Agilent OpenLAB CDS
Functional Design Specification

Control for GC, LC, GC/MS-SQ, LC/MS-SQ, A/D and 3rd party Instruments

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1 Introduction

OpenLAB CDS is developed according to the quality process and software lifecycle followed by the Life Science and Chemical Analysis divisions of Agilent Technologies. It has a number of features specifically to help users document that their analyses meet current regulations and quality standards including, but not limited to the Food and Drug Administration’s (FDA) 21 CFR Part 210 (Current Good Manufacturing Practice In Manufacturing, Processing, Packing, Or Holding Of Drugs), 21 CFR Part 211 (Current Good Manufacturing Practice For Finished Pharmaceuticals), 21 CFR Part 58 (Good Laboratory Practice For Nonclinical Laboratory Studies). These features help users validate and specify methods, verify that methods are fit for their intended use, verify system performance and operation and ensure the traceability, integrity and security of the data.

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

- Mandatory login
- Security policies including configurable session locking
- Configurable user roles and privileges
- Full data traceability through audit trails
- Full result data versioning
- Electronic signatures

For those specifically concerned with 21 CFR Part 11 or the European Medicine Agency’s (EMA) Good manufacturing practice (GMP) Guidelines - Annex 11 (Computerised Systems) compliance please consult the white paper on this topic available from Agilent (see section 24.3 at the end of this document).

1.1 Software Development Process and Validation

The Agilent Declaration of Software Quality 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.

1.2 OpenLAB CDS Compliance Services

Agilent offers compliance 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 CrossLab and are delivered by certified support personnel. For more information on Agilent CrossLab Compliance Services please refer to the section 24.3.
2 General Description

2.1 Overview

Agilent OpenLAB is an industry-leading suite of software products designed to capture, analyze and share scientific information throughout its lifecycle, across the laboratory and the enterprise. OpenLAB provides instrument control, data acquisition, data processing, reporting and secure storage for GC, GC/MS-SQ, LC, LC/MS-SQ, A/D and 3rd party instruments.

OpenLAB CDS scales from a single workstation to large client/server systems connecting up to 300 instruments. You can safely archive, store, and share electronic files in a central repository that can meet the needs of all laboratory sizes. It provides the necessary controls for managing system access, data transfer handling and detailed audit trail functionality. OpenLAB CDS ensures secure record keeping, record audit trailing, versioning, as well as provides means for electronic signatures and data archival. The central data repository provides several storage options such as PostgreSQL Server or Microsoft SQL Server or Oracle database.

Agilent OpenLAB CDS uses LAN to communicate between servers, workstations and instruments.

2.2 Supported Instruments

Agilent instruments as well as instruments from other manufacturers are supported on OpenLAB CDS:

Agilent Gas Chromatography:

- Agilent 7890 series gas chromatographs
- Agilent 7820A gas chromatographs
- Agilent 6890 series gas chromatographs
- Agilent 6850 gas chromatographs
- Agilent 490 Micro gas chromatographs
- Agilent 7697A and G1888 Headspace Autosamplers
- Agilent CTC PAL Autosamplers with Agilent GC
- Agilent 35900E series A/D converters

The Agilent 5890 GC can only be controlled via a 35900 series A/D converter.

Agilent Liquid Chromatography:

- Agilent 1260 Infinity LC modules and systems
- Agilent 1290 Infinity LC modules and systems
- Agilent 1100/1200 Series LC modules and systems
- Agilent 1220 Infinity LC systems
- Agilent 1120 and 1220 Compact LC systems
- Agilent CTC PAL Autosamplers with Agilent LC
- Agilent 35900E series A/D converters

Agilent Mass Spectrometry:

- Agilent 6120C/6130C Single Quadrupole LC/MS
- Agilent 5975 Series and 5977 Series Single Quadrupole GC/MS
- Agilent 35900E series A/D converters

In addition OpenLAB CDS supports a wide variety of instruments from other manufacturers. For supported 3rd party manufacturer instrumentation see section 22.4 of this document.
2.3 Configurations

OpenLAB CDS is available in two different topologies:

- Workstation (standalone with local administration and secure local data repository)
- Client/server system with a central administration and secure central data repository

In all cases data is managed in a relational database.

OpenLAB CDS workstations or client/server systems are managed via the OpenLAB Control Panel, which provides:

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

OpenLAB CDS may be installed and configured in two primary configurations:

- A **workstation configuration** where an OpenLAB CDS workstation directly controls up to four instruments. The workstation configuration allows direct control of instruments from a standalone PC workstation without requiring server-based network resources. All data is securely stored in a local secure repository using a relational database.

- A **client/server configuration** where instruments are controlled via dedicated Agilent Instrument Control (AIC) servers and access is provided through OpenLAB CDS clients. Users, instruments and licenses are managed on a central OpenLAB Server. Data is centrally managed in central repository using a relational database. The client/server 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. This central license management on the OpenLAB Server allows for dynamic license allocation.

For more detail see the licensing chapter (chapter 8) of this document.
3 Network Requirements

3.1 General Requirements

OpenLAB CDS systems rely on network infrastructure in order to support the communication between various system nodes. TCP/IP networking in a LAN is required for all products. This communication is based on standard TCP/IP protocols. In order to provide optimum performance and uptime, the network must meet design criteria for available bandwidth, IP address assignment, name resolution and appropriate isolation of the lab subnet from the corporate network. IP v6 is not supported and must be deactivated.

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

WAN’s (wide area networks) are not generally supported. If you plan to implement OpenLAB CDS in a WAN please contact Agilent CrossLab’s Informatics Enterprise Services (IES) for consultancy services.

For more details on the individual topics outlined below please refer to the OpenLAB CDS Requirements Guide (see section 24.4 for the Agilent publication number).

3.2 Instrument Controller Communication

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.

3.3 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 OpenLAB CDS client/server system must reside within the same domain or have the appropriate cross domain trusts to allow name based communications between all components in the system.

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

3.4 Firewall Settings

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

3.5 Environments with Proxy Servers

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

The terminology for computer hardware in client/server 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. The version of Microsoft Windows installed on each machine is assumed to be at least “Professional” and not a starter or home edition. PCs are used for:

- OpenLAB CDS Workstations,
- OpenLAB CDS Clients, and
- OpenLAB CDS Agilent Instrument Control (AIC) servers.

A server is a computer with hardware suitable for continuous service in a client/server environment running a Windows Server operating system. Servers are used only for dedicated OpenLAB Data Store servers.

In most cases the personal computer is interfaced to the analytical instruments through a LAN card, in cases where third party hardware is connected, specific interface cards may be required. Signals from third-party instruments can be acquired via the Agilent 35900E A/D-Converter interface. The separate hardware components that comprise a particular instrument configuration, including third party instrumentation, may need to be coordinated through a remote cabling system for time-critical events such as injection.

The following sections focus on the hardware and software requirements for OpenLAB CDS. For additional information regarding hardware and software requirements please refer to the OpenLAB CDS Requirements Guide. All current OpenLAB CDS manuals with publication numbers are listed in the section 24.4.

4.1  Agilent Original PC Bundles

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

To learn more about the Agilent Original Bundle PC please refer to the technical overview Agilent Technologies Original Bundle PC (please refer to section 24.3 for publication number). Current hardware specifications can also be found at www.agilent.com/chem/bundlePC.

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

4.2  Support for Varying Computer Manufacturers

OpenLAB CDS 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 software mainly on Hewlett Packard equipment. All configuration information listed in the manuals applies to Hewlett-Packard computers and may not be optimized for other vendors’ PCs. For a non-Hewlett-Packard computer, use the setup utility program supplied by the manufacturer to configure your computer. Although the software is also designed to be run on other compatible hardware Agilent Technologies will not necessarily accept responsibility for defects solely observed and reported on third party hardware.

Agilent offers a variety of preconfigured Agilent Original Bundle PCs that provide lots of benefits over computers from other manufacturers. For details refer to section 4.1.
4.3 OpenLAB CDS Workstations

There are two types of workstation hardware configurations – small and standard. Unless otherwise stated, small workstations are tested and supported with any combination of two instruments; standard workstations are tested and supported with any combination of four instruments, both with up to one Headspace or CTC Sampler running simultaneously. LC’s containing DAD and/or FLD count as 2 instruments. Single Quadrupole (SQ) LC/MS or Single Quadrupole GC/MS count as 3 instruments and can only be connected to a standard workstation.

4.4 OpenLAB CDS AICs

In a client/server configuration instruments are controlled via dedicated Agilent Instrument Control (AIC) servers and access is provided through networked clients. In such a configuration a limit of 6 instruments with 2D detectors can be configured on a single OpenLAB CDS AIC. LC’s containing DAD and/or FLD count as 2 instruments. Single Quadrupole (SQ) LC/MS or Single Quadrupole GC/MS count as 3 instruments. With instruments entirely equipped with 3D detectors such as the LC diode array detector the limit therefore drops to 3 instruments per AIC. Similarly, a single AIC can handle up to two LC/MS or GC/MS Single Quadrupole instruments.

5 OpenLAB Server and Database Requirements

OpenLAB CDS manages system information and scientific data in a database on the OpenLAB server. The OpenLAB server can be configured to use an Oracle, Microsoft SQL Server or PostgreSQL database.

OpenLAB CDS includes OpenLAB Data Store as a storage location for scientific data. For Workstations Data Store is installed on every Workstation PC. For client/server system configurations, the Data Store service and database are installed on a dedicated server to ensure acceptable performance of the system.

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

For detailed OpenLAB server requirements please refer to the OpenLAB Data Store Hardware and Software Requirements Guide. All current OpenLAB CDS manuals with publication numbers are listed in the section 24.4.

6 Installation

The OpenLAB Installer is the central utility to prepare, install or uninstall OpenLAB CDS and OpenLAB Data Store. It consists of five panels: Planning, Installation, Recommended Software, Documentation and Online Resources.

The Planning panel gives access to user documentation on

- minimum hardware, software, network and firmware requirements needed to run OpenLAB CDS, and supported instrumentation
- installation, configuration, administration, and maintenance of OpenLAB CDS workstations and client/server systems.

It includes a System Configuration Check that checks the system hardware, operating system and installed software. The OpenLAB Installation Wizard provides for a guided installation of the OpenLAB CDS software suite. At the end of the installation, the Software Verification Tool verifies a successful installation.

The Recommended Software panel comprises software products that are recommended, but not mandatory to use OpenLAB CDS. The Documentation panel provides access to additional documentation and enables the installation of the OpenLAB CDS Help and Learning system on systems that will not be used as an OpenLAB CDS workstation or client.
The following components can be installed by the OpenLAB Installer:

- OpenLAB CDS Workstation (incl. local OpenLAB Server)
- OpenLAB CDS Clients and Instrument Controllers (AICs)
- OpenLAB Server
- OpenLAB Data Store Server

In addition the OpenLAB Installer has the following capabilities:

- **OpenLAB Repair Wizard** – Software installation repair using the repair utility in the maintenance section of the OpenLAB Installer.
- **OpenLAB Uninstall Wizard** – Software uninstallation of OpenLAB CDS.
- **Scripted installation of clients and AICs** – An XML file may be exported at the end of the installer parameter definition which can then be used to install an identical configuration on other computers.

Installation of OpenLAB CDS requires the installer to be logged into the machine as a domain user that is also a local administrator. This enables the OpenLAB CDS Installer to apply network exceptions to the Microsoft Windows firewall under the domain profile which is necessary to configure a functional system.

### 6.1 OpenLAB Configuration

The OpenLAB Configuration tool is used to connect an AIC to the OpenLAB Server and to register it as an instrument controller. It can be used at any time for reconfiguration purposes, for example when an AIC was moved and needs to be registered on a different OpenLAB Server.

### 6.2 Software Verification

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

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

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

### 7 Virtualization

OpenLAB CDS clients (not AICs) can be virtualized on application virtualization platforms like Citrix. VMWare ESX hosted virtual machines are also supported for use as OpenLAB Server systems. Microsoft Terminal Services can be used to remotely access CDS client. Please contact your Agilent support representative for specific requirements and details.

When using virtual machines as OpenLAB CDS clients, the network connections to instruments and application components should be as direct as possible. Each additional router or switch will adversely affect the performance of the entire system.

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

For the virtualization of OpenLAB CDS the participation of a VMWare application expert is strongly recommended. More details are available in the OpenLAB CDS Requirements Guide and the OpenLAB Data Store Hardware and Software Requirements (see chapter 24).
8 OpenLAB Licensing

Agilent OpenLAB CDS supports the use of a central licensing server for the distribution and tracking of license entitlements. FlexNet Publisher is used for this purpose and is installed with the installation of OpenLAB CDS. More details on licenses are provided in section 12.3.9.

9 Language Compatibility

The English version of OpenLAB CDS is validated on Windows English and Western European language operating systems. Localized versions of OpenLAB CDS are supported on localized language versions of Windows, using default system fonts:

- Chinese: SimSun;
- Japanese: MS UI Gothic;
- Brazilian Portuguese: MS Sans Serif.

