



Agilent OpenLAB CDS EZChrom Edition for GC, LC, and A/D Instruments

OpenLAB CDS EZChrom Edition A.04.05 OpenLAB Shared Services A.01.05

Functional Design Specification

General Description

Agilent OpenLAB is a family of systems providing analytical information creation and management. Agilent OpenLAB CDS EZChrom Edition provides instrument control, data acquisition, and data evaluation for GC, LC, and A/D instruments from a variety of manufacturers. Data can be stored in centralized file storage or in a database to extend Agilent OpenLAB CDS EZChrom Edition into an analytical information management system.

There are two database options for Agilent OpenLAB CDS EZChrom Edition, Agilent OpenLAB Data Store, and Agilent OpenLAB Enterprise Content Manager (ECM). Both options offer centralized chromatography data storage and retrieval, and the comprehensive security, audit trails, and e-signature authorization required for US FDA 21 CFR part 11 and EU Annex 11 compliance capability.

Agilent OpenLAB Data Store provides:

- Automated workflow scheduling and workflow management
- Efficient laboratory event and asset tracking
- Affordable deployment, administration and maintenance
- Agilent OpenLAB Enterprise Content Manager (ECM):
- Automated file indexing for powerful search capability
- Scheduled storage of files gathered from any vendors instruments or network storage location
- Scalable for enterprise data storage

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.



Agilent OpenLAB CDS EZChrom 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.

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 EZChrom Edition and OpenLAB CDS ChemStation Edition. This specification document covers Agilent OpenLAB CDS EZChrom Edition. Agilent OpenLAB CDS ChemStation Edition is covered in a separate document.

Instruments supported on OpenLAB CDS EZChrom Edition include:

- Agilent 7890A gas chromatograph
- Agilent 7820A gas chromatograph
- Agilent 6890N, 6890 Plus and 6890A gas chromatographs
- Agilent 6850A gas chromatograph
- Agilent 6820A gas chromatograph
- Agilent 5890 gas chromatograph (out of support life)
- Agilent 490 Micro GC
- Inficon 3000 Micro GC
- CTC Autosamplers (Agilent and CTC)
- Agilent 35900E A/D Converter
- Agilent SS420X 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 1120 and 1220 Compact LC systems
- Alltech Associates HPLC Detectors
- Hitachi LaChrom and LaChrom Elite, LaChrom Ultra, and Chromaster HPLCs
- PerkinElmer Nelson Interfaces
- PerkinElmer Series 200 HPLCs
- PerkinElmer Autosystem XL GCs
- Valco Valves
- Varian CP-3800, 3900, and Micro GCs
- Waters Alliance HPLCs

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

- A workstation configuration where an Agilent OpenLAB CDS EZChrom Edition workstation directly controls up to four instruments with 2D detection, or two instruments with 3D detection 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 EZChrom 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) computers 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.

Any of these configurations can be combined with OpenLAB Data Store or OpenLAB ECM to integrate the system with centralized data storage.

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.

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

Network Requirements

General Requirements

OpenLAB CDS EZChrom 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. LAN communication hardware should be 100/1000 or Gigabit speed capable. LAN cards should not be teamed for system communications.

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 is required for all products. WAN's (wide area networks) are not supported.

When using virtual machines as OpenLAB CDS EZChrom Edition clients, AICs, or networked workstations, the network connection must allow access to other system components with no routing between instruments and the instrument controller or workstation.

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

See the Options Installation Guide located on the EZChrom Edition Drivers disk for further information regarding vendor specific instrument connections to an EZChrom edition system.

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 EZChrom 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 EZChrom 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 EZChrom 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 EZChrom Edition is installed, open these firewall ports to allow communication between the system components of OpenLAB CDS EZChrom Edition:

- Port 67 and 68: These ports are used for the receipt and response, respectively, of BootP server communications.
- Port 80: This port is used by OpenLAB Data Store or OpenLAB ECM.
- 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 8084-8089: These ports are used as an alternative to port 8090 if that port is in use by another page or process.
- Port 8090: This port is used to host the viewing page of current license grants and consumptions found in the OpenLAB Control Panel administration interface.
- 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 9753 (default): This port is used for all task-based messaging communication between acquisition controllers and chromatography clients. It is configurable during AIC registration. It is required that all ports designated during AIC registration be opened for access.
- 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, an ISA or 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. Specific instruments may also support SCSI or USB interfaces. Signals from third-party instruments can be acquired via an 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 EZChrom 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 EZChrom 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 vendor's 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 and Software Requirements

Requirements for All OpenLAB CDS Computers

In an OpenLAB CDS EZChrom 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 12x DVD ROM drive.

OpenLAB CDS EZChrom 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. See Network Requirements section for restrictions regarding implementation of virtualized instrument controllers.

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

Minimum Hardware Configurations

The following table lists the minimum hardware configurations for the different computers within an OpenLAB EZChrom CDS system:

Item	Workstation, Client, or EZChrom AIC (Any OS)	Shared Services Server (32- or 64-bit OS)	Data Store Server	
			Entry Level*	High-End*
Processor Speed (CPU)	2 GHz (Windows XP) 3 GHz Dual Core (Windows 7)	3 GHz Dual core	2x (Intel Xeon 2.0 GHz 4 Core) OR 1x (Intel Xeon 3.0 GHz 6 Core)	2x (Intel Xeon 3.0 GHz 4 Core)
Physical memory (RAM)	2 GB (Windows XP) 4 GB (Windows 7 - 32 or 64-bit)	4 GB (32-bit) 6 GB (64-bit)	8 GB (1333 GHz)	12 GB (1333 GHz)
DISK (OS, DB, Indexes for Data Store)	Total 80 GB Available 40 GB	Total 80 GB Available 40 GB	2x (150 GB 7.2 K rpm SATA) RAID 1	2x (250 GB 15 K rpm SCSI) RAID 1
DISK - Data	NA	NA	3x (150 GB 7.2 K rpm SATA) RAID 5	3x (500 GB 7.2 K rpm SATA) RAID 5
Optical Device	DVD ROM (12x)	DVD ROM (12x)	DVD ROM (12x)	DVD ROM (12x)
Network	100/1000 LAN	100/1000 LAN	1 GB	1 GB

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

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

On AIC's with more than 6 instruments, it is recommended to have at least 10 GB of RAM if you plan to work under heavy load (e.g., simultaneous acquisition and reprocessing of long sequences with sequence summary reports).

OpenLAB CDS EZChrom Edition AICs

Agilent Instrument Controllers that support installation of OpenLAB CDS EZChrom Edition :

AIC Model	CPU	RAM	Disk Space
5000	2.8 GHz	2 GB	80 GB
7800	2.3 GHz Dual-Core	2 GB	135 GB
7900	3.0 GHz Dual-Core	2 GB	232 GB (2x116)
8000	3.16 GHz Dual-Core	4 GB	250 GB
Z210	3.10 GHz Quad-Core	4 GB	250 GB
Z220	3.20 GHz Quad-Core	4 GB	250 GB

Revision A and B Agilent instrument controllers are not supported for use with Agilent OpenLAB CDS. AICs must be updated to meet minimum memory requirements as needed.

A limit of 4 instruments with 2D detectors can be configured on a single OpenLAB CDS EZChrom Edition AIC. With 3D detectors such as the LC diode array detector the limit drops to 2 instruments per AIC. LC/MSD, CE and CE/MSD instruments are not supported. Each

instrument can consist of several modules, as in the case of Agilent modular LC systems.
There is no limit to the number of AICs allowed in an OpenLAB CDS EZChrom Edition distributed system.

Operating Systems

The following table lists the Operating systems that are supported for the installation and use of the specified OpenLAB CDS components. This includes support for professional editions and above of the stated operating systems. Home editions of these systems are not supported.

OpenLAB CDS component	Operating System			
	Windows XP SP3	Windows 7 SP1 (32/64bit)	Windows server 2003 R2 SP2	Windows server 2008 R2 SP1
Shared Services Server	N	N	Y	Y
EZChrom Edition Workstation/NWS (includes VL and compact)	Y	Y	N	N
EZChrom Edition Client	Y	Y	Y	Y
EZChrom Edition AIC	Y	Y	Y	Y
Data Store Server	N	N	N	Y
EZChrom Edition Workstation / NWS with OpenLAB Data Analysis	N	Y	N	N
OpenLAB Data Analysis stand-alone Workstation/ NWS	N	Y	N	N

OpenLAB Data Store General Requirements

In order for OpenLAB CDS to use Data Store as a file storage location, and to use the Data Store Lab Applications, you will need the following Data Store product revisions:

- Agilent OpenLAB Data Store A.01.02
- Agilent OpenLAB Data Store Add-in A.01.02

The OpenLAB Data Store server system is installed on the following platforms:

- Windows 2008 R2 SP1 (English, Chinese, and Japanese)
- MS SQL Server 2008 R2 SP1

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 SP1 and the Agilent OpenLAB ECM API v. 1.0.25.x (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 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 Minimum	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 Win7	200 GB
Client	1.5 GHz		512 MB XP 1 GB Win7		40 GB

Application Virtualization/Delivery

OpenLAB CDS Shared Services servers, instrument controllers and client systems can be run on virtual machines that meet the requirements outlined above. Agilent will support vSphere 4.x and vSphere 5.x software for host machines.

OpenLAB CDS EZChrom Edition clients are also supported to run via terminal services and Citrix XenApp 5.x and 6.x.

Other Software

The following software must be installed on any supported operating system prior to installing OpenLAB CDS components:

- Microsoft.Net Framework 3.5 with Service Pack 1 or Microsoft.Net Framework 4.0 (required for OpenLAB Data Analysis)
- Windows Installer 4.5 (required for SQL Installations on Shared Servers and platform updates)
- Adobe Flash must be installed in order to view all graphic features of the Data Store user interface.
- In order to view site prep or administrative reports (such as system reports), you need version XI of Adobe PDF reader.
- If a PDF reader is not installed on your system, you can install Adobe Reader from the OpenLAB CDS installation DVDs. It is available on disk6/Adobe Reader in 4 language versions (English, Japanese, Chinese and Portuguese).
- For Data Store with Lab Applications, Java Runtime Environment Revision 7 Update 11 must be installed separately. It is provided on Disk1\Tools

Language Compatibility

The English version of OpenLAB CDS EZChrom Edition is validated on English and Western European language operating systems.

Localized versions of OpenLAB CDS EZChrom Edition are supported on localized language versions of Windows, using default system fonts (Chinese: SimSun; Japanese: MS UI Gothic; Brazilian Portuguese: MS Sans Serif (Workstations only)).

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

- IEEE-488 GP-IB Support Matrix
- Instruments Supported on GP-IB (not on AICs)
- Agilent 6890 GC
- Agilent 5890 GC
- Agilent Capillary Electrophoresis (CE) G1600
- Agilent Capillary Electrophoresis/Mass Spectrometry (CE/MS)

82350A/B GP-IB Interface Cards

Analytical instruments can communicate with the Agilent OpenLAB CDS EZChrom 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 SB/GP-IB (USB port on PC is used, not on AICs):

- Agilent Capillary Electrophoresis (CE) G1600
- Agilent Capillary Electrophoresis Mass Spectrometry (CE/MS)

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.

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

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.

- 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 G1356C 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)

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 Microsoft TCP/IP protocol needs to be installed and configured as a network protocol on the PC.

The boot strap 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.
- BaseT coaxial cabling with the appropriate tee connectors and terminators can also be used to configure single and multi-instrument systems.

LAN Transmission Rates

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

Printers

The Agilent OpenLAB CDS EZChrom 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 manufacturer's 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 EZChrom Edition on-line sessions.

The Agilent OpenLAB CDS EZChrom Edition has a central print server. The features of the print server are covered in the printers section in OpenLAB Shared Services Control Panel Administration.

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 for configuration of a series of named storage locations to allow organization of method, sequence and data files according to the desired scheme.

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. 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 supported instrument types. An optional contact field offers space for entry of a contact responsible for the instrument. A default project can be selected for the instrument and a checkbox locks the instrument to the default project to ensure all activity on the instrument is saved to the storage locations specified for the project. 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. If the instrument has been in service and data from the instrument is available, the instrument configuration can be retrieved from the data and applied to the new instance. 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 control and data processing are performed through associated OpenLAB CDS EZChrom 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 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.

The Select Printer button allows assignment of a printer to the instrument from the list of printers configured to the print server service. Printers can also be selected for a location and the selection will apply to all instruments within the location.

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.

A Close Connection button can be used to disconnect the session from the associated instrument.

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:

- Name
- Project
- Location
- Application
- Type
- Controller
- Description
- Last Configured By
- Last Configured Time Stamp
- Created Time Stamp
- Used By
- Run Status

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. Unless specific privileges are set for individual instruments, 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 EZChrom Edition sessions can be locked manually or be set to lock based on a timeout after the configured period of user inactivity. Any valid user can open a locked session.

The Timeout period can be set in the OpenLAB Control Panel in the Security Policy section of the Administration view.

Selecting Lock from the Window 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.

Email Notifications

When an email server is configured into the OpenLAB Shared Services Server, notifications can be configured for each instrument so selected events on an instrument will trigger an email message to one or more recipients. When notifications are configured for a location, all instruments within the location will share the notification profile.

When you Edit Notifications for an instrument or location, you create a table where each row defines a triggering event, recipients for the message and an optional Custom Message. The triggering events can be selected from the following list.

- All
- Change
- SequenceStart
- SequenceStop
- CalibrationFailure
- QCFailure
- SystemSuitabilityFailure
- HardwareError
- HardwareNotification

OpenLAB Projects

The Projects view within the OpenLAB Shared Services Control Panel provides for the creation and managements of projects to store all the files associated with analyses performed on the OpenLAB CDS EZChrom Edition. Project definitions contain the storage locations, access privilege profiles, and a detailed set of project options. Projects allow the work performed in your operation to be accessed and stored using a logical organization defined according to individual needs for each department, project or even user. Because each profile has individual option settings, restrictions can be tight or access can be open as needed for each project.

Basic Project Properties

Projects are created and organized with controls very similar to those for instruments. Projects or Project Groups can be created in the project root node of the navigation tree. Project Groups allow projects to be organized and to have common properties and options managed but settings at the group level.

When a project is created it must be given a unique name within the selected location and project folder path. When the storage type is set to the file system, the location of project folders is not restricted as long as the folder is assigned proper access privileges, but it is common to locate the folders within a Projects folder that is automatically created within the EZChrom Enterprise folder. Existing project folder paths may be used but only one project can be assigned to a given project folder path at the same time.

Creation of the project folder also creates the following subfolders; Method, Result, Sample Prep, Sequence and Template to store the corresponding files.

With OpenLAB ECM as the storage type, the project folder is an ECM LCDF storage location within the ECM database. In a similar manner, when Data Store is the storage type, the storage locations are folders within the Data Store database.

An optional project description can be added, typically to indicate the appropriate use or assignment of the project.

Projects can be edited and deleted but deletion of a project does not delete the files in the corresponding project folder.

Privileges and Signature Levels

If users are assigned access roles in the Administration view, these access roles apply to all projects unless inheritance is turned off in Edit Privileges. Users can be assigned specific access roles for individual projects or project groups.

Up to three signature levels; Technician, Shift Supervisor, and Lab Manager, can be enable for any project. Users or User Groups are then assigned to each signature level as appropriate for the project.

A list of predefined reasons for the signature is provided which contains:

- I am the author
- Ready for review
- Reviewed
- Ready for approval
- Approved

Additional user defined reasons can be added. Existing reasons can be deleted and the list can be ordered by moving entries up or down in the list.

EZChrom Project Options

File Locations

When a project is created, a set of default folders within the project folder are created to organize the files for the project. The default folders are; \Method, \Result, \Sequence, \Sample Prep and \Template. These folders cannot be edited within the project.

The Project Options

This section contains a checkbox to enable the saving of all analytical results within the data file, and another to enable users to print results from modified results files on their clients.

Result Set Mode

In File Mode, Data files and PDF reports are saved to a path selected during acquisition or processing. Method, sample prep and report template files are used directly from their original folders. This is the classic approach used in EZChrom prior to OpenLAB CDS EZChrom Edition. This mode requires the storage type to be set to File System and is not compatible with using OpenLAB ECM data storage.

In Result Package Mode, the individual data files, result files and meta-data are stored together in a result package. It is optional but preferable to include method, sample prep and report template files in the result package. This creates a complete and self-contained data package for each acquisition. If the automation or reprocessing modifies the contents of the package, the original methods, sample prep and report template files are unchanged. This allows completed sets to be reopened and examined or processed without affecting current analyses.

When OpenLAB ECM is used for file storage these result packages are zipped and uploaded to the database. Each revision is stored and previous data revisions can be retrieved easily.

For labs with completely automated analysis, checking the option to "Update Original Methods During Acquisition with Analysis Updates" will keep the master methods current with each set of analyses while maintaining the independence of each set for reprocessing.

Audit Trail Settings

Just as with electronic signatures above, a list of reasons can be configured to allow the user to select reasons from a list when making audit entries that prompt for a reason. A single list can be configured for all entries or individual lists can be created for Method, Sequence, Sample Prep, and Advanced Report audit entries.

There is a tab for each audit trail type where you can check an option to allow users to enter their own reason. A second check Automatically Enables the Audit Trail for each new file created. If the audit trail is automatically enabled a radio button allows control of prompting for reasons. The options that can be selected are:

- Prompt for reason at every change (except report templates which change during editing)
- Prompt for reason when saving
- Do not prompt for a reason

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.

Users can select the Change My Password button to set a new password for their account.

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 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
- All 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.

The storage location can be selected to assign the destination of OpenLAB EZChrom data. If EZChrom is not connected to a database the storage can be set to file location or to a network storage location. When OpenLAB Data Store is installed it should be set as the storage location. In a similar way, OpenLAB ECM can be set as the storage location and if OpenLAB ECM is the authentication provider it will also be the storage location.

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

These settings configure the mail settings for the server. An email address for a valid account on the email server must be provided as the From Address. The email server is specified by setting the server URL as the Host. The TCP port for outgoing mail can be set. If Authorization is checked a user name and password can be supplied for authentication of the source of the messages. Once the email server is configured a test email can be sent to an address entered from the test message dialog.

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 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.

With authentication from Windows, the password policies are controlled by the operating system and only the inactivity timeout is configured.

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 EZChrom Edition. Each role may be assigned or removed for the user. More information on roles is provided in the roles section of this document.

For internal users, you can change the user password, set the account so the password cannot be changed, or flag the account so the password must be changed on the next logon.

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 EZChrom 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	EZChrom Analyst
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	✓		✓			
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 EZChrom Edition Method						
Save Method	✓					✓
Edit Method Properties	✓					✓
Open Method	✓					✓

Role Name	Everything	System Administrator	Instrument Administrator	Project Administrator	Instrument User	EZChrom Analyst
OpenLAB CDS EZChrom Edition Method (cont'd)						
Instrument Setup	✓					✓
Integration Events	✓					✓
Peak Groups	✓					✓
Advanced Parameters	✓					✓
Custom Reports	✓					✓
System Suitability	✓					✓
Review Calibration	✓					✓
Calibrate	✓					✓
Edit Running Method	✓					✓
Update Master Method	✓					✓
OpenLAB CDS EZChrom Edition Data						
Save Data	✓					✓
Open Data	✓					✓
Edit Properties	✓					✓
Manual Integration Fixes	✓					✓
OpenLAB CDS EZChrom Edition Sequence						
Open Sequence	✓					✓
Sequence Save	✓					✓
Process Sequence	✓					✓
Sequence Properties	✓					✓
Edit Any Running Sequence	✓					
Edit Own Running Sequence	✓					✓
OpenLAB CDS EZChrom Edition Sample Prep						
Open Sample Prep	✓					✓
Save Sample Prep	✓					✓
Edit Sample Prep Properties	✓					✓
Edit Running Sample Prep	✓					
Update Master Sample Prep	✓					✓
OpenLAB CDS EZChrom Edition Control						
Preview Run	✓					✓
Single Run	✓					✓

OpenLAB CDS EZChrom Edition Control						
Sequence Run	✓					✓
Print Setup	✓					✓
Manual Control (idle only)	✓					✓
Manual Control	✓					✓
Monitor All Data	✓					✓
Abort Any Run	✓					
OpenLAB CDS EZChrom Edition Standard Report						
Add Standard Report Template	✓					✓
OpenLAB CDS EZChrom Edition Instrument						
Modify Instrument Configuration	✓					
OpenLAB CDS EZChrom Edition Advanced/Intelligent Report						
Open Advanced/Intelligent Report	✓					✓
Save Advanced/Intelligent Report	✓					✓

Printers

OpenLAB Shared Services for the EZChrom Edition has a Print Server. When the Printers node is selected a table of printers configured to the Agilent OpenLAB CDS Print Server is displayed. Pressing the Add button opens the print server status and configuration dialog. You can see the status of the print server and start or stop the print server.

When you select Add Monitor you can enter or select a folder for the printer to monitor, a printer from those available to the operating system. Each printer and folder combination can be given a display name and a comment can be entered for the configuration. The print server will print files added to a monitored folder. Folder Monitoring can be turned on or off.

Printer configurations added to the printer server can be selected as the printer assigned to an individual instrument.

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

- Gas chromatography (GC)
- Liquid chromatography (LC)
- Analog data acquisition with external even protocol (A/D)

One OpenLAB CDS EZChrom Edition core license is required for each OpenLAB CDS EZChrom 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 is one add-on license for 3D UV detectors. One of these licenses is required per instrument. Sessions without a 3D UV license will have spectral data processing disabled.

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.

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 Controllers

OpenLAB Shared Services administers instrument controllers. For standalone or networked workstations, the instrument controller is a service on the local PC. 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.

Instrument controllers provide BootP services if needed. 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

Installed Components

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, opens 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 EZChrom 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 standard 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 and holds sample information for the individual samples, references to the method to be used for each injection and specifications for automation.

With the creation of Result Sets enabled, when the acquisition based on the sequence 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. Component Name

Software User Interface

OpenLAB CDS EZChrom Edition User Interface Concepts

The OpenLAB CDS EZChrom Edition user interface is a unified graphical interface that provides direct access to typical analytical tasks and their associated parameters within a single application window. Data and software dialogs open as individual windows within a common workspace.

Access to the task and data windows is provided by three types of controls which can be used interchangeably for most display windows. All windows can be opened from the menus at the top of the application. Most commonly used functions can be opened from a toolbar just below the menus.

A Navigation Pane on the left contains the Navigation Buttons, which organize the task windows and allow rapid switching between analytical tasks. Each button opens an explorer panel which presents tasks and views in tree structures. The selections in the tree are links to specific task windows, to task oriented window arrangements in the workspace, or to items such as report templates.

The following buttons are available; Method, Sequence, Reports, Control, and Views. Method provides direct access to parameters in each section of the current method. Sequence provides the same access for the current sequence. Reports offers direct access to standard report formats to report the current results. Control offers links to instrument and acquisition status. Views provide links to the different data loaded and to displays combining or isolating elements of the data.

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 EZChrom Edition electronically and stored in the signal data file. For detectors without a digital interface to the OpenLAB CDS EZChrom 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 project path on the system. Storage locations can be on the local PC or on a network storage location. Note, however that delay or interruption in access to a storage location can cause data acquisition to fail.

When the storage location is configured to an OpenLAB Data Store or ECM server, the project selected for the instrument in the OpenLAB CDS EZChrom Edition Control Panel allows selection of the location on the server for data storage.

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 aborted. Single runs will stop immediately when aborted. Aborting sequences will halt the current run and pause the current sequence.

Sequences or single injections 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:

- Dark Grey – Offline
- Light 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

The currently loaded method and sequence are displayed in the title bar for the application window.

When an analysis is in progress, the elapsed time is displayed.

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 signals. 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.

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 EZChrom Edition can be used through the offline copy. While acquisition is running, pressing the Analyze button will integrate the signals displayed for the analysis in progress. Data for each completed run is available in offline data analysis.

Data Analysis

Opening Result Sets

The data acquired is stored as individual data files (.DAT) for each injection. When the data is processed an RST file is created with the processing results in format specific to EZChrom and an ACAML (Agilent Common Analytical Markup Language) file in XML result format. When the project is set to file mode, the files reside in a common folder. In result package mode, each sequence creates a folder that contains the data and result files along with methods, sequence and report template files.

OpenLAB CDS EZChrom Edition allows either data to be opened from the File menu or from a dropdown list on the toolbar. Opening data opens the signals from a selected file, a single injection or one injection from a sequence of injections.

The Open Data dialog has data identification and location features. When a data file is selected, the Description button opens a panel with detailed descriptive information for the run. The preview button shows a chromatogram preview, or for 3D data, an isoabsorbance plot. A File Name dropdown menus has the currently selected file and a list of recently opened files.

Search allows files to be filtered based on the sample name and analyst with filters for the acquisition and modification time stamps.

Available time filters are:

- Yesterday
- Today
- Last 7 days
- This Week
- Last 30 Days
- This month
- Any time

Options allow selection of the method to be loaded with the data. Current loads the data without loading a method so the current method is still loaded. From Results loads the method used for the most recent processing. Original/Acquisition opens the method as it was when the data file was created. Results are saved for each processing so when multiple result versions are available the Results to be opened can be selected from a dropdown list. The default is to open the Most Recent results.

A checkbox enables the option to load the Sample Prep with the data.

OpenLAB CDS EZChrom Edition can open data files from a number of manufacturers. The following file type selections are supported:

- SSI (*.dat)
- AIA (*.cdf)
- SSI Ascii (*.asc)
- SAMPL (*.SAMPL)
- BioCAD (*.bxx)
- PE Nelson (*.pts)
- TurboChrom (*.raw)
- ChemStation 32-bit (*.ch)
- ChemStation (*.ch)
- GAML (*.GAML)

Opening a result set loads the signals from first run in the set with the method and sequence from the result set. When results are opened from a sequence, the sequence table can be used to navigate the data set.

Trace Window

When a signal is loaded, it opens in a trace window. If the current run has more than one signal they can be displayed in separate trace windows or together in the same trace window. The title bar of the trace window has the signal definition for the trace. By default, the graph of the trace has both the signal description and the sample name.

The trace cursor is a cross and its X and Y coordinates are displayed in real time at the upper left above the graph of the trace. Left click and drag defines a zoom box on the trace display. Double clicking returns to the last zoom level, double clicking again toggles the zoom level back again. The context menu (right click) has an option to zoom all the way out.

The context menu is a primary access to trace functions. Functions are organized into groups that enable related sets of functions.

Add Trace

Add Trace offers; From Current Data that is another trace from the current data file, From Other Data Files which opens the file selection dialog to add a trace from a different file, or From Method which allows selection of instrument traces such as temperature or pressure if they are available with the current method settings. Clear Overlays removes all of the overlaid signals and returns the display to only the original signal.

Axis Setup

Axis Setup opens the axis settings dialog which has options for the x-axis and left or right y-axis. The scale can be set, the margins for the display, the orientation, and legend options.

Annotation

Annotation opens a dialog controlling the items annotated on the traces. Each trace can be selected individually and its annotation settings controlled separately. A field selector allows selection of the peak values to be used to annotate the peaks. For Instance, you could select Retention Time, ESTD concentration and USP Resolution. The number of digits for the numeric displays can be set.

In the Other section, the following graphical annotations can be turned on or off via a set of checkboxes.

- Baseline
- USP Width
- RT Window
- Undetected Peak Names
- Group Ranges (Peak Groups)

Appearance

Appearance allows selection of colors, line styles and fonts for each element of the trace graph. The settings can be saved as named schemes.

Properties

When the Properties item is selected, a dialog opens combining the trace selection, axis setup, annotation, and appearance settings into a single tabbed settings dialog.

Trace Operations

- The Trace Operations menu items enable mathematical and physical manipulations of signals. The following controls are available:
- Move Signal – prompts the user to click on a signal which they can then drag to move it within the display window to offset or align it with other signals.
- Stack Signals – Prompts the user for an X and/or Y offset to create a stacked display of multiple signals.
- Align – Prompts for selection of an alignment point on each trace. Once the points are selected the traces automatically shift to align the selected points.
- Stretch – Prompts for selection of two points on each signal. The selected points are then aligned by stretching the chromatograms as necessary.
- Normalize – Prompts for the start point and apex of a peak in each signal. Once the points are selected, the chromatograms are sized vertically to normalize the chromatograms based on the selected points.
- Smooth – Mathematically smooths the selected signal
- 1st Derivative – Copies the selected signal and takes the first derivative
- 2nd Derivative – Copies the selected signal and takes the second derivative
- Add, Subtract, Multiply, or Divide – applies the selected mathematical operation to the selected signals

Trace Utilities

Trace Utilities offer three utility operations.

Print – Prints the trace window to the default printer.

Copy to Clipboard – Copies the trace window to the clipboard. The image will appear as it does in the trace window.

Save Trace – The user is prompted to select a trace. The user is then prompted for a file name and a new .DAT file is created containing the selected signal. This function can be used to save mathematically manipulated signals to new files.

Graphical Programming

The menu items under Graphical Programming are for the interactive setting of integration parameters and peak properties. These functions are mirrored in a set of tool buttons at the bottom of the EZChrom application window. The functions in these sections and their application are covered in the sections on integration and calibration.

Integration Task

The OpenLAB CDS EZChrom Edition integrator algorithm is a very sophisticated design tested against a very wide variety of chromatograms to provide, 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 EZChrom Edition integration.

Initial Events –Integration Core Controls

The integration process is controlled by integration events. Integration events may be entered into an integration events table directly or defined using graphical programming to create the events using a cursor to place the events by selections in the trace window. Parameters for graphically placed events are entered or adjusted in pop-up dialog boxes. Events can be set in a table within the method that will be applied to each data file processed using the method or into the MIF table, a table of events stored with each run that can store modified integration events specific to each data file.

The sensitivity of the integration is controlled by the initial threshold and peak width. These values may be set by the operator or tools can

set the values based on the calculated characteristics of the signal over selected time ranges.

Time-Based Integration Events

Graphical programming 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 - Threshold, Width, Shoulder Sensitivity, Minimum Area
- Baseline placement - valley to valley, horizontal baseline, backward horizontal baseline, lowest point horizontal baseline, Disable Peak End Detection, Reset Baseline, Reset Baseline at Valley
- Peak skimming - Tangent Skim, Front Tangent Skim, Exponential Skimming, Front Exponential Skim
- Area summing over selected time ranges using Area Sum ON/OFF events
- Integration through Integration ON/OFF events
- Recognition of negative peaks

Manual Integration

When the integration algorithm is unable to establish the correct baseline or when adjusting the parameters might be too tedious, graphical programming provides tools allowing the operator to draw baselines by selecting points on the chromatogram. The tools allow:

- Manual Baseline
- Force Peak Start
- Force Peak Stop
- Splitting a Peak
- Move Baseline

As each baseline is drawn the event can be placed into the integration event table for the method, in the table for this run only, and an Analyze button updates integration results immediately. Manual baselines are indicated in reports through the use of specific peak-type codes.

Calibration – Peaks/Groups

The Agilent OpenLAB CDS EZChrom Edition calculates quantitative results for peaks defined in the Peaks/Groups table. The Named Peaks tab has a table of individual named peaks identified based on retention time. The Groups tab has a table of grouped peaks which are based on summing peaks over a time range or by combining individual named peaks into groups. The definition of a peaks and groups can be created and managed with graphical programming tools.

The following features are an overview calibration capability and precise details are available in the online help for EZChrom Calibration.

Quantification can be based on peak area or height, and results can be selected for either response mode for each named peak. Groups containing combinations of named peaks must be based on consistent response selections. Calibrations may be multi-level and may include multiple internal standard definitions.

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

- Equal – All calibration points have equal weight in the curve.
- Linear (Amnt) – A calibration point with the amount x has the weighting $1/x$ normalized to the smallest amount so that the largest weight factor is 1. Normalization is done by multiplying the weight with the smallest amount. For example the weight of a calibration point with the amount x is $(1/x) * a$, where a is the smallest amount of the calibrated compound prepared in the calibration standards. If the origin is included it is assigned the mean of the weightings of the other calibration points.
- Linear (Resp) – A calibration point with the response y has the weighting $1/y$ normalized to the smallest response so that the largest weight factor is 1. Normalization is done by multiplying the weight with the smallest response. For example the weight of a calibration point with the amount y is $(1/y) * b$, where b is the response corresponding to the smallest amount of the calibrated compound prepared in the calibration standards. If the origin is included it is assigned the mean of the weightings of the other calibration points.
- Quadratic (Amnt) – A calibration point with the amount x has the weighting $1/x^2$ 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.

For multi-level calibrations the curve can be forced through the origin.

Compounds are identified based on a defined retention time and a retention time window. Compound identification may be refined by defining individual retention time windows. The expected retention time for a peak can be adjusted based on the location of a reference located based on the biggest peak in the defined window. Expected retention time can be updated based on each run or each calibration run or both.

Resolution can be calculated relative to the preceding peak or on any selected peak. Any peak can be designated as the internal standard for any other peak and more than one internal standard can be defined. ISTD calculations based the calculated concentration on the ratio of the responses for the peak and its internal standard and the ratio of the concentrations in the standard.

Fit Type determines how the calibration curve will be fit to the data. There are five choices for how the calibration curves will be drawn: point-to-point, linear, and quadratic, cubic, and Average RF fits. You must have at least two calibration levels for a linear fit (not including zero), three levels for a quadratic and four levels for a cubic fit.

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 unit label can be specified and since all quantitation is based on ratios the units for the standard concentration entered into the calibration table are the units the result is calculated in.

The calibration curve may be scaled for all the compounds or for each compound individually by selecting one of the following calculations; None, 1/Amount, 1/Amount², ln[Amount], 1/ln[Amount], sqrt[Amount], Amount², 1/Response, 1/Response², ln[Response], 1/ln[Response], sqrt[Response], Response², Log (Amount), 1/ log (Amount), log (Response), 1/ log (Response), ln (Amt)&ln(Resp), or log(Amt)&log(Resp)

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.

Groups can also define peak sum ranges for quantitation. Ranges are defined as rows in the table with a start and an end time. Each range can be named.

Once the peaks and groups are defined and standards have been analyzed, the method has been calibrated and the calibration can be reviewed. From Review Calibration, you can:

- Look at the calibration curve for each calibrated peak.
- Change and overlay calibration curve fit types.
- Review the equations for curve fit types, and examine the R-squared (goodness of fit) value for each.
- Temporarily remove points from the calibration curve.
- View response factors, replicate areas, and standard deviation values.
- Use the concentration calculator to calculate amounts from manually entered areas.

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 EZChrom Edition has three types of reporting; Standard reports, Advanced reports, and Intelligent Reporting, an entirely new reporting engine introduced with OpenLAB CDS EZChrom Edition. Intelligent Reporting populates reports with analytical results stored in ACAML format using report templates defined in Microsoft's Report Definition Language (.RDL files).

Quantitation Settings

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 Peaks/Groups table.

5 Multiplier and 5 Dilutors can be entered; both Multiplier will be multiplied with the calculated concentration and Dilutors will be divided. These factors are entered into the sequence table at the time of analysis or later to be applied during reprocessing.

Standard Reporting

When Report is selected in the Method menu, a report template editor opens allowing the user to define the report to be used for the method. Reports can be built from scratch using individual report field or graphic elements selected from the right-click context menu.

Inserting a report opens a predefined section or a wizard to define a section allowing reports to be assembled quickly without tedious field by field definition or programming. The available report tables are:

- Baseline Check Report
- Calibration Info
- Calibration Table
- Data Audit Trail
- Electronic Signatures Table
- Extra Sequence Columns
- Fraction Report
- Generic Report - a report table file that was created by a user program
- Instrument Activity Log
- Instrument Configuration Report
- Library Definition Report
- Library Search Report
- Method Audit Trail
- Method Report
- Purity Report
- Run Report
- Sequence Audit Trail
- Spectrum Report

Importing a report opens a list of the predefined report templates, those included with OpenLAB EZChrom Edition and those defined by the users in the report template editor. Reports provided with EZChrom include a selection of the most commonly used styles including; Area%, External Standard, Internal Standard and Normalized reports. Useful variations are offered such as portrait and landscape orientations.

Advanced Reporting

The Advanced Reporting feature uses a "spreadsheet format" to create customized reports that can include results from across a sequence of injections. Advanced report templates are provided that illustrate the advanced reporting functions and can be modified to create the desired reports. Advanced reports can take the results from a sequence of runs and perform statistical calculations on selected results.

In the Advanced Method parameters there is an Advanced Report Tab that allows selection of an advanced report template, an export path and an automatic file naming mask for the automated export of advanced reports.

Advanced reporting supports templates created in earlier versions of EZChrom but many of the reports which would have been created as an Advanced report before can now be more easily developed as Intelligent Reports.

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 patented extension of the XML (eXtensible Markup Language) standard. 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 EZChrom Edition 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 EZChrom Edition can report at the injection or single sequence level, but when ECM is used as the central data store, OpenLAB Intelligent Reporter can be installed on ECM to extend reporting across your entire data repository.

Intelligent Report Items

Fields can be selected and placed into the template for all result values generated by OpenLAB CDS EZChrom 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 EZChrom 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, an open result set is automatically propagated to the report template editor. 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 or saved as PDF files. For more accurate or complete testing, saved templates can be opened and applied to any dataset available in OpenLAB CDS EZChrom Edition.

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. The report destination can be a printer or a PDF file.

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 EZChrom 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

File Support

The OpenLAB CDS EZChrom Edition can import data files in many formats. The following formats are supported:

- SSI (*.dat)
- AIA (*.cdf)
- SSI ASCII (*.asc)

- SAMPL (*.SAMPL)
- BioCAD (*.bxx)
- PENelson (*.pts)
- TurboChrom (*.raw)
- ChemStation 32-bit (*.ch)
- ChemStation (*.ch)
- GAML (*.GAML)

Data Export

Previewing Intelligent Reports Automated data export can be defined in the Advanced parameters of the OpenLAB CDS EZChrom Edition. Once export is enabled, export can be defined for: AIA (*.cdf)

- Peaks
- Groups
- Standard Reports
- Chromatograms
- Spectrum
- PDA Data

For Peaks and Groups, a dialog allows selection of the fields to be exported, the field separator character and the destination path for the file.

Standard reports offers a list of report templates where each report provides a different selection of results, (Area%, ESTD, ISTD, etc.) to the export file.

Chromatograms can be exported as AIA, ASCII, or ASCII Double.

Spectra can be exported as ASCII, or ASCII Double.

PDA Data can be exported as ASCII 3D, or ASCII Double 3D.

Graphics Export

The Graphics Export tab on the Advanced Method parameters allows definition of the traces to be plotted and formatting options for the plot. The plot is produced and exported as a .WMF file in the specified destination folder.

Customization

Custom Fields

Per sample and per compound custom parameters are available and can be used to enter, store and export information for reporting not defined by standard OpenLAB CDS EZChrom Edition operation. The fields are defined in the advanced method parameters, so fields can be defined differently for each method. Each field has a selectable type to return numeric or text values. Fields have a user defined name.

Field values are filled by a selection of script files or through a user defined script file. The document CDS_EE-script-custom-param.pdf provided in the \Docs folder on disk 6 of the OpenLAB CDS installation media contains a reference guide to EZChrom scripting.

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 EZChrom Edition sequences can assign a different method to the injections on each line in the sequence table.

The acquisition can automatically name data files using a naming mask generated from selected naming elements. The user may select to run full analyses or data acquisition only.

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 not set or is set to Unknown, the injections are treated as unknown samples and are evaluated and reported according to the method specification. When the type is Calibration, samples are used to update the calibration table of the method.

For each calibration injection, the calibration level is selected and the calibration is updated based on the calibration type selected. A calibration injection can clear the calibration for all levels or for the level assigned to the injection. This causes the current injection to calculate a new response factor for each compound on the level. Subsequent injections from the same level average the new response values with the previous calibration information to calculate new response factors based on the average. The average is the average of all calibration injections for the level.

The new sequence wizard provides a simple and rapid way to build the sequence using advanced calibration options. The sample and data file naming can be automated through the use of naming masks including, Line Number, Increment Number, Injection Vial, User Name, Method Name, Instrument Name, Calibration Level, Calibration Set, and Data and Time. The naming of samples and calibration injections can be defined differently.

If Multiple Calibration Sets is selected, a recalibration interval is set and recalibration becomes cyclic where the standard is injected after the defined number of unknown samples has been injected. The sequence can be setup to use one set of vials for all calibration injections or to add a new set of vials interspersed with the samples for each calibration set. When multiple calibration sets are run, update can be set to bracketing, during repossessing. For each bracket interval, the samples can be quantitated based on the average response of the standards immediately before and after the unknown samples in the bracket interval or the bracketing can use all of the calibration injections over the whole sequence.

Special sample types can be used to designate injections for; System Suitability calculations, QC Check Standard calculations, to define the beginning and end of injections to be included in sample summary calculations, and to define Spike Samples and calculate Spike Recovery.

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.

A special Action column allows result based modification of the sequence automation. For each Action entry a Test is selected to be based on Calibration, QC, System Suitability, Hardware Status or Concentration Limit. An entry is also available to perform the action at the selected point in the sequence for Any Condition. The Result field selects whether Pass or Fail triggers the action. The Action can then be selected from; Abort, Pause, Reinject, Run User Program, Run Shutdown, Alarm, Goto, Restart Sys Suit, or Continue. If the action requires additional information, the Parameter field becomes active and appropriate dialogs are made available.

The user can select the columns to be displayed in the sequence table. An anchor can be set to fix the columns to the left of the anchor and scroll only the columns to the right. The individual column widths can be set by clicking and dragging the column boundaries. 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 right click fill-down functions.

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.

Running Partial Sequence

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

Queuing Sequences

Multiple and different sequences can be added to the queue. Additional sequences are added to the end of queue, and the order in which the sequence is run can be changed. Pauses may be added to the queue to cause the execution of the queue to pause and wait for a required operator activity. The queue can then be resumed to perform the remainder of the queued sequences. Sequences or injections can be scheduled to run as soon as the instrument is available or to run at a scheduled time in the future.

New Sequence from Existing Data

When the New Sequence Wizard is run, a selection can be made at the beginning to create the sequence based on existing files rather than creating an acquisition sequence. The dialog allows for browsing the available data and selecting runs for the new sequence. This allows runs originally from different sequences to be combined for reprocessing and reporting.

Sequence Reprocessing

When reprocessing results, the sequence can be used to navigate the data and load individual injections. An individual injection can be analyzed to apply the current processing parameters or the method can be saved and the sequence reprocessed as a whole.

Good Laboratory Practice

OpenLAB CDS EZChrom 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.

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 EZChrom 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.

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 EZChrom 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 EZChrom 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 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 activity log 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 audit trail records the start and end of each individual analysis, and error messages generated within the scope of the sequence. Audit trails can be enabled at the project level to ensure they are enabled for all sequences. 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.

As specified in the project, user may be required to enter reasons for specific changes or activities which will be recorded with the user's identity and a time stamp in the applicable audit trails.

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 or OpenLAB Data Store are 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 database as a new revision. Once the data are stored in the database, each operation that modifies the data will result in a new revision once the data are uploaded again to the database.

A transaction log is maintained in 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 EZChrom Edition may be expanded through the purchase of additional instrument modules 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 EZChrom Edition and GC

The Agilent OpenLAB CDS EZChrom Edition 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 EZChrom 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 EZChrom 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
- Table-driven system scheduler which permits clock time programming for all Agilent 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.
- Capillary columns can be calibrated to properly specify length and diameter for pressure and flow calculations.
- Automatic method transfer from the 6890 to the 7890 GC.

The Agilent OpenLAB CDS EZChrom 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 EZChrom 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 100-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 EZChrom Edition allows random sample access and priority sample injection.

The following autosampler parameters may be controlled:

- number of syringe pumps
- number of syringe washes
- the injection volume
- the bottle number for each injection
- a viscosity delay
- on-column injection setup
- syringe size
- depth of needle penetration
- multiple injections per run in cooperation with PTV for large volume injection
- For the Agilent 7683 Series, plunger speed may be controlled from a maximum of 100 $\mu\text{l}/\text{sec}$ to a minimum of 5 $\mu\text{l}/\text{sec}$ when using a 10 μl syringe.
- For the Agilent 7683B, larger turret for 2x increase in solvent and waste capacity with the 7890A GC.
- For the Agilent 7683B, solvent saver made for 4x increase in solvent usage (6890, 6850 only).
- For large volume injections a 100- μl syringe can be used with the Agilent 7683 Series.

The G1926A bar code reader attachment is supported in the 100-vial tray configuration of the autosampler. The bar code reader 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.

The G2615A bar code reader is used with the 7683 automatic liquid sampler tray.

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 EZChrom 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 EZChrom Edition and LC

The OpenLAB CDS EZChrom 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:

- Standard autosampler (G1313A / G1329A thermostatable with illumination)
- Thermostatted standard autosampler (G1327A)
- High performance autosampler SL (G1367C high pressure compatible with illumination)
- High performance autosampler (G1367B)
- Well-plate autosampler (G1367A)
- 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

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:

- Isocratic pump (G1310A)
- Binary pump (G1312A)
- Binary pump SL (G1312B)
- Quaternary pump (G1354A / G1311A)
- 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)

Valves

The Agilent OpenLAB CDS C EZChrom 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 1200/1100 Series 2-position/10-port valve (G1157A)
- Agilent 1200/1100 Series 2-position/6-port (standard) valve (G1158A)
- Agilent 1200/1100 Series 6-position selection valve (G1159A)
- Agilent 1200/1100 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

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 EZChrom 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.

OpenLAB EZChrom Edition for Other Instruments

OpenLAB CDS EZChrom Edition provides control, data acquisition, and data evaluation capabilities instrument systems from vendors other than Agilent. The information below is current as of the release of this revision, but instrument drivers and supported instruments are made available as the drivers are released. The latest driver packages and their documentation are made available on Agilent's SubscribeNet website. Module by module information along with the required firmware revision and support communication interface is available in the Supported Instruments and Firmware Guide (Manual Part Number M8300-90013). The sections below are an overview of the instrument systems supported by manufacturer.

CTC Analytics LC Injectors

HTC PAL Injection System - G4270-CTC

HTS PAL Injection System - G4271-CTC

Alltech Associates LC Detectors

Evaporative Light Scanning Detector - ELSD-2000

Conductivity Detector - CD-650

Hitachi LaChrom LC

System - D-7000 Interface Module (IFM)

A/D - D-7000

Autosamplers - L7200, L7250

Detector - L7400, L7420, L7450, L7455, L7480, L7485

Oven - L7300

Pump - L7100

Hitachi LaChrom Elite LC

System - USB Interface Board (IFB)

A/D -

Autosamplers - L-2200

Detector - L-2400, L-2420, L2450, L-2455, L2480, L-2485, L-2490

Oven - L-2300, L-2350

Pump - L-2100, L-2130

Hitachi LaChrom Ultra LC

System - USB Interface Board (IFB)

A/D -

Autosamplers - L-2200U

Detector - L-2400U, L-2420U, L-2455U, L2480U

Oven - L-2300, L-2350

Pump - L-2100, L-2130

Hitachi Chromaster LC

System - Interface Control Board (ICB)

Analog Input Device

Autosamplers - 5210

Detector - 5410 UV, 5420 UV-VIS, 5430 Diode Array, 5440 FL, 5450 RI

Oven - 5310

Pump - 5110

PerkinElmer Series 200LC

Autosamplers - Series 200, ISS-200

Detector - Series 200 UV

Pump - Series 200

PerkinElmer Nelson Interfaces

A/D – 760, 940/941A, 950/950A, 960/960A, 970/970A, NCI 901/902

Valco LC Valves

Valve - EMHCA-CE, EMTCA-CE, EMHA-CE

Waters Alliance LC

Integrated LC - 2690 Separations Module, 2695 Separations Module

Detector - 2487 Dual Wavelength Absorbance Detector, 996 PDA, 2996 PDA

Waters Acquity LC

Sample Manager

Sample Organizer

Binary Solvent Manager

Column Manager (CM)

TUV Detector

PDA Detector

PDA Detector eLambda

Fluorescence Detector
ELSD Detector

Waters Acquity H-Class LC

Sample Manager FTN
Sample Organizer
Quaternary Solvent Manager
Column Manager (CM-A)
Column Manager Aux
TUV Detector
PDA Detector
PDA Detector eLambda
Fluorescence Detector
ELSD Detector

PerkinElmer Autosystem XL GC

GC - Autosystem XL
Inlets - Capillary, Programmable On-Column - Inlet Pgm Mode, Programmable On-Column - Oven Track Mode, Programmable Split/
Splitless - Inlet Pgm Mode, Programmable Split/Splitless - Oven Track Mode
Detectors - FID, ECD, TCD, PID
Autosampler - (Built-in)
Other – PPC

Varian CP-3800 GC

GC - CP3800
Detector - FID, ECD, TCD, TSD, uTCD, PFPD
Autosampler - CP8200, CP8400, CP8410

Varian 3900-GC

GC - CP3900
Inlets - Split/Splitless, On Column
Detector - FID, TCD
Autosampler - CP8200, CP8400, CP8410

Varian Micro-GC

CP2002(P), CP2003(P)
CP2003 Quad

Inficon 3000 Micro GC

Micro GC Standard
Micro GC Quad
3000 Micro GC

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 peak
- 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 smoothing, first derivative, and second derivative

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.

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.

The OpenLAB CDS EZChrom Edition allows users to use libraries both interactively and automatically. The OpenLAB CDS EZChrom 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.

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 EZChrom Edition software
- Using OpenLAB CDS EZChrom Edition software
- Customizing OpenLAB CDS EZChrom Edition

Installation

The Agilent OpenLAB CDS EZChrom 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))
- 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)

Learning and Using

The OpenLAB CDS EZChrom 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.

Agilent OpenLAB Chromatography Data System (CDS) EZChrom Edition Users Guide (M8201-90013) provide detailed information about the functionality of the software and way in which the functions are implemented.

The OpenLAB Report Template Designer Guide (G4635-90007) included on the OpenLAB CDS 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 EZChrom Edition, or who want to build in additional features, may implement Quick Launch. Documentation is provided in the Agilent OpenLAB Chromatography Data System (CDS) EZChrom Edition Quick Launch Guide.

Custom parameters, provided by scripting provide a power mechanism for implementing calculations. The Agilent OpenLAB Chromatography Data System (CDS) Scripting Custom Parameters Guide is a detailed reference for programming EZChrom scripts.

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

Microsoft is a U.S. registered trademark
of Microsoft Corporation

Information, descriptions, and specifications in this
publication are subject to change without notice.

© Agilent Technologies, Inc. 2013

Printed in the USA July 3, 2013

5991-2549EN



Agilent Technologies