel interface. These interfaces allow OpenLAB CDS ChemStation Edition to acquire data from instruments that are not capable of being interfaced for data acquisition through the GP-IB system or LAN. One or two analog signals per instrument may be configured; if only one is used the other is available for use with another instrument running on another timebase. 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.

LC Spectral Evaluation

Using OpenLAB CDS 3D UV Add-on (M8360AA) 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 the 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 the spectra, the spectral differences, the signals, signals 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.

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 the 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 $\pm 5\%$ 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.

Compatible Software Modules

Additional compatible add-on software modules for OpenLAB CDS ChemStation Edition Workstation stand-alone and Networked Workstation without OpenLAB ECM

- Control for CTC PAL Autosampler (G3382AA, G3383AA)
- LC/MS Easy Access (G2725AA)
- LC/MS Deconvolution & Bioanalysis SW (G2720AA)
- LC/MS Trap Software (G2440A, G2450A)
- LC/MS Trap Bioanalysis SW (G1981AA)
- Active Splitter
- SIMDIS Software (G2887BA)
- RTL Pesticide Library (G2081AA)
- Method Scouting Wizard (G2196AA)
- Integrated Headspace Software (G7318AA, G2924AA)
- GC & GC/MS Instrument Utilities (G4600AA)
- Lab Advisor (G4800AA)
- MassHunter Analytical Studio Reviewer Software (G3772AA)
- Agilent LTM Control Software (G6586AA)
- Easy SamplePrep (G7300AA)

Additional compatible add-on software modules for OpenLAB CDS ChemStation Edition Workstation and Networked Workstation with OpenLAB ECM

- Control for CTC PAL Autosampler (G3382AA, G3383AA)
- LC/MS Deconvolution & Bioanalysis SW (G2720AA)
- Active Splitter
- Method Scouting Wizard (G2196AA)
- Integrated Headspace Software (G7318AA, G2924AA)
- GC & GC/MS Instrument Utilities (G4600AA)
- Lab Advisor (G4800AA)
- MassHunter Analytical Studio Reviewer Software (G3772AA)
- Easy Sample Prep (G7300AA)

Additional compatible add-on software modules for OpenLAB CDS ChemStation Edition Distributed System (with OpenLAB ECM)

- Control for CTC PAL Autosampler (G3382AA, G3383AA, LAN-only)
- Method Scouting Wizard (G2196AA)
- Integrated Headspace Software (G7318AA, G2924AA, LAN-only)
- GC & GC/MS Instrument Utilities (G4600AA)
- Lab Advisor (G4800AA)
- Easy Sample Prep (G7300AA)

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

Documentation

Documentation is provided as PDF file on the software disks 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

Installation

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

- Hardware and software requirements: (Hardware and Software Requirements (M8301-90041), Network Requirements Guide (M8301-90051), Supported Instruments and Firmware Guide (M8300-90011)
- Upgrade preparation: Agilent OpenLAB CDS ChemStation Edition Upgrade Preparation Guide (M8301-90031)
- Installation manuals specific to the purchased configuration: Workstation Installation Guide (M8301-90001), Networked Workstation Installation Guide (M8305-90001), Distributed System Installation Guide (M8203-90001), Software License Installation Guide (M8301-90070), Creating OpenLAB Shared Services Databases on Oracle Systems (M8301-90110)
- Instrument installation: (Agilent OpenLAB CDS ChemStation Edition Instrument Configuration Guide (M8300-90001)

Learning and Using

The Agilent OpenLAB CDS ChemStation Edition software includes a task-based tutorial that is built into the online help. This tutorial is designed to let users learn specific topics at their own pace. Each analytical task is divided into a number of clear, guided steps.

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.

Understanding OpenLAB CDS ChemStation Edition

A pair of manuals, Agilent OpenLAB CDS ChemStation Edition Concepts and Workflows (M8301-90011) and Agilent OpenLAB CDS ChemStation Edition Reference to Operation Principles (M8301-90021), 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 Agilent OpenLAB CDS ChemStation Edition with ECM Concepts Guide (M8301-90080) provides additional concepts relating to the combined functionality.

The OpenLAB Report Template Designer Guide (G4635-90007) included on the OpenLAB CDS ChemStation Edition C.01.02 installation media is dedicated to detailed information on creating Intelligent Report templates.

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 Interface, RC .NET Module Driver in OpenLAB CDS ChemStation Edition C.01.02, provides a detailed syntax reference for the instrument control commands.

Interfacing

The Agilent OpenLAB CDS ChemStation Edition XML Connectivity Guide (M8301-90100) 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.

To learn more about OpenLAB CDS, visit us at
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