OpenLAB CDS can run on other language versions of Windows as well, but the user interface will be in English. Non-localized instrument drivers are supported, and will appear in English even when running localized versions of OpenLAB CDS. For details please refer to the OpenLAB CDS Requirements Guide (see section 23.3 for the publication number).

10 Printers

The Agilent OpenLAB CDS 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 locally connected to the computer or connected through a Local Area Network.

Networked printers must be shared by a network server running a network protocol supported by the Microsoft operating system. Agilent recommends similar printer specifications as offered with our software bundle PCs (see www.agilent.com/chem/bundlePC).

Agilent Technologies has not tested all printer and printer driver combinations that are supported in the Windows environment. Print performance and results may vary on other manufacturers’ printers and appropriate drivers.

11 Instrument Communication

OpenLAB CDS provides standard LAN-based communication with the instrument, using TCP/IP. All Agilent instrument hardware that is currently supported by OpenLAB CDS is controlled over LAN. Please refer to the instrument specific sections in chapter 22 for details.

11.1 LAN Interfaces

OpenLAB CDS provides network-based instrument control and data acquisition for network-capable Agilent instruments, optional A/D controllers and 3rd party instruments (for compatibility information please refer to the section 22.4). For general networking requirements see also the chapter 3.

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

For further information please refer to the OpenLAB CDS Requirements Guide (see section 24.4).
11.2 LAN Communication Protocols

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

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

For details please refer to the respective hardware manuals and the OpenLAB CDS Requirements Guide.

11.3 Additional Hardware Required for LAN Instrument Control

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

12 OpenLAB Control Panel

The OpenLAB Control Panel provides access to the instrument management and system administration tools of OpenLAB CDS. All functions in the OpenLAB Control Panel are under system access controls, so the access each user has to the OpenLAB Control Panel is dependent on the roles he has been assigned. The OpenLAB Control Panel connects to the OpenLAB Server which runs the Shared Services application that internally manages the system information.

If access control is not required, the OpenLAB Control Panel can also be used in a mode where user authentication is not enforced. In this mode all functions of OpenLAB Control Panel are available to all users. More details are provided in the section 12.3.

OpenLAB Control Panel functions are divided into views selected through view selection buttons in the lower left pane of the application’s user interface. The Instrument view provides a display of the instruments connected to the system, instrument session launch controls, and tools for configuring and managing instruments. The Administration view provides access to system administration functions. In addition, a Projects view is available for defining project level CDS settings and to configure storage locations for method, sequence and data files according to the desired scheme.

12.1 OpenLAB Control Panel – Instruments

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

12.1.1 The Navigation Pane

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

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

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

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

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

Most current instruments can be configured automatically by providing the IP address of the instrument and waiting for the system to locate and identify the instrument. Once an instrument is identified, it may have modules and associated configuration items that can be accessed by opening each module.

Instrument control and data processing are performed through associated OpenLAB CDS application sessions. For standalone workstations, these sessions are running on the workstation itself and can only be accessed on that workstation. In such a configuration instrument control is restricted to the workstation the instrument was created and configured on. Therefore, this workstation must be running and connected to the instrument whenever data acquisition is active.

With a client/server system, instrument control sessions run on their assigned AICs and an instrument’s session is accessed remotely from any OpenLAB CDS client. 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. Likewise, while an instrument is acquiring data the session can be accessed by another client, for example to schedule a sequence of additional samples and add them to the queue, again without impacting ongoing acquisition.

Users with the Service Instrument privilege can lock instruments to prevent users from starting runs on the instrument, for example during it is serviced. After completion the instrument can be unlocked.

Instruments can be disconnected from OpenLAB Control Panel using the Close Connection function.

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

12.1.3 Instrument Status Displays

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

- Grey – Not Connected
- Green – Connected and Ready
- Yellow – Connected and Not Ready
- Red – Error
- Purple – Prerun or Injecting
- Blue – Running
- Teal – Sleep (7890B GC) or Standby
- Orange – Maintenance Due
By default all status columns are displayed including:

- Name
- Project
- Location
- Application
- Type
- Controller
- Description
- Last Configured By
- Last Configured
- Created
- Used By
- Run Status
- Current Sample

Selecting “Edit Columns” from the toolbar, users may hide table columns that are not of interest or change the order of appearance.

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.

Instruments can be launched from any of the views described above.

### 12.1.4 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. As a result 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 are not automatically applied to a child node. They can be explicitly copied down to the item or set from scratch. Users or User groups can then be assigned or removed and the specific roles added or removed. User privileges are detailed in section 12.3.7.

### 12.1.5 Instrument Session Locking

The OpenLAB Control Panel and the OpenLAB CDS sessions can be locked manually or be set to lock based on a timeout after the configured period of user inactivity. The Timeout period can be set in the OpenLAB Control Panel in the Security Policy section of the Administration view. The operator opening a locked session must supply login credentials based on the authentication configured for the system.

### 12.1.6 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.
12.2 OpenLAB Control Panel – Projects

The Projects view within the OpenLAB Control Panel provides for the creation and managements of projects. Projects store all the files associated with analyses performed with the OpenLAB CDS. 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 just as needed for each individual project. All methods, sequences, analysis templates and report templates required for a given analysis task must reside within the same project.

Selecting a project in the Projects tree will display information on the project in the project window. There are two available tabs, the Project Properties and the CDS Settings tab.

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

12.2.1 Project Properties

Projects are created and organized with controls very similar to those for instruments (including privileges, activity log and desktop shortcuts). 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 by settings at the group level.

When a project is created the storage locations are folders within the Data Store database. The project must be given a unique name within the selected location and project folder path. Existing project folder paths may be used but only one project can be assigned to a given project folder path at the same time.

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

12.2.2 Project CDS Settings

12.2.2.1 Project File Locations

When a project is created, a set of default folders within the project folder is created to organize the files for the project. The default folders are: \Methods, \Results, \Sequences \Analysis Templates, and \Report Templates. These folders cannot be edited within the project once it is created.

12.2.2.2 Project Options

This section contains a checkbox to enable users to print unsaved results on their clients. This setting can be changed by editing the project.

12.2.2.3 Project-wide Audit Trail Settings

A list of reasons can be configured to allow the user to select from when making audit entries that prompt for a reason. A global list applicable to all audit trail types can be configured as well as individual lists for Method, Sequence, and Results audit entries. By editing both, global and individual lists, the system can have a set of common reasons available for all entries as well as individual reasons defined per item.

For each audit trail type the administrator can enable two additional options: to allow users entering their own reason, and to automatically enable the audit trail for any newly created file. For results the “silent” audit trail is always on and cannot be turned off.

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 when saving
• Do not prompt for a reason
12.2.2.4 Project-wide Sample and Compound Custom Parameters

Custom parameters are defined per project. OpenLAB CDS supports two types of custom parameters – Sample Custom Parameters and Compound Custom Parameters. Custom parameters can be completed during sequence submission or after the acquisition in the data analysis client. When setting up custom parameters for a project the administrator has to define the following values:

- **Name** – name of the custom parameter; appears as a label for the custom parameter in the sequence table (acquisition client), the injection list (data analysis client) and reports.
- **Type** – a custom parameter can be of type: Text, Numeric or Date.
- **Default Value** – an optional default value can be set for text or numeric parameters.
- **Mandatory** – completing a custom parameter before sequence submission can be enforced by flagging it as “mandatory”.

12.2.3 Project-wide Privileges

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.

12.2.4 Signature Levels

Up to five signature levels, Technician, Shift Supervisor, Lab Manager, QA Manager and Operations Manager, can be enabled for any project. The default signature level names can be changed. Users or User Groups are then assigned to each signature level as appropriate for the project.

A list of predefined signature meanings is provided which contains:

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

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

12.3 OpenLAB Control Panel – Administration

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

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

12.3.1 My Settings

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

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

“My Settings” is only available when user authentication is enabled.
12.3.2 Local Configuration

This item displays the URL for each available OpenLAB Server. Depending on the system topology the OpenLAB Server may be local or on a central server. For client/server systems, the “Local Configuration” item displays the server selected for the current connection, and the current connection status. The configured server connection can be tested to make sure the server is available.

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 Servers.

12.3.3 System Configuration

12.3.3.1 System Settings

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

- **No Authentication** – eliminates the requirement for users to provide any credentials to access the system. The generic user name SYSTEM will be used for logs and reports.
- **Internal** – the user accounts are created by and stored within OpenLAB Server.
- **Windows Domain** – Domain users and groups defined in the Active Directory services can be granted access to the OpenLAB CDS with the Windows domain controller providing user authentication.
- **Windows Local** – Local Windows users and groups can be granted access to the OpenLAB CDS with the local Windows operating system providing user authentication.

12.3.3.2 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.

12.3.3.3 Email Server

An Email Server can be set up in order to send notification emails:

- **From Address** – the name of a valid email account on your mail server

The following items can be specified for the SMTP (Simple Mail Transfer Protocol) Server:

- **Host** – the URL of the mail server
- **Port** – the TCP port used for outgoing mail.
- **Authorization** – if authorization is required it can be enabled.
- **TLS** – If your email server requires a Transfer Layer Security connection, enable the TLS option.
- **User Name, Password** – If you have enabled Authorization or TLS, enter the User Name and Password required for authorization.

A test message can be sent to verify the Email Server configuration. An email address and message for the recipient has to be created and can be sent.

12.3.4 Security Policy

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

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

12.3.5 Users

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

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

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

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

12.3.7 Roles

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

The tables below list the default roles (Table 1) and privilege groups (Table 2) delivered with OpenLAB CDS. These roles should serve as a starting point and can be modified according to the operation's needs.

Table 1: OpenLAB CDS Roles

<table>
<thead>
<tr>
<th>Role</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Everything</td>
<td>All Privileges</td>
</tr>
<tr>
<td>System Administrator</td>
<td>Manage users and security settings</td>
</tr>
<tr>
<td>Instrument Administrator</td>
<td>Manage instruments and locations</td>
</tr>
<tr>
<td>Project Administrator</td>
<td>Manage projects and project groups</td>
</tr>
<tr>
<td>Instrument User</td>
<td>View and run instruments</td>
</tr>
<tr>
<td>Archivist</td>
<td>Archive and Dearchive content</td>
</tr>
<tr>
<td>Data Store Approver</td>
<td>View, Read, Add, Modify and Sign Content</td>
</tr>
<tr>
<td>Data Store Contributor</td>
<td>View, Read, Add and Modify Content</td>
</tr>
<tr>
<td>Data Store Reader</td>
<td>View and Read Content</td>
</tr>
<tr>
<td>Technician</td>
<td>Laboratory Technician</td>
</tr>
<tr>
<td>Chemist</td>
<td>Analytical Chemist</td>
</tr>
</tbody>
</table>

Table 2: OpenLAB CDS Privilege Groups

<table>
<thead>
<tr>
<th>Privilege Group</th>
<th>Privileges</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acquisition Method</td>
<td>Access to method editing functions, Create and modify acquisition method</td>
</tr>
<tr>
<td>Audit Trail</td>
<td>Access to audit trail related functions, Review audit trail, Add manual audit trail entry, Change method audit trail settings</td>
</tr>
<tr>
<td>Control</td>
<td>Access to instrument control related functions, Manual control (idle only), MS autotune, Abort any running sample, MS autotune and manual tuning</td>
</tr>
<tr>
<td>Data</td>
<td>Access to data related functions, Export data, Import data, Save Reports to disk</td>
</tr>
<tr>
<td>Data Processing</td>
<td>Access to data processing related functions, Do manual compound identification, Reprocess data, Do manual integration, Update master processing method, Create new result set, Launch Custom Calculation Editor</td>
</tr>
<tr>
<td>Data Store</td>
<td>Archive Content</td>
</tr>
<tr>
<td>E-Signature</td>
<td>E-Signature Sign Data Files, E-Signature Revoke</td>
</tr>
<tr>
<td>File and Folder Operations</td>
<td>Access to file and folder delete operations</td>
</tr>
<tr>
<td></td>
<td>Delete analysis templates, Delete methods, Delete report templates</td>
</tr>
</tbody>
</table>
### Table 2: OpenLAB CDS Privilege Groups

<table>
<thead>
<tr>
<th>Privilege Group</th>
<th>Privileges</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Instrument Management</strong></td>
<td>View instrument or location, Manage instrument or location, Manage instrument or location access, Run instrument, Service instrument</td>
</tr>
<tr>
<td><strong>Lock</strong></td>
<td>Lock Results, Unlock Results</td>
</tr>
<tr>
<td><strong>Processing Method</strong></td>
<td>Access to processing method functions, Edit Custom Calculation Parameters, Create processing method, Save master method, Save result set method, Edit sample information, Edit integration parameters, Edit identification parameters, Edit calibration parameters, Edit spectra parameters, Edit system suitability parameters</td>
</tr>
<tr>
<td><strong>Project Management</strong></td>
<td>Project Privilege Group, View project or project group, Manage project or project group, Edit content of project, Manage project or project group access</td>
</tr>
<tr>
<td><strong>Report Template</strong></td>
<td>Access to Report Template Designer, Create report template, Lock/unlock report template items, Validate report template</td>
</tr>
<tr>
<td><strong>Sample Prep</strong></td>
<td>Create and modify sample prep</td>
</tr>
<tr>
<td><strong>Sequence</strong></td>
<td>Access to sequence related functions, Edit users own running sequences, Edit any running sequences, Create and modify sequence</td>
</tr>
<tr>
<td><strong>Sequence Template</strong></td>
<td>Create and modify sequence template</td>
</tr>
<tr>
<td><strong>System Administration</strong></td>
<td>Administration Privilege Group, Manage printers, Edit activity log properties, Create administrative reports, Manage system components, Manage security, Manage instrument controllers, Unlock any locked UI</td>
</tr>
</tbody>
</table>

For further details on assigned privileges per default role please refer to the current guides for installation and configuration (see section 23.3 for more information on available guides and section 24.4 for publication numbers).

#### 12.3.8 Links

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

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

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

#### 12.3.9 Licenses

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

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

The MAC address and name of the current license server are displayed in the user interface. All installed licenses are listed.
OpenLAB CDS provides the following license types:

- OpenLAB CDS Workstation software
- OpenLAB CDS AIC software
- OpenLAB Data Store Server
- Agilent instrument connection for GC, LC, DAD or A/D
- Agilent MS instrument connection
- 3rd-party GC or LC instrument connection

The OpenLAB CDS Workstation license enables acquisition, data analysis and reporting for the following separation techniques:

- Gas chromatography (GC and SQ GC/MS)
- Liquid chromatography (LC and SQ LC/MS)
- Analog data acquisition (A/D)

For instrument control Agilent instrument connection licenses are required in addition.

One “OpenLAB CDS Workstation license” is required for each OpenLAB CDS Workstation PC and is shared by all required instrument sessions residing on the workstation.

A pure data analysis client in a client/server environment requires no particular license.

One “OpenLAB CDS AIC license” is required for each OpenLAB CDS AIC computer and is shared by all required instrument sessions residing on the AIC.

Each Agilent GC, LC, or A/D instrument, or Diode Array Detector requires an instrument connection license. For Agilent MS instrument acquisition an “Agilent MS instrument connection” is required. For 3rd party instrument acquisition a “3rd-party GC or LC instrument connection” is required.

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

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

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

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

For more details related to licenses please refer to the current guides for installation and configuration (see section 23.3 for more information on available guides and section 24.4 for publication numbers).
12.3.10 Instrument Controllers

The OpenLAB Control Panel facilitates the administration of instrument controllers. For standalone workstations, the local PC is the instrument controller. For client/server systems Agilent Instrument Controllers (AICs) run on one or more independent computers.

A status table lists all available instrument controllers. For each instrument controller the table displays:

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

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

12.3.11 Diagnostics

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

12.3.11.2 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

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

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

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

12.3.11.3 Log Files
All local or server log files or a subset of them can be selected and saved for diagnostics, during a support call or for documentation purposes.
12.3.12 Data Store
The synchronization of users, groups and permissions to Data Store can be triggered after the change to immediately enforce the changes.

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

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

The Create Report tool opens the selected report in a viewer. The report can be printed to a printer or saved as a file in .pdf, .xls or .docx format. The Export XML tool saves reports as XML export files.

13 OpenLAB Tools
OpenLAB CDS includes additional tools, the OpenLAB Shared Services Maintenance utility, the MAC Address tool and the File Upload Queue, which are installed with the OpenLAB software and are available from the Windows Start Menu, in the OpenLAB Shared Services program group.

13.1 File Upload Queue
The file upload queue buffers all jobs that are pending for upload to Data Store. It allows privileged users to monitor upload requests, be notified of errors, and access details about such errors. This information can then be used to troubleshoot and fix upload issues. In the event of an upload error a taskbar notification occurs. During a network or server outage pending jobs are securely stored in the queue. A table shows a listing of all pending activities on the AIC with the following details:

- Group
- State
- Source File
- Destination Folder
- File Size
- Submitter
- Submit Date
- Error Message

Additional details are available if needed.
13.2 MAC Address

The MAC Address utility provides a list of MAC addresses for the current computer that can be used for licensing. SubscribeNet requires that one of these be provided for the license server. Clicking one of the addresses copies it to the clipboard, allowing users to paste it into SubscribeNet.

13.3 OpenLAB Shared Services Maintenance

Privileged users may access the OpenLAB Shared Services Maintenance utility. The Activity Log tab is used 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.

The Shared Services database can be backed up or backups can be restored from the Backup and Restore tab. A backup directory and a retention time in days for old backup files can be specified. Available backups are listed in a table sorted by date.

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

The Server Settings tab shows a table listing all configured OpenLAB servers and the default server connection. The content is identical with the Local Configuration in the Administration view of OpenLAB Control Panel (see section 12.3.2). While OpenLAB Control Panel only permits viewing, the maintenance utility enables administrators to edit OpenLAB servers. The default server can be switched, new servers can be added or existing servers edited or deleted. A check mark enables a function allowing users to choose the server during login.

14 OpenLAB CDS Data Model and Definitions

14.1 Methods, Single Samples and Sequences

For a single sample the control file is called “Single Sample”. The system may be set up for automated analysis of a number of samples using the same or different methods. The control file for multiple samples operation is called a sequence and holds sample information for the individual samples, references to the methods to be used for acquisition and processing of each injection and specifications for automating recalibration.

When the acquisition based on the sequence begins, a copy of this sequence and of all required methods are placed into a uniquely named folder, called a “result set”, which also receives all data files and log files thereby creating a result set.

14.2 Method Specification and Use

The Acquisition and Processing methods are the primary instantiation of the analysis procedure in the OpenLAB CDS. The methods are specifically designed to support accurate, complete and secure maintenance of system operating parameters.

The OpenLAB CDS acquisition method fully describes how a particular analysis is performed. It contains all the parameters for instrument control and data acquisition. The processing method specifies all parameters for data evaluation, including integration, quantitation and reporting.

The complete instrument and data analysis specification is stored in a parameter file each, which are again stored in one folder in the storage location. The parameter files are in a proprietary, binary format to prevent editing outside the control of OpenLAB CDS.

The acquisition and processing methods are saved with the data file to record the settings at the time of the analysis.
14.3 Result Set

In the course of automated data acquisition and processing in a sequence, data is written to a Result Set. The result set comprises all data that was used and generated during the sequence:

- raw data,
- acquisition and processing methods,
- report templates,
- Injection list,
- calculated results,
- reports, and
- audit trails (if enabled).

When the data is processed, integration, identification and quantitation results are saved to files in Agilent Common Analytical Markup Language (ACAML) into the result set, thereby creating a self-contained, transportable result set for the entire analytical process.

For a single sample run the results are written to a Single Sample Result. A single sample result only references the master methods and the report template used for the analysis.

15 Software User Interface

OpenLAB CDS consists of three application subsystems that share a common client user interface design:

- OpenLAB CDS Acquisition
- OpenLAB CDS Data Analysis
- OpenLAB CDS Intelligent Reporting

The software has been designed to provide an easy to understand user interface aiding the transition for existing Agilent CDS users and enabling new or occasional users to easily start using the software.

15.1 General Concepts

OpenLAB CDS introduces a new user interface (UI) design concept with focus on ease of learning and work efficiency. A consistent navigation and coloring scheme helps users to find their way; Microsoft ribbon controls make it easy for users to quickly learn how to use the software. The main UI elements are the ribbon toolbar and windows that can be organized in layouts. In some client user interfaces there is an additional navigation pane on the left side of the application window.

15.1.1 Ribbon Toolbar

The ribbon toolbar is a graphical control element that is always shown on top of the application window. The ribbon consists of tabs with graphical controls grouped by functions. Main tabs are always visible (for example the Home tab) giving access to functions which are generally needed. Contextual tabs appear only when a user needs them in a specific context, based on the focused (selected) window.

15.1.2 Layouts and Windows

The workspace consists of single elements called windows organized in layouts. A window is a single UI component available in a certain task context. Windows can have graphical toolbars, context menus or other input elements. Layouts define which windows are shown in the workspace and how they are positioned. Each application provides a set of predefined layouts that can be selected from the Layout ribbon group. Each layout combines the elements required for a particular user task or workflow. Users may design their own layout and organize windows to meet the workflow-specific needs. They may modify predefined or create new layouts. Modifications as well as new layouts are automatically saved per user for future use. Each window can be individually sized and docked within the workspace, either side by side or tabbed. Defaults can be restored at any time.
15.2 OpenLAB CDS Acquisition Client User Interface

The Acquisition subsystem of OpenLAB CDS provides all means for instrument control, automation and monitoring. OpenLAB CDS instrument control is based entirely on RC.Net instrument drivers and supports LC and GC instruments including mass spectrometry based and 3D UV detectors as well as simple time vs. response (A/D converter) detectors, all in a single environment with the same user interface. More details on the supported instrument hardware are provided in the chapter 22.

The system uses a queue based approach that allows multiple analyses to be queued up by different operators. The instrument status window displays the intuitive instrument dashboard consisting of individually dock-able windows, one per instrument module, which graphically show the most important information for each module – even visible from a distance.

The Acquisition client user interface (in the following referred to as “acquisition client”) comprises all workflows related to setting up and running data acquisitions, from simple single sample analyses to complex sequences. It has been designed to provide rapid sequence creation from configurable analysis templates.

In more detail, the acquisition client provides two main Ribbon tabs – File and Home. On the File tab users can create new instrument methods by importing the instrument settings from existing ChemStation or EZChrom methods (see chapter 19 for details). It provides access to the online help system and general information on the acquisition client. A lock function provides the ability to protect the acquisition session window from unauthorized access.

The Home tab hosts the main user interface elements for control, automation and monitoring. It offers 4 different layouts that support users in their daily tasks – “Status” (instrument and queue status monitor), “Method” (method viewing and editing), “Single Sample” and “Sequence” (sequence setup and submission).

The available windows in all layouts are: Activity Log, Instrument Status, Run Queue, Online Signals, Spectrum and Status. Additional windows appear depending on the selected layout and can be added to fill the workspace. These Windows are:

- Method layout – Single Sample Analysis, Sample Prep
- Single Sample layout – Acquisition Method
- Sequence layout – Sequence Creation Template

15.3 OpenLAB CDS Data Analysis Client User Interface

The Data Analysis subsystem of OpenLAB CDS handles the entire data processing workflow – automated processing as part of an acquisition sequence or interactive review and reprocessing using the data analysis client. It has been designed for most efficient data handling, high throughput (fast generation of high quality results) and intuitive use. Innovative data visualization techniques allow for accelerated processing, review and reporting of large numbers of samples.

The Data Analysis client user interface (in the following referred to as “data analysis client”) comprises all workflows related to integration, identification, calibration, quantitation, UV and MS spectral analysis, custom calculations and report generation for single injections or sequences. It automatically adjusts to the type of loaded data (2D signals, 3DUV or MS).

The data analysis client groups functions of the overall workflow into three distinct views:

- Data Selection
- Data Processing
- Reporting

In the Data Selection View users can browse and choose data and methods for review – samples originating from multiple folders, complete result sets, or distinct single samples. Data selected for review and reprocessing is automatically loaded into the Data Processing View, where all data analysis tasks can be performed and the selected data is processed. Processing methods can be developed and stored. In the Reporting View users may interactively create and preview reports with a predefined report template or develop new report templates with the Report Template Editor (see chapters 17 and 18 for more details).
15.3.1 Navigation Pane

The navigation pane mainly consists of a title bar and a navigation tree for the selection of data. Depending on the context additional sections are present, for example for method or report template selection. The navigation pane is always present and located at the left of the application.

Some functions are additionally divided into views. View selection buttons in the lower left part of the navigation pane allow switching between different views. The title bar of the navigation pane shows the name of the currently selected view.

The layout and purpose of the navigation tree depends on the selected view:

- Data Processing: Injection Tree
- Data Selection: Data Selection Tree
- Reporting: Reporting Tree

15.3.2 Data Selection View

In the Data Selection view there are three main Ribbon tabs — File, Home and Export/Import. Similar to the acquisition client, the File tab hosts functions, such as opening, printing or saving existing processing methods or creating new processing methods from scratch or based on MACAML files, or by importing the compound identification settings from ChemStation or EZChrom methods. Results can be saved too. It provides access to the online help system and general information on the data analysis client. A lock function provides the ability to protect the data analysis session window from unauthorized access.

From the Home tab of the Data Selection view users can browse the content of the entire project the session was started from. The navigation pane displays the folder structure of the project in a tree view and provides for the selection of data and browsing of the available sequence templates, methods and report templates in the project. The workspace next to the navigation pane displays a table listing the content of the folder or item selected in the tree. Users may change the order of appearance of the table columns by drag and drop. The latest or an older version of the selected data can be loaded, for single samples the selection can be limited to some or all files in a folder. For methods and templates the table displays the name, the type and last modification date.

The Import/Export tab of the Data Selection view provides functions for the import of ChemStation or EZChrom raw data, the export of selected data to an archive file, the import of archive files and the import of the default report templates into the current project.

15.3.3 Data Processing View

The Data Processing View hosts four main ribbon tabs — File, Home, Processing and Audit/E-Sign. The File tab is identical to the one outlined for the Data Selection view.

All main user interface elements and functions needed for data review and processing are located on the Home tab. It consists of 4 different default layouts targeting different aspects of the review workflow — “Results”, “Chromatograms”, “Compounds” and ”Method”. By default the Layouts contain the following windows:

- Results layout – Chromatograms, Injection Results, Sample Information
- Chromatograms layout – Chromatograms
- Compounds layout – Chromatograms, Injection Results, Peak Details, Calibration Curve
- Method layout – Chromatograms, Processing Method

The data selection in each window is synchronized with the selections in other windows. For example, if a user selects an identified peak in the Chromatograms window:

- the corresponding line will be selected in the compound table of a linked processing method
- the corresponding line will be selected in the Injection Results window
- the peak will be shown in the Peak Details window and highlighted in the Peak Explorer window
- the calibration curve for the corresponding compound will be shown in the Calibration Curve window
- associated UV or MS spectra will be shown in the UV Spectrum and MS Spectrum windows

Vice versa, if a user selects a different compound in another window, the corresponding peak will be selected in the Chromatograms window.
The following additional windows are available, but not included in the default layouts: Acquisition Setpoints, Injection List, and Peak Explorer. The Chromatograms window and Peak Explorer window have their own toolbars with icons. The content of graphical windows such as the Chromatogram window or the Peak Explorer window can be exported to the clipboard or to a file, either as Enhance Meta File (EMF) or Portable Network Graphic (PNG).

Additional injections or methods can be opened or closed from the respective ribbon groups. The data can be reprocessed to apply method changes and new results can be saved to the backend storage as a new version.

Contextual tabs provide additional tools when editing processing methods (e.g. adding compounds or groups to the method), customizing the chromatogram display (e.g. signal scaling or manual operations) or working with Peak Explorer. The same toolset is available in the local toolbars, context menus or other input elements of the windows. The Contextual tabs provide short textual descriptions in addition to the graphical elements, which help novice users finding their way.

The Processing ribbon tab contains three ribbon groups – Methods, Processing and Tools. It combines all tasks associated with reprocessing data. When switching from the Home tab to the Processing tab the current layout is retained. Users can reprocess complete result sets or just selected injections, or requantify injections with the current method. Custom calculations can be created with the Custom Calculation Editor which is launched from the Tools ribbon group.

Users can open and review injection and result set audit trails of the currently selected injection in the Audit/E-Sign tab. Besides the Audit Trails ribbon group there are two others – Signature and Lock Results. They provide means to electronically sign data and lock results.

15.3.4 Reporting View

In the Reporting view there are two main Ribbon tabs – File and Home. The File tab is identical to the one in the Data Selection and Processing views. The Home tab consists of two default layouts, the Report Preview and the Report Editor, each hosting one window of the same name. Users can switch between layouts in the Layouts ribbon group. In addition there are two more ribbon groups: The Reporting ribbon group provides means to save a report in different file formats. It is only active if the Report Preview window is displayed. And the Report Editor ribbon group provides template management tools for to the Report Editor window.

15.4 OpenLAB CDS Intelligent Reporting Client User Interface

The Intelligent Reporting subsystem of OpenLAB CDS 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. The Reporting client is integrated into the Data Analysis client as an additional view. The user interface is described in the previous section 15.3.
16 Data Acquisition

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

16.1 Analysis Control

OpenLAB CDS is specifically designed to facilitate the occasional or new user to rapidly understand the system and become productive in the shortest possible time. The user just has to select which of the 4 discrete screen layouts better suits their needs.

- **Status** – The status layout provides a view of the overall system status: A graphic status monitoring window which supplies the operator with up to the minute information about the instrument, a view of the current Online Signals and Spectrum, if available, and a view of the Run Queue which is controlling the analysis.

- **Method** – This layout provides access to the Acquisition parameters available for the current instrument. These may then be set and saved as an Acquisition Method.

- **Single Sample** – Once you have a method, the Single Sample layout provides simple scheduling of individual samples, viewing the Run Queue, Online Signals and, if available, spectral information.

- **Sequence** – The Sequence Layout allows the operator to create, edit, save and run sequences. Operators may create the new sequence using the sequence table user interface or based on prepared sequence templates that require minimal input. Again the online signal, spectral and queue information is available.

The operator can start a single sample analysis or a sequence controlled analysis. Both are submitted to a queue for the instrument. Sequences and single samples run in the queued order.

Once the analysis has begun and the sequence is controlling the analysis, the system provides the ability to pause the analysis, if needed. If the operator has the appropriate permission a running sequence 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 immediately aborted or paused at the end of the current injection.

The sequence table view provides for monitoring of the sequence progress. The view can be closed to allow for submission of new sequences. From the queue window users can always switch back to view the currently running sequence.
16.2 Instrument Status Monitoring

The status of the instrument is continually monitored and updated on the Status Layout. The instrument dashboard gives a view of the available states of each module of the instrument. Both, setpoints and instrument actuals are available at a glance. Icons reveal more information on installed accessories, such as interface boards, RFID tags or flow cells. If users have appropriate permissions they can also use instrument direct control to help with maintenance tasks.

This layout provides a large single status bar which allows the current instrument status to be viewed from a distance. 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:

- Yellow – Not Ready
- Green – Ready but not running
- Grey – Not connected
- Purple – Pre-run (waiting for injection), Injecting or Post-run
- Blue – Running
- Orange – Tuning
- Teal – Standby
- Red – Instrument Error

Note: The color-coding applies to Agilent RC.NET drivers only. 3rd party RC.NET driver providers might show different colors in their device status.

16.3 Acquisition Methods

OpenLAB CDS acquisition methods include the parameters for all instrument modules associated with the instrument. Users can create new or load existing methods for a launched instrument, make modifications as needed and save the acquisition method with the same name or under a new one. When loading an acquisition method from a different instrument configuration, method parameters get resolved for the new instrument configuration. Since parameters may not be automatically resolvable or default values might be added after the conversion, it is always recommended to review the content of a converted method before using it for new data acquisitions.

In the Acquisition Method layout users can manually download the method to the instrument to prepare it for the next run or sequence. Likewise, the upload of the current method from the instrument to the Acquisition client is possible.

For instrument configuration with an auto sampler an additional window Sample Prep is available. The Sample Prep window hosts the editor for sample preparation methods (formerly known as “Injector Program”). Users can create new or open existing methods, and manually upload a method from or download to an instrument.

16.4 Submission of Single Samples and Sequences to the Run Queue

OpenLAB CDS supports running Single Samples and Sequences. Both are submitted into a run queue. There’s a separate run queue for each instrument which controls all runs for an instrument.

Whenever submitting a Single Sample or a Sequence run the item is first added to the Run Queue and is then automatically started from there. Before starting the run the queue is first validating the submitted jobs. The Run Queue allows users to schedule a whole series of samples and sequences. With the Run Queue, automation of lengthy operations such as overnight or weekend jobs is a simple task.

The minimum that needs to be specified for submitting runs is the acquisition method *.amx (used to acquire the data), the processing method *.pmx (used to process the results and create a report) is optional. If not specified, data acquired will not be analyzed at the end of a run. The data can be processed interactively with the Data Analysis client after the acquisition has completed. If the user doesn’t enter a result path (location where the data file will be saved at the end of the run) or result filename (data file name) the defaults are used.
A series of tokens facilitate naming of both single runs and sequence runs. The tokens are available for sample and data file naming. For single injections data files can be named automatically using simple prefix-counters or pattern based naming using tokens. Users can combine any or all of the following elements:

- Acquisition Method Name
- Instrument Name
- Local Data & Time
- Processing Method name
- Sample name (data file name only)
- Sample Prep Method Name
- Sequence Line number
- Short Local Date & Time
- User name
- Vial number

16.4.1 Submitting Single Sample Runs

The Single Sample Analysis panel consists of four different sections, where the user can enter the required information for a single sample run and submit it to the queue:

- *Run Information section* – This section holds the general sample information: Sample name, Acquisition method (mandatory), Processing method, Result path, Result filename. Provided field tokens help users to simplify data entry.
- *Autosampler section* – This section contains the parameters required to support an automated liquid sampler. For example: Injection source, Injection volume, Vial location, Sample prep method (formerly known as injector program, shown only if applicable).
- *Processing section* – This section is used for quantitative analysis and provides the following input fields: Sample amount, Internal Standard Amounts (up to five ISTDs), Multipliers (up to five injection multipliers), Dilution factors (up to five dilution factors, Target (mass Spectrometry only, used for specifying a formula or molecular mass of a target molecule), Calibration Level.
- *Sample Description* – User may enter a short note or description of the sample being run.

Finally the user selects “Run” to add the single sample run to the run queue. A consistency check is done. If an error prevents the system to submit it into the run queue, this is shown to the user (like “acquisition method can’t be empty”).

16.4.2 Sequence Submission using the Sequence Table

A sequence automates the analysis of multiple samples. The samples to be analyzed are listed in the sequence table. The user has to enter information into the sequence table and then submit it to the run queue which finally executes the sequence.

There are five ways to complete a Sequence table:

- Complete the Sequence table manually
- Load and edit a saved sequence
- Import or drag a *.CSV (Comma Separated Value) or *.TSV (Tab Separated Value) file into the Sequence table
- Import the sequence from an existing result file and reuse it
- Use a predefined sequence template.

For fast and convenient data entry the sequence table user interface can be easily customized by hiding or “pinning” columns, rearranging the order of appearance or resizing columns. These changes are retained per instrument and user and will be provided to the user upon restart of the acquisition client for the instrument. New sequence lines can be inserted after a selected line or added to the end of the sequence table. Redundant sequence lines can be deleted. A “Fill Down” function assists the user in completing the sequence table by automatically filling the entire table, or just a selection of rows or columns based on the content of the first row.
The sequence table provides input fields for the following items for each run in a sequence:

- Sample name
- File name
- Acquisition and processing methods
- Sample type
- Sample amount
- Calibration level
- Run type (for calibration standards only)
- Number of replicated injections (Inj/Vial)
- Vial (injection location)
- Injection source
- Sample Prep Method
- Injection Multiplier 1-5
- Dilution factor 1-5
- ISTD 1-5
- Target 1-5 (MS only)
- Custom parameters
- Sample description
- Bracket (defined in sequence template)
- Expected Barcode (only available for some instrument configurations)

Custom parameters are defined in the OpenLAB Control Panel. In the sequence table they can be filled according to this definition. See section 12.2.2.4 for more details.

The following sample types can be specified in the sequence table:

- **Sample** — sample with unknown amounts to be analyzed. May also include ISTD(s).
- **Calibration Standard** — calibration sample with known amounts for recalibration or update of the calibration table. May include ISTD(s).
- **Blank** — sample without any analytes that is treated like a sample (incl. ISTD). Used as signal-to-noise reference for all subsequent samples and for system suitability calculations.
- **Double Blank** — Same as blank, but does not contain ISTD(s).
- **System Suitability** — this sample type can be used for reporting the suitability of the instrument for use. It is treated like a sample.
- **QC Check** — calibration sample that is treated like a sample to demonstrate that the method is calibrated correctly. May include ISTD(s).
- **Spike** — this sample type can be used for Reporting. It is treated like a sample.

After the editing is completed, the sequence can be saved to the sequence folder under the same or a new name or just submitted to the Run Queue without saving. A copy of the sequence is always stored in the result set, but retaining a copy in the sequence folder is optional by explicitly storing it before selecting “Run”.

Optional is to add barcodes to the sequence table. This is done either by hand, or automatically using the Scan Barcodes option to populate the **Expected Barcode** column with the scanned values.

When enabled in the Run Options of the sequence, the barcode label of the sample vial is automatically scanned before each injection of a running sequence and is compared to the previously entered expected barcode. OpenLAB CDS alerts the user with an error message if the barcodes don’t match. Depending on the run options, the current injection is injected or aborted on barcode mismatch. Both expected and actual barcode are stored with the sample data (see section 17.2.5).

The OpenLAB CDS acquisition subsystem stores barcode values during sequence execution as a means to trace inputs of samples as well as data outputs. This feature is only available if the instrument is configured for Sample Identification (like Agilent GCs, see section 22.1.2.1).
16.4.3 Using Predefined Sequence Templates

Sequence templates are defined in the Sequence Template Creation window. Sequence templates identify the order of runs to be included in a sequence, such as when to process calibration and blank runs and when to process samples. Users can easily apply predefined templates to a provided list of samples or to the empty sequence table.

For example, the sequence template could specify a complex order of calibration standards, QC checks and blank runs with bracketing, and can be applied with a single click. You can only specify bracketing in the sequence creation template.

Users can be even faster to complete their work with using a combined approach. For example, they import sample lines via drag & drop or CSV import, then apply a sequence template to the imported samples and finally submit the sequence to the queue.

From the Run Queue users can view and manage all submitted runs and sequences for an instrument. A separate Run Queue is managed for each instrument. Privileged users may stop, pause, resume, or delete lines from the queue.

In more detail, the queue offers the following options:

- **Stop current run** — the current run is aborted and the next run is started,
- **Stop current run and sequence** — the current sequence is aborted and the next sequence or single run is started,
- **Stop sequence after current run completes** — the sequence is stopped and the next sequence or single run is started,
- **Stop all items submitted by current user** — all current and pending sequences or single runs submitted by the current user are aborted,
- **Stop all** — the complete instrument queue is aborted,
- **Pause / Resume** — pause current sequence or resume paused sequence,
- **Delete** — delete line from queue.

The instrument’s Run Queue display is shown by default in the Status, Single Sample and Sequence layouts. It provides an instant overview of the status of samples queued for the current instrument. In addition the operator may select the current sequence to obtain a detailed, injection-by-injection view of the sequence status.

Selection of a completed sequence in the Run Queue allows single click access to the OpenLAB CDS Data Analysis client for review of the collected data.

The Sequence Editor allows the currently running sequence to be edited to add more samples or remove sample that are pending analysis. The operator may choose to review the samples that have already been acquired with a single click. For example System Suitability samples may be immediately evaluated to ensure the measurement system is suitable for the analysis, rather than waiting until the sequence execution is complete.

A color-coded status for the analysis is displayed either line by line in the Sequence Editor (to distinguish at a glance between completed, running and pending samples) or one sequence at a time in the Run Queue. The following color scheme is applied in the run queue colors:

- light brown — validating,
- grey — pending,
- blue — acquisition,
- light green — processing,
- green — completed,
- red — aborted.
16.5 Signals and Spectrum Online Plots

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 milli Absorbance Units (mAU), Volts (V), degrees Celsius (°C), pico Amps (pA) or bar.

The Signals window may show multiple overlaid chromatographic or instrument curves, which monitor the change of an instrument parameter, such as pressure, over time (depending on the capabilities of the instrument). The user may choose between display modes:

- **Overlaid** – All the signals selected are shown together. Selecting one of the signals displayed will bold that signal line and display that signal’s Y-axis units on the left,
- **By unit** – Signals that are part of the same unit are shown in panels together,
- **Separate** – Each signal is shown in a separate panel.

Users can further adjust the signal display settings to a fixed range per axis and signal.

If the instrument generates spectral information e.g. mass spectrum or UV spectrum this may be viewed in a Spectrum window in real time as the analysis proceeds. For UV detection it shows absorbance as a function of the wavelength in a continuously updated display. Users can adjust both the displayed wavelength range (in nm) and the absorbance scale (in mAU). For MS detection the online spectra monitor displays the abundance as a function of the m/z range with the same means for adjustment.

Both, Signals and Spectrum window have a zoom capability and the cursor may be used to display a specific signal’s response at any point in time. Users may enlarge the real time plot by clicking and dragging a zoom area one or multiple times. Zoom steps are easily undone using double-clicks.

16.6 Acquisition Resilience during Network Interruption

In case the connection between Acquisition server and the OpenLAB server gets interrupted, the acquisition will continue to run. All pending instrument run queue items (sequences and single runs) that were scheduled up to the point of interruption will get completed on the AIC without any potential for data loss. Acquired data and calculated results will be securely stored in a protected location on the AIC. The buffered data will automatically upload to the OpenLAB Data Store server when the connection to the central storage is re-established. Precondition for taking advantage of the described safeguarding against failure is a stable, isolated LAN connection between the AIC and the instruments.

16.7 Data Review During Acquisition

Data from any completed injection of a running sequence may be reviewed in the Data Analysis while the remaining injections continue to be acquired. The full range of capabilities of OpenLAB CDS Data Analysis is transparently available for the review. The user simply needs to right click on the completed run he or she wishes to review and select the review option.
17  Data Processing

The data acquired with OpenLAB CDS is processed automatically during sequence execution or interactively with the Data Analysis client. The OpenLAB Data Analysis offers extensive review capabilities for GC and LC data facilitating the use of the same integration, calculation, calibration and reporting across the entire laboratory. The OpenLAB Data Analysis offers 3D capabilities to further analyze data generated by a Diode Array Detector (DAD) or Mass-Selective Detector (MSD). For backwards compatibility it can also process data originating from OpenLAB CDS EZChrom Edition and ChemStation Edition.

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

17.1  Selecting and Loading Data

The OpenLAB CDS Data Analysis client opens in the Data Selection view when it is launched from the Projects view in the OpenLAB Control Panel or from the respective desktop shortcut. The user can browse the content of the entire project in the navigation pane and select the data of interest for review. The user can load an entire sequence (result set) or a choice of single injections from a single folder. To load multiple single injections from different folders, the load operation has to be repeated multiple times, once per folder. Multiple result sets or single runs can be opened and reviewed in parallel. If a result set has been processed before, the user can choose whether to load the most current version (default) or an earlier version of the data. The application automatically switches to the Processing view when the data is selected and loaded.

Alternatively, users can choose to review a just completed sequence or completed injections of a running sequence from the Acquisition client. In this case the Data Analysis client already opens in the Data Processing view with the chosen data loaded.

If no processing method was assigned during sequence or sample submission, the user can create a new method before starting the review or just load the data without linking a method to it. A wizard facilitates the choice of the appropriate default parameter set to start from.

The user can choose whether to just link the method to the data or immediately reprocess the data with the selected default parameter set.

17.1.1 Injection Tree

In the data processing view, the injection tree displays the loaded injections in a hierarchical tree. It shows the sequence names, sample names and data file names of the injections. For each injection users can expand the available signals to see more details. Extracted spectra, if available, will also appear in this section.

The tree is grouped by sequence or sample, where the grouping nodes are alphabetically sorted by name. The injections in each node are sorted by sample order number, injection order number, and acquisition date/time. The sort order can be expanded to include the injector source.

Symbols next to the injections reveal additional information regarding the status of the injection. This includes processing status, method linkage, the presence of manual integrations and warnings. The following symbols are used in this context:

- The data is linked to the selected processing method.
- Manual integration has been added to the data.
- The data file could not be reprocessed. There is no processing method linked to the data file.
- Warnings occurred during reprocessing.
- Reprocessing has been stopped, or an error occurred.
- The data file has successfully been reprocessed

Below the injection tree the Signal Selection area (also referred to as Signal Selector) shows all signals of all injections in the injection tree. The signals are alphabetically ordered by detector. If the user changes the signal selection, the content of the different windows is automatically updated.
Below the signal selector the Instrument Traces area lists all instrument traces such as pressure, solvent ratio, or temperature, that have been recorded during data acquisition. The list contains all available traces for all currently loaded injections. The selected instrument traces are shown in the Chromatograms window and are handled the same way as signals. By default no instrument traces are enabled.

The Methods area (also referred to as Method Selector) lists all methods associated with the loaded data. The methods are arranged in alphabetical order. When selecting an injection with a linked method, the method is automatically selected and marked in the method selector. If the user opens another method or creates a new one it additionally appears in the method selector.

### 17.1.2 Creating new result sets

Users can easily create new result sets from the loaded injections, either as a subset of a sequence of injections or a combination of selected injections from one or more sequences and single runs. After selecting the injections the user can assign a processing method to the new result set and save it to the data backend under a new name. Typical use cases for self-assembled result sets are:

- Combining a sequence of calibration samples with a sequence of samples (unknowns) for results calculation,
- Applying custom calculations to a set of samples from different sources.

### 17.2 Data Review

In the default Results layout users can do a first review of data. When selecting an injection in the injection tree or from the injection list, a concise summary is shown to the user with chromatograms, sample information, and injection results. The injection list table additionally provides an overview of all loaded single injections or all injections in the selected results set. All windows are synchronized with the data selection in the navigation tree.

#### 17.2.1 Chromatograms

A graph with one or more chromatographic signals from the selected injection is displayed in the Chromatograms window. The graph is annotated with sample name, signal name and data file name.

The Chromatograms window displays all signals and instrument traces belonging to the focused injection. To zoom into a specific section of a chromatogram, the user simply drags the mouse over the required section. To move the x- or y-axis, it is sufficient to grab the axis and move the mouse. For better overview a Zoom Overview Window can be enabled. This additional window will always display the entire chromatogram with the zoomed section annotated as a red rectangle. It is shown in the upper right corner of the Chromatogram graph.

Users may stepwise zoom into a chromatogram and zoom out of it. If several chromatograms are loaded, the zooming area can be automatically applied to the other loaded chromatograms as well. To do so, the user first defines which axes are linked and in a second step zooms into the area of interest. The link is applicable to the x- or y-axis, or to both axes.

The Signal Selector in the navigation pane shows all signals of all injections in the injection tree. To show or hide particular signals in the Chromatograms window the user can check or uncheck them in the signal selector. The signals can be displayed all separated, all overlaid, overlaid per detector, overlaid per sample, or in a stacked mode (overlaid with an offset). Instrument traces can be enabled or disabled for display in the same way as signals.

All integrated peaks are annotated. Identified compounds are labeled with their compound names and retention times. For not identified compounds, only the retention times are shown. Annotations can be customized to include additional information.

There are further scaling options to adjust the display. These include the same scale globally for all graphs, individual scales per graph or normalized scales where each signal is displayed using its own signal maximum (100%).

The scaling options interact with the different display modes. For particular use cases custom scaling provides more sophisticated scaling capabilities:

- **Ignore n largest peaks**

  This option can be useful, for example, for GC chromatograms, where the solvent peak is integrated and the sample peaks are located on the shoulder of the solvent peak. It can also be useful if the overall baseline is rising or going down to a great extent.
17.2.1.2 Scale to fraction of \( n \)th largest peak
This option can be useful, for example, for GC chromatograms where the solvent peak is not integrated: With the option Ignore \( n \) largest peaks, the system would not ignore the solvent peak, as it is not integrated and therefore not recognized as a peak. In this example, scaling to the largest integrated peak would be the most suitable option.

17.2.1.3 Scale to baseline (ignore all identified peaks)
The system ignores all integrated peaks. Only the baseline signal is considered for the custom scaling. This option can be useful to examine the baseline, or to check if there are any not identified peaks that are not, but should have been, integrated.

17.2.2 Sample Information
The Sample Information window is structured in three sections — sequence, sample and injection. It provides all information that was entered during single sample or sequence submission and meta data generated by the system, such as operator or date and time stamps.

In more detail, the Sequence Information lists all sequence-related information:
- **Name** — Name of the result set (sequence).
- **Description** — Description of the result set as entered in the sequence properties.
- **Creation date** — Date and time when the sequence or result set was created.
- **Created by** — User name of the user who created the sequence or result set.
- **Modification date** — Date and time when the sequence or result set was last modified.
- **Modified by** — User name of the user who last modified the sequence or result set.

The Sample Information section contains all data related to the sample:
- **Name** — Name of the sample as entered in the sequence table or single sample analysis window.
- **Description** — Description of the sample as entered in the sequence table.
- **Type** — Defines the type of sample for data analysis (e.g. Sample, Control, Calibration).
- **Level** — If the sample is a ‘Calibration’ type, this value shows the defined calibration level of the calibration curve.
- **Sample Amount** — Amount of analyzed sample as entered in the sequence table.
- **Multiplier** — Injection level multiplication factors as entered in the sequence table per sample; up to five injection multipliers are displayed, separated by semicolon.
- **Dilution factor** — Dilution factors as entered in the sequence table per sample; up to five dilution factors separated by semicolon.
- **Order No.** — Order number of the sample in the sequence (sequence line).
- **Injector position** — Position of the injector on the instrument; only available for specific instrument configurations; can be "undefined"
- **Acquisition method** — Name of the acquisition method.
- **Replicate number** — Injection count of total number of injections per sample.
- **Vial** — Vial number or plate location.
- **Volume** — Injection volume as defined in the acquisition method.

The Injection Information section lists all data related to the injection:
- **Data file** — Name of the data file.
- **Injection date** — Date and time when the sample was injected.
- **Acquisition operator** — User name of user who created the data.
- **Instrument name** — Name of the instrument as configured in the software.
- **Actual injection volume** — Injection volume as injected.
- **Modification date** — Date and time when the injection was last modified.
- **Modified by** — User name of user who last modified the injection.
- **Processing method** — Name of the processing (data analysis) method.
- **Method modification date** — Date and time when the method was last modified.
17.2.3 Acquisition Setpoints

The Acquisition Setpoints window shows all available information on the data acquisition method of the focused injection. The information, for example oven temperature or flow rate, is read from the method defined in the acquisition client. The availability of information and the degree of detail depends on the origin of the data. For example, data imported from the Multi-technique ChemStation does not include any acquisition information.

17.2.4 Injection Results

The Injection Results window consists of two tabs, the Peaks tab and the Summary tab. The Peaks tab contains the results table of the focused injection, including the custom calculation results for peaks, groups, or compounds. The Summary tab displays the custom calculation results for signals of the focused injection and results calculated across multiple injections of the whole result set. Custom calculations are described in detail in section 17.3.9.

The Peaks tab lists the calculated integration results by peak. The table can be easily customized by hiding columns, rearranging the order of appearance or resizing columns. The following list shows examples for columns that can be configured for the injection results table. A complete list of all available columns is documented in the Online help system of OpenLAB CDS.

- **Peak#** — index of the peak according to its retention time.
- **Name** — compound name, empty if the peak is not identified.
- **Signal description** — name of the signal on which the peak is integrated.
- **RT (min)** — peak retention time, corresponds to the time at the peak apex.
- **Area** — peak area, area between the signal and the baseline between the two peak edges (peak start and stop markers).
- **Area%** — relative area of the peak (in %) to the area sum of all peaks in the integrated signal.
- **Height** — peak height, difference between the value of the signal at the apex of the peak and the value of the baseline at the same time.
- **Height%** — relative height of the peak (in %) to the height sum of all peaks in the integrated signal.
- **Width** — peak width as estimated by the selected integrator.
- **Amount** — amount and unit of the compound as calculated from the calibration curve (before applying any multipliers and factors).
- **Concentration** — concentration (with unit) or mass percentage, of the compound after applying injection multipliers, compound multiplier and factors.
- **RF** — calculated response factor (RF) of the compound. See section 17.3.5 for more details.
- **Start time (min)** — time at the beginning of the peak (in minutes).
- **End time (min)** — time at the end of the peak (in minutes).
- **UV Conf. Match Factor** — number indicating the similarity of the current peak’s apex spectrum with the UV reference spectrum (0 = no match, 1000 = identical). See section 17.4 for details.
- **UV Purity** — number indicating the UV purity of the current peak (0 = surely impure, 1000 = most likely pure). See section 17.4 for details.

17.2.5 Injection List

The Injection List window displays a table with all injections that are part of the selected item in the navigation tree:

- For a result set, the window lists all injections of this result set.
- For one or more single samples, the window lists all loaded single sample injections.

The details on the available injections are shown in this table. Each row represents an injection. Like any other table, it can be easily customized by hiding columns, rearranging the order of appearance or resizing columns. The following columns are available:

- **Order number**
- **Injection number** — Injection count of total number of injections per sample
- **Sample name**
- **Sample type** — see section 16.4.2 to read more about the available sample types.
- **Bracket** — Shows how calibration standards are bracketed according to the selected Bracketing mode, see also section 17.3.5.3.
- **Run type** — for calibration samples only. Determines how calibration points are calculated when processing the standard.
- **Calibration level**
- **Injection date**
- **Modification date** – Date when the injection was last processed.
- **Sample amount**
- **ISTD amount** – ISTD amount as entered in the sequence table (up to 5), but can be modified for a single injection afterwards.
- **Multipliers** – Can be modified for a single injection afterwards. Used to calculate the concentration for all compounds; up to five multipliers are displayed.
- **Dilution factors** – Can be modified for a single injection afterwards. Used to calculate concentration for all compounds.
- **Acquisition method**
- **Processing method**
- **Sample description**
- **Vial number or plate location**
- **Injector position**
- **Data file name**
- **LIMS ID** – Keys required for connection from and to a LIMS system.
- **Barcode** – Barcode label as it has been automatically read from the sample vial during a sequence run (read only). It is only filled when this feature was enabled in the run options of the sequence.
- **Expected barcode** – The expected barcode is filled in during sequence creation, either by hand or automatically using the “Scan Barcodes” option.
- **Compound amounts** – The compound amount is defined in the calibration parameters in the method, but may be adjusted for individual injections. When clicking in the Compound amounts column of a calibration standard, part of the window shows the actual amounts in the sample and the amounts defined in the method.
- **Target** – For mass spectrometry: Masses or formulas (up to 5) that are used for the MS sample purity calculation.
- **Custom Parameters** – If custom parameters have been configured for the project, values can be viewed and edited here. The Sample Custom Parameters are shown in the corresponding table column just like any other sample-related information. Clicking on the Compound Custom Parameters column shows the corresponding parameters and values in a separate part of the window. Custom parameters are described in detail in section 12.2.2.4.

### 17.2.6 Viewing and Comparing Chromatograms

The default Chromatograms layout provides for a visual inspection and comparison of multiple injections. The scaling and zooming options offer many options for comparing single peaks or entire chromatograms. The chromatograms may come from different injections, from different samples, or even from different sequences.

By pinning two or more injections in the navigation tree these can be compared in the Chromatograms window. The appearance can be easily changed from the toolbar. The following display modes are available:

- **Separate** – each chromatogram is shown separately
- **Overlaid** – all chromatograms are overlaid in a single graph
- **By detector** – the chromatograms are displayed in one graphs per detector
- **By sample** – the chromatograms are displayed in one graph per sample
- **By Signal name** – the chromatograms are displayed in one graph per signal
- **By injection** – the chromatograms are displayed in one graph per injection

There are several scaling options to further adjust the display. These include the same scale globally for all graphs, individual scales per graph or normalized scales where each signal is displayed using its own signal maximum (100%).

If the injections contain more than one signal or additional instrument traces, the displayed items can be limited by unchecking signals or traces that are not of interest in the signal selector or trace selector in the navigation pane.
For comparison with other injections the user can step through the injections in the navigation tree while the pinned injections will persist in the Chromatograms window.

Chromatograms can be easily zoomed by dragging a rectangle across the area to be zoomed in the chromatogram. For the display mode Separated only the selected chromatogram will be zoomed. The x-or y-axes of the chromatograms can be linked with the buttons Link x-axes over panes or Link the y-axes over panes, respectively. Linked axes will all be zoomed automatically if one chromatogram is zoomed. The same linkage occurs automatically if the display mode is switched from Separated to Overlaid. A zoom region is also kept when selecting a different injection. This allows users to zoom into a specific region and then review injection by injection without a need for repetitive zooming.

For chromatograms originating from different detectors a delay of specific signals can be adjusted using the signal alignment defined in the processing method.

### 17.2.7 Viewing and Comparing Results

The Data Analysis client of OpenLAB CDS is perfectly suited for the fast review of large numbers of samples. The content of the windows is always synchronized. For example, the data selection in the Injection List window is synchronized with the injections selected in the Chromatograms window or the navigation tree. When a peak is selected in the Chromatogram, the corresponding line in the Injection Results window is automatically highlighted.

The synchronization of the windows facilitates the comparison of results from different injections. When a particular peak is selected for an injection in the Chromatograms window (or Injection Results window) and another injection is chosen for display, the system will automatically highlight the corresponding peak in the injection results of in the new focused injection, if it exists.

### 17.2.8 Peak Details

The Peak Details window shows an enlarged representation of the peak currently selected in the chromatogram or injection results table. It includes details on the peak such as time, area, height, and compound name, Due to its size the user can easily check the peak’s appearance. The header of the window shows the sample name, the name of the data file, and the signal. If calculated, the window includes UV purity information or system suitability annotations. Both are enabled in the processing method.

With the arrows to the left and right of the peak, you can navigate to the previous or to the next peak in the chromatogram. The peak selection is synchronized with the selections in other windows.

### 17.2.9 Peak Explorer

The Peak Explorer is a tool perfectly suited for the review of sequences with a large number of samples. For such sequences, a chromatogram in the display mode Overlaid may not be helpful any more. With a rising number of signal traces it becomes close to impossible to identify the single graphs. Users would still see, for example, that retention times are varying, but not, whether a systematic shift is underlying.

The Peak Explorer provides an overview of retention times and peak sizes in the form of a bubble chart. The y-axis shows the currently loaded injections, as a function of the retention time (x-axis). The injections appear from top to bottom in the same order as in the injection tree. For each peak in an injection a bubble is plotted on an invisible horizontal line corresponding to that injection (y-value) and at the retention time of the peak (x-value). The bubble size represents a value related to the peak size. When zooming in, details can be inspected and artefacts such as a systematic shift become visible. The injections and peaks selected in the Peak Explorer are synchronized with the data selections in other windows. For example, if a user selects an injection in the injection tree, this injection is also highlighted in the Peak Explorer.
The Peak Explorer window is enabled from the ribbon toolbar. The Peak Explorer diagram shows all loaded sequences and single runs with one bubble diagram per selected signal. If pinning is used, only the currently selected injection and all pinned injections are shown. The bubble size can relate to a choice of different peak values, which is picked from the Peak Explorer toolbar:

- Area
- Height
- Area%
- Height%
- Width
- Amount
- Concentration

Users may toggle between seeing identified peaks, not identified peaks, or both, in the diagram. The bubbles are displayed in different colors for identified and not identified peaks. When hovering over a bubble, a tool tip will display results associated with the peak, if available. The tool tip contains compound name, amount and concentration for identified peaks; retention time, area, height, area%, height%, peak width, peak start, and peak end as determined by the selected integrator for both identified and unidentified peaks.

To choose a peak and view the details in another window, users can simply click the bubble. This enables them to immediately inspect deviations for their potential root cause, for example a bad integration becomes immediately visible in the Peak Details window.

17.3 Processing Data

The Processing ribbon tab provides the necessary toolset for reprocessing data. Users can reprocess all loaded or just selected injections, or requantify selected injections (no update to integration, identification and calibration). Single injection reports are automatically generated, when this function is enabled and reporting is turned on in the method. Further, the user can choose to retain or clear manual corrections, such as manual integration or compound identification corrections, during reprocessing.

The data must be reprocessed in order to apply any method changes. Such changes can be for example modified integration or calibration parameters or custom calculations. Methods can be loaded, edited and immediately applied to verify the impact. Method changes can be saved to the result set method as well as to the master method. Processing Log files are created and can be viewed.

17.3.1 Processing Methods

Processing methods are used in the Data Analysis context. They contain the information and parameters needed to process the data and generate results. A processing method must be linked to the data in order to apply its parameters during reprocessing. When linking data to a processing method, the data is reprocessed automatically.

The Processing Method window consists of a method navigator on the left and a parameter screen on the right. The method name displays above the navigation element. Adjacent to the method name, a link symbol shows if this method is linked to an injection. When a user selects an item from the navigator on the left, the corresponding information appears on the right. Depending on its nature this may be one or more checkmarks, radio buttons or selection boxes, or tables with entry fields. Sometimes the information is arranged in multiple tabs. To edit the parameters in this window, a user needs the corresponding privileges.

The processing method is broken down into several sections:
17.3.1.1  General
The general section hosts method information and global method settings. It consists of two sub sets, the Properties and Signals. Under Properties users may provide a description and view general information on the processing method such as the file location, version, creation date, modification date, or name of the users who created or last modified the method. The method audit trail viewer is accessible from here.

There is a choice of two different integrators, the ChemStation or EZChrom integrator. Both integrators can be equally well used to automatically locate peaks in a signal and calculate their sizes. The integrators provide the same integration algorithms as available in earlier versions of OpenLAB CDS, namely OpenLAB CDS ChemStation Edition and OpenLAB CDS EZChrom Edition. The processing method supports all the initial and timed events from ChemStation or EZChrom. In each method, users must select the integrator that they want to use.

Under Signals, users can adjust the delay of specific detectors in order to align their signals in the Chromatograms window. The delay is automatically calculated from the entered retention time for a particular peak.

17.3.1.2  Extraction
Users may specify the parameters for Extracted Ion Chromatograms (EICs), Mass Spectra and UV spectra. The extraction section is only applicable to 3D UV or MS data. The settings apply to both: manual workflows like spectra extraction as well as automated workflows like EIC extraction. For more details please refer to the sections 17.4 and 17.5.

17.3.1.3  MS Sample Purity
All parameters related to the calculation of the MS sample purity are set in the MS Sample Purity Properties. For more details, please refer to section 17.5.3.

17.3.1.4  Integration Events
In the Integration Events section users may configure integration events as required for the analysis. This includes adding or deleting timed integration events or configuring signal-specific integration parameters. For more details please refer to the section 17.3.3.

17.3.1.5  Compounds
The Compounds section contains all parameters related to compound identification, calibration, quantitation and spectral confirmation. This includes the use of references as well as grouping. For more details please refer to the sections 17.3.4 and 17.3.5.

17.3.1.6  System Suitability
The calculation of column performance and noise can be enabled and required parameters defined in the System Suitability section. Users may choose which calculation formulas are applied, based on the European Pharmacopeia (EP), Japanese Pharmacopoeia (JP) or United States Pharmacopeia (USP) requirements. Please refer to section 17.3.8 for details.

17.3.1.7  Tools
The tools section provides means to embed or link one or more Custom Calculations to a method. More details about custom calculations are given in the section 17.3.9.

17.3.1.8  Reports
Under Injection Report users may specify the Report template and Report destination for automatically created injection reports. Up to two different injection reports per injection can be created automatically. Reports can be printed to a printer or file. The available file formats are: PDF (*.pdf), Excel Workbook (*.xls), Word document (*.doc), or plain text (*.txt). The file-based report is automatically stored with the data. A copy may be additionally saved to a specified storage location (folder) in the backend storage or on the Windows file system.
17.3.2 Creating new Processing Methods

A new processing method is always based on a fixed configuration. The user can select from four predefined method configurations that represent different application areas. Based on the choice certain sections of the method are visible and editable in the Processing Method window. The available choices are:

- **GC/LC Area Percent** – for qualitative GC/LC analysis
- **GC/LC Quantitative** – adds the calibration method section to enable quantitative analysis
- **3D UV Quantitative** – adds method sections related to UV spectra extraction, UV impurity checking and UV spectral confirmation
- **MS** – adds method sections related to MS spectra extraction and MS Library Search
- **LC/MS Sample Purity** – adds method sections related to LC/MS Sample Purity. This configuration doesn’t have method sections related to calibration, MS Library Search and System Suitability.

During method creation the fixed configurations are listed including the available method sections for each method configuration. The MS method configuration corresponds to a method “super set” and contains all method sections apart from LC/MS Sample Purity. To use a method section that is not present in the currently loaded method a new method has to be created from an appropriate configuration that includes this section. The table details the default parameter sets provided in the method configurator.

<table>
<thead>
<tr>
<th>Method Configuration</th>
<th>GC/LC Area Percent</th>
<th>GC/LC Quantitative</th>
<th>3D UV Quantitative</th>
<th>MS</th>
<th>LC/MS Sample Purity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Integration and Area% / Height% Calculations</td>
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<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
</tr>
<tr>
<td>Manual UV Spectra Extraction</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
</tr>
<tr>
<td>Manual MS Spectra Extraction</td>
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<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
</tr>
<tr>
<td>MS Sample Purity</td>
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<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
</tr>
<tr>
<td>Compound Identification</td>
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<td>✔️</td>
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</tr>
<tr>
<td>Calibration</td>
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<td>✔️</td>
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<td>✔️</td>
<td>✔️</td>
</tr>
<tr>
<td>UV Impurity Check &amp; Spectra Confirmation</td>
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<td>✔️</td>
<td>✔️</td>
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</tr>
<tr>
<td>MS Library Search</td>
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<tr>
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<tr>
<td>Custom Calculation</td>
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<tr>
<td>Reporting</td>
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<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
</tr>
</tbody>
</table>
17.3.3 Integration

Two integrators are available for use in the Data Analysis — the ChemStation and the EZChrom Integrator. Which integrator is applied is defined per method. Depending on the choice, the processing method will contain and apply the integration parameter set of the ChemStation or EZChrom integrator.

With integration events, users can configure how the signals are integrated at specific time ranges. The method can include one set of global integration events and a signal-specific set for each available signal. Global integration events are used for all signals that have no signal-specific events defined in the method.

Users can add, change or delete integration events in two different ways:

- By adding, editing or deleting the values in the integration events table in the linked processing method, or
- Graphically, by adding, editing or moving events in the chromatogram with the mouse pointer.

To work graphically users need to enable the functions for displaying and changing timed events in the Chromatograms window properties. Additional annotation options for integration events allow further extending or reducing the degree of detail shown in the Chromatograms window.

17.3.3.1 ChemStation Integrator

The ChemStation integrator provides a large set of standard integration events complemented by some advanced events for tangent skimming and baseline correction.

The Standard integration events are either signal-specific or global and consist of two groups:

- **Initial events** are those that apply from the start of integration. These events cannot be deleted, but may be changed. There are only few initial events.
- **Timed events** take place after the start of integration. Timed events may change the value of an initial event, or may switch on or off additional integration parameters.

All available standard integration events are listed below. If not otherwise noted, they are of type “timed”.

- Slope sensitivity (initial and timed)
- Peak width (initial)
- Area reject (initial and timed)
- Height reject (initial and timed)
- Shoulders mode (initial and timed)
  - Drop
  - Tangential
- Area sum (On/Off)
- Area sum slice
- Auto peak width
- Baseline at valleys (On/Off)
- Baseline backwards
• Baseline hold
• Baseline next valley
• Baseline now
• Detect shoulders (On/Off)
• Fixed peak width
• Maximum area
• Maximum height
• Negative peak (On/Off)
• Set baseline from range
• Set low baseline from range
• Slope sensitivity
• Solvent peak
• Split peak
• Tail tangent skim (On/Off)
• Tangent skim mode
  ○ Exponential
  ○ New exponential
  ○ Standard
  ○ Straight
• Unassigned peaks
• Use baseline from range

The *Advanced* integration events always apply to all signals:

• Tangent skim mode (for modes see above)
• Tail skim height ratio
• Front skim height ratio
• Skim valley ratio
• Baseline correction mode
  ○ Classical
  ○ No penetrations
  ○ Advanced
• Peak-to-Valley ratio

More details are given in the *OpenLAB CDS Data Analysis reference guide* (reference information on the principles of calculations) or the online help ("How To"), see chapter 23.
17.3.3.2 EZChrom Integrator

There are different types of integration events. For some events only a time range with start and stop time is required, during which the parameter is active. For others, users can define a specific value to be used from a start time or during a time range.

The available integration events are:

- Width
- Threshold
- Shoulder sensitivity
- Integration off
- Valley to valley
- Horizontal baseline
- Backward horizontal baseline
- Lowest point horizontal baseline
- Tangent skim
- Front tangent skim
- Exponential skim
- Front exponential skim
- Minimum area
- Negative peak
- Disable end of peak detection
- Manual baseline
- Manual peak
- Split peak
- Force peak start / Force peak end
- Reset baseline
- Reset baseline at valley
- Maximum area
- Maximum height

More details are given in the OpenLAB CDS Data Analysis reference guide (reference information on the principles of calculations) or online help (“How To”), see chapter 23.
17.3.3.3 Manual Integration

Manual integration is especially helpful when dealing with complex chromatograms and many not baseline-separated peaks. In such cases, the automatic integration may not easily lead to the desired quality of integration. OpenLAB CDS Data Analysis uses a unique approach to manual integration. A single context sensitive tool, the Integration Wheel, provides all means for the manual correction of the integration. It replaces traditional toolbars by a more intuitive practice. Manual integration is activated by selecting the corresponding button from the Chromatograms window toolbar or activating it from the Manual operation ribbon group in the Chromatograms contextual tab.

Peak integration adjustments are achieved by simply dragging and moving baseline points. The Integration Wheel automatically offers the right toolset for a particular integration problem and allows an easy selection of the possible options. The Integration Wheel appears automatically when the user moves the mouse pointer close to a baseline start/end point or to the connection point of a drop line with a baseline segment. It consists of several colored segments. Each of these segments is associated with a specific action that is possible for the active baseline point. Visual feedback is continuously given to indicate what tool is active and what part of the data will be modified by the currently active tool.

Many of the manual integration tools interact with attractors. Attractors are usually visible on the signal and at baseline points of the adjacent elements. They are indicated by four small arrows. When the cursor approaches an attractor, it will automatically snap to the attractor. This allows to position new elements directly on the signal or directly attached to adjacent baseline segments.

Depending on the type of baseline point (for example, end point of a baseline segment, drop point on a baseline segment etc.), the integration tools offered within the Integration Wheel will vary. The system automatically offers the tools which are appropriate to use for the selected baseline point. The available manual integration tools are:

- New baseline
- New nested baseline
- Merge baseline segments
- Merge peaks
- Delete peaks
- Delete range
- Change baseline type
- Move baseline point
- Move common baseline point
- Move drop line
- New connected baseline
- Split peaks
- Select peak

Some tools are part of the integration wheel, some not. When manual integration is enabled, the manual integration tools are automatically activated by moving the mouse pointer over the chromatogram. Approaching a peak apex, baseline point or baseline segment without any integrated peak, from a particular angle with the mouse cursor will reveal a suitable tool or the Integration Wheel with all appropriate options. For example, The New baseline tool is automatically activated, when moving the mouse pointer below the signal in an area without any integrated peaks.
17.3.4 Peak Identification

Peak identification determines the compounds in an unknown sample based on their chromatographic characteristics. The identification of these compounds is a mandatory step if the analytical method requires quantitation. If not required, processing methods may also be created without identification or quantitation steps.

The characteristics (e.g. expected retention time) of each compound of interest are stored in the compound table for identification, which is part of the compound section of the processing method. The peak identification process compares each peak in the signal with the peaks stored in the compound table.

The identification is based on

• expected retention time,
• absolute retention time window, and
• relative retention time window in %,

all of which are specified in the compound table. The final retention time window is the sum of relative and absolute windows, applied symmetrically to the expected retention time.

If multiple peaks are within the determined retention time window, there are different peak matching criteria that may be applied to identify the correct peak (first peak, last peak, closest peak, largest area or height). If an unambiguous assignment is not possible (e.g. no or more than one peak in the time window fulfills the criteria), none of the peaks will be identified and a warning will be written into the processing log.

Users may enter the expected retention time as absolute time value or calculated from a relative retention time. Time reference compounds may be used to correct the expected retention times based on possible shifts observed by specific reference compounds.

For details on the peak identification capabilities of OpenLAB CDS (such as calculations) please refer to the OpenLAB CDS Data Analysis reference guide (reference information on the principles of calculations) or the online help (“How To”), see chapter 23.

17.3.4.1 Relative Retention Times (RRT)

The retention time of a compound is compared to the retention time of a reference. The ratio of the two retention times is the RRT, normally a known or previously determined number.

OpenLAB CDS supports the use of relative retention times to determine the expected retention times of compounds or timed groups. In addition at least one RRT reference compound is required. Compounds are marked as RRT reference compounds in the compound identification table of the processing method. The expected retention time of an associated compound or timed group is calculated from its RRT value and the expected retention time of the RRT reference compound.

RRT values themselves have no impact on peak identification. Only the calculated absolute retention time values (possibly corrected by a time reference) are used.

17.3.4.2 Using Time Reference Compounds

To adjust for possible retention time shifts OpenLAB CDS supports the use of one or more time reference compounds to correct the absolute retention time window based on a shift of the selected time reference compound. Compounds can be marked as time reference compounds in the compound identification table of the processing method. For each non-reference compound the user chooses a time reference to be used for the correction of the peak’s expected retention time.

The extent of correction can be adjusted per compound by an individual correction factor. The calculation of the updated expected retention time of a compound is done by adding the shift, determined from the time reference and multiplied by the user-defined individual correction factor, to the expected retention time.

For timed groups, the expected start and stop times are calculated accordingly.

If time reference compounds are used with RRT reference compounds, the retention time shift is applied to the RRT reference compound. If internal standards and time reference compounds are used the internal standards are by default set as time reference compounds.
17.3.4.3 Retention Time Updates in the Processing Method

As retention times may shift in the course of a sequence, the data analysis subsystem provides means for the consecutive update of retention times in the processing method. Based on the selected retention time update type (*Never*, *After each run*, or *After calibration standards*), the expected retention times of all or selected identified compounds or timed groups in the processing method are automatically updated after the corrected expected retention times have been calculated. If the compound can be found based on the corrected value, the corrected value becomes the new expected value in the method.

To correct the expected retention times, the application uses the current retention time to calculate the shift to the expected retention time. This shift, multiplied by a user-defined weighting factor, is added to the expected retention time. The weighting factor is a compound-specific percentage value that is specified in the compound identification table.

In addition to updating the retention times during the run, users can also manually shift all retention times by a given value. This is done by specifying an absolute and relative (%) value for the shift in the contextual ribbon tab.

17.3.4.4 Named and Timed Groups

OpenLAB CDS provides grouping as a means for quantifying one or more segments in a chromatogram as a single entity. A group may consist of one or more time regions – forming a timed group, or of a set of identified peaks, or timed groups, or a combination of both – forming a named group.

A timed group is defined on a specific signal. The overall area and height of the group are calculated by summing the area and height of all peaks included in the time regions. Users may define in the processing method whether to include or exclude identified peaks. The expected retention time of the group is for sorting purposes only and can be entered manually.

A timed group is treated like any other compound during calibration and quantitation. Optionally peaks contained in a group can be individually quantified in addition to the group quantitation. If a peak belongs to several groups, or if identified peaks are quantified as part of the group, the following rules will apply:

- If an unknown peak belongs to several groups, it is quantified with the response factor of the group with the smallest retention time.
- If an identified peak is quantified as part of the group, but has its own calibration parameters defined, it is quantified with its own response factor and not with the group response factor.
- If an identified peak is quantified as part of the group and has no specific calibration parameters defined, the compound is quantified with the group response factor. The response type (area or height) of the group is used.

The following parameters can be edited for timed groups:

- Include identified peaks
- Quantify each peak individually
- Region start
- Region stop
- RRT start (if applicable).
- RRT end (if applicable).

A named group may consist of user-selected compounds and timed groups. Each compound or timed group is identified and quantified on its own. ESTD and ISTD calculations are based on the calibration data of the individual compounds. The calculated group area, height, amount, and concentration of the group are the sum of the individual areas, heights, amounts, and concentrations. The named group itself is not calibrated. One compound can be in multiple named groups.

The following parameters can be edited for named groups:

- Assign compound to a named group.
- Name of the group.
- Retention time (RT) of the group (used for sorting purposes only).
17.3.4.5 Compound Identification Table
The compound table in the peak identification sub set of the processing method displays the following columns:

- **Order number** – order number of the compound (as sorted by retention time).
- **Icon** – indicator whether the compound is an internal or external standard, a normal or time reference compound, or a group compound.
- **Name** – name of the compound.
- **Signal** – detector signal used to identify and quantify the compound.
- **Is time ref.** – set the compound as a time reference compound.
- **Associated time ref.** – name of the associated time reference compound.
- **Factor** – correction factor applied to the shift that is calculated for the time reference compound.
- **Is RRT ref.** – set the compound as an RRT reference compound.
- **Associated RRT reference** – name of the associated RRT reference compound.
- **Exp. RT** – expected retention time of the compound.
- **RRT** – relative retention time (RRT).
- **Absolute RT Window (min)** – window in minutes around the expected retention time.
- **Relative RT Window (%)** – window in percent (%) around the expected retention time.
- **RT Update** – set the mode of the automated RT update.
- **Peak match** – relevant if there is more than one peak in the retention time window.

The compound table is synchronized with other windows. For example, selecting a compound in the table highlights the corresponding peak with its annotations in the corresponding chromatogram. At the same time the Peak Details window and the Calibration Curve window show information related to the peak or compound.

Depending on the Chromatograms window properties the graphs are annotated with information related to peak identification: For expected compounds or timed groups the compound or group name, name of associated signal, the retention time (RT) window, in which the compound is expected, and the name of the processing method can be added as annotations to the peaks or peak groups. The RT window is shown as two dashed lines at the beginning and end of the RT window. If the Chromatograms window shows several graphs for different injections, the annotations can be optionally restricted to the focused injection only. Users can select to draw a border around the annotated peak identification information to delimit it from other information in the chromatogram.

17.3.5 Calibration
After the peaks have been integrated and identified, the calibration transforms the measured responses into amounts. For the quantitative analysis the method is calibrated with calibration standard that contain the compounds with known amounts.

The following calibration modes are available for quantitation and can be selected per compound:

- **Curve** – Compound specific calibration using External Standard Calibration (ESTD) or Internal Standard Calibration (ISTD).
- **Reference** – Indirect quantitation using a calibration or response factor from another compound or group, and
- **Manual Factor** – Fixed response factor.

For using another compound’s calibration curve the applicable reference calibration curve must be selected from the curves stored in the method. This is done by selecting the calibration mode “Reference” and the suitable calibrated compound as Curve Reference in the compound calibration table. The response factor of the reference can be adjusted by applying an optional response correction factor which is specific to a compound.

OpenLAB CDS enables single level as well as multi-level calibrations. There is one global number of calibration levels defined per processing method (up to 99 levels are theoretically possible). Based on this selection the compound table of the calibration subset is automatically populated with the corresponding number of columns, one per level. The user calibrates each calibration level by processing the corresponding calibration sample.

All calculation formulae are documented in the OpenLAB CDS Data Analysis reference guide as well as in the calibration section of the Calculations and Background References chapter of the context-sensitive OpenLAB CDS Online Help (see also chapter 23 of this document).
17.3.5.1 Compound Calibration Table

The compound table in the calibration subset of the processing method can display the following columns:

- **Order number** – Order number of the compound (as sorted by retention time).
- **Type** – Icon indicating whether it is an internal or external standard, a normal or time reference compound, or a group compound.
- **Name** – Name of the compound.
- **Amount unit** – The amount unit of the compound.
- **Concentration unit** – The concentration unit of the compound.
- **Response** – Selection of the response type used to calibrate and quantify the compound.
- **Is ISTD** – Define whether the compound is an internal standard.
- **ISTD amount** – Amount of the internal standard.
- **Associated ISTD** – Name of the associated internal standard.
- **Mode** – Defines the calibration mode.
- **Weighting method** – Method for calibration point weighting.
- **Manual Factor** – Define value of the manual factor (if selected as calibration mode).
- **Curve reference** – Compound whose calibration curve is used for quantitation (if selected as calibration mode).
- **Ref. correction** – Response correction factor.
- **Curve model** – Calculation model for the calibration curve.
- **Origin** – Define how the origin is used for calculating the equation of the calibration curve.
- **Multiplier** – Compound multiplier entered for a specific compound or timed group.
- **Level** – Compound amount of the calibration standard for this level.
- **Last calibration date** – Date when the last calibration curve for the compound has been created.

Like any other table in the Data Analysis client, the displayed columns are configurable, so that columns not of interest can be hidden.

Compound amounts are required to calculate a calibration curve. By default, OpenLAB CDS uses the compound amount values that are defined for each calibration level in the compound table of the processing method. However, users may apply different amount values for each injection of sample type calibration standard. This can be useful if you have weighed in slightly deviating amounts when preparing the calibration standards.

17.3.5.2 Calibration Curve

The response types available to calibrate and quantify a compound are Area, Area%, Height, or Height%. For timed groups and named groups, only Area and Height are available.

The ESTD calibration curves and calculations are based on measured responses (Area or Height) of given amounts. The ISTD calibration curves and calculations are based on relative responses (Response / ISTD Response) and relative amounts (Amount / ISTD Amount).

The calculated response factors can be defined as the ratio of the response to the compound amount or vice versa. This is set globally per processing method.

For each compound, the calibration curve can be inspected in the user interface. It shows the average calibration points and individual points that have been used to calculate the averages. Users may choose per processing method how calibration points are used for the calculation of the calibration curve. The following modes are available:

- **From average per level** – Amounts and responses of all calibration points contributing to a level are averaged and used in the algorithm to calculate the best calibration curve.
- **From individual calibration points** – All amounts and responses of the individual calibration points are used directly to determine the calibration curve.
The following curve models can be applied:

- **Linear**: \( y = a + bx \)
- **Quadratic**: \( y = a + bx + cx^2 \)
- **Exponential**: \( y = a \exp(bx) \)
- **Logarithmic**: \( y = a + b \ln(x) \)
- **Log/log**: \( \log(y) = a + b \log(x) \)

For the log/log calibration curve the axes are changed to \( \log(x) \) and \( \log(y) \) to show a linear curve.

If required, calibration points can be weighted using one of the following calibration point weighting methods:

- **None** – All calibration points have the same weight
- **1/Amount** – Calibration points are weighted by the factor \( 1/\text{Amount} \)
- **1/Amount^2** – Calibration points are weighted by the factor \( 1/\text{Amount}^2 \)
- **1/Response** – Calibration points are weighted by the factor \( 1/\text{Response} \)
- **1/Response^2** – Calibration points are weighted by the factor \( 1/\text{Response}^2 \)

For the response, the value defined under Response is used for weighting (Area, Area%, Height, or Height%). For ISTD calibrations, relative amounts or relative responses are used. With the calibration curve model log/log, the logarithm of the amount, response, relative amount, or relative response is used for weighting.

Individual calibration points can be disabled if required. The icon of the disabled calibration point in the calibration curve window changes to make it distinguishable from other points. Likewise, disabled calibration points can be printed in reports.

There are different options for the origin usage when building the calibration curve. Users can choose among the following modes:

- **Ignore** – The origin is not used.
- **Forced** – The calibration curve is forced to the origin.
- **Include** – A virtual point \((0;0)\) is taken into account to calculate the equation of the calibration curve.
- **Connect** – The curve is connected to the origin by a linear segment from the lowest calibration level point.

The quality of the fit of the calibration curve to the calibration levels, and the presence of outliers can be evaluated using statistical calculations. The calibration curve calculation provides a correlation coefficient and a relative standard deviation for each curve, as well as a relative residual value for each calibration level.

The calibration curve calculations are verified and warnings are set if any of the following cases apply:

- Number of calibration points not sufficient for the curve calculation,
- Curve slope of zero or negative,
- Infinite curve slope, or
- Curve cannot be calculated.

### 17.3.5.3 Bracketed Calibration

With bracketed calibrations, the samples are bracketed by pre-sample and post-sample calibrations. The calibration standards from opening and closing brackets are processed first, and a calibration curve is calculated. This curve is then used to calculate the samples in between the calibration standards. A Clear all calibration operation is performed for all opening brackets. Brackets can be defined prior to acquisition in a sequence template (see section 16.4.3) or for processing in the injection list.

Users may choose from the following bracketing modes:

- **None** – No bracketing, calibration standards and injections are processed in order of acquisition.
- **Overall** – The calibration curve is calculated with all calibration standards in the sequence. All samples are reprocessed after the calibration curve has been calculated.
• **Non overlap** — Each calibration standard is only used for one calibration curve (bracket). A standard closing a bracket is followed by another standard opening the next bracket.

• **Overlap** — All standards apart from the first and last one are used in two calibration curves (with the preceding and with the following block).

• **Custom** — Users can manually create brackets as required and choose which calibration levels are cleared and when. For each bracket the user can choose whether the level is averaged with the predecessor, the level is cleared or all levels are cleared before the update.

17.3.5.4 Recalibration

When re-running a calibration sample, or when processing further calibration samples of a given calibration level, the calibration point for the level can be updated. It is updated by the average value of the new measured point and the already existing value(s). How the point is evaluated depends on the configured curve calculation.

The update of calibration points can be controlled by the Run Type as follows:

• **No selection** — A new point will be added to the calibration curve, or, if the calibration point already exists, the application calculates the average value of all existing calibration points for the given level.

• **Clear all calibrations** — All previous calibration points for all calibration levels are deleted before the new calibration data (response factor) is saved.

• **Clear Calibration at Level** — All previous calibration points for the given calibration level are deleted before the new calibration data (response factor) is saved.

If a level is cleared, the respective calibration points are removed from the calibration curve before new ones are added during processing of the standard.

Reprocessing the same calibration sample injection multiple times will update the same calibration point in the curve and not add new points.

17.3.6 Quantitation

OpenLAB CDS offers the following modes for quantitation to determine the amount of the compounds present in a sample:

• **Area or Height Percent (Area% or Height%)**

• **External Standard (ESTD)**

• **Internal Standard (ISTD)**

For uncalibrated compounds the following modes are available:

• **Quantitation using a fixed Response Factor (manual factor), optionally in combination with ISTD**

• **Indirect quantitation using a calibrated compound**

Not identified peaks can be captured in timed groups (see section 17.3.4.4) and treated like uncalibrated compounds.

The quantitation calculation uses different correction factors, the multiplier (compound or injection multiplier) and dilution factor. Dilution factors are set on the injection level and can be configured as divisors or additional multipliers per processing method. Multipliers are set on the injection or compound level. Overall up to five injection level multipliers, five dilution factors and one compound level multiplier can be applied during the calculation.

Optionally compound amounts are calculated relative to the sample amount as mass percentage (Mass% calculation).

Like area or height the calculated amounts can be normalized using the Norm% calculation. By default the normalization is based on a total amount of 100%. However, a different percentage value can be set in the processing method. The total amount is the sum of all calculated compound and timed group amounts, independent of the main compound signal. Optionally ISTD compounds can be included in the calculation.
17.3.7 Signal Alignment

If signals are reviewed in combination with signals from other detectors (for example a UV and MS signal), the signal alignment parameters in the processing method can be set to correct for the delay of a specific detector signal. The correction is automatically applied during reprocessing. For example, by incorporating a signal delay time, the extraction of mass spectra corresponding to peaks in a non-MS detector signal is possible.

17.3.8 System Suitability Calculations

For checking the system performance before and during routine analysis OpenLAB CDS provides the toolset for automated System Suitability calculations. To calculate, collate and statistically evaluate the system suitability tests the application provides a set of predefined report templates for result set summary reports. Users may also adapt these templates to their needs. The following parameters are calculated by OpenLAB CDS:

- peak retention time,
- peak area,
- amount,
- peak height,
- peak width values at specific heights,
  - tangent (4 sigma) peak width,
  - at 4.4% of height (5 sigma) peak width,
  - at 5% of height (tailing) peak width,
  - at 10% of height peak width,
  - at 50% of height (true half-height or 2.35 sigma) peak width
- peak symmetry and asymmetry,
- USP peak tailing factor (identical with EP and JP Symmetry factor),
- capacity factor (USP) or capacity ratio (ASTM), also called k prime or k',
- Number of theoretical plates per column,
  - Tangent method (USP, ASTM)
  - Half-width method (EP, JP, ASTM)
- Number of theoretical plates per meter,
- resolution between peaks, and
- selectivity relative to preceding peak.

To calculate system suitability results and populate the injection results with the computed values, the respective data has to be reprocessed. Extended performance results are calculated only for calibrated compounds. The tangents and peak widths are annotated in the peak details window. The displayed peak widths are from top to bottom: 50 %, 10 %, 5 %, and 5 sigma. For more details and calculation formulas please refer to the OpenLAB CDS Data Analysis reference guide as well as to the related chapters in the OpenLAB Help and Learning System.

17.3.8.1 Noise Determination and Signal-to-Noise Calculation

If the Signal-to-Noise (S/N) calculation is enabled, OpenLAB CDS provides a choice of three different methods for the noise calculation from the data points in the defined time range of a given signal:

- as six times the standard deviation of the linear regression of the drift ($6\text{SD}$),
- as peak-to-peak (drift corrected) noise ($P2P$), and
- as defined by the ASTM method E 685-93 ($\text{ASTM}$).

The user may either define a fixed time range or select the automatic mode. The automatic mode requires a blank preceding the sample.
In this mode, the noise is calculated from the last blank run (sample type = Blank) which was acquired before the injection. The noise is calculated from the corresponding signal of the blank, in a range determined by the retention time of the peak -10 and +10 times the half-height peak width. With a fixed range the noise is calculated in this range either of the current signal or the last blank signal.

The automatic mode combined with the P2P method corresponds to Agilent’s interpretation of the EP, JP and USP pharmacopeia requirements for the S/N determination.

17.3.8.2 Performance Test Definitions

Peak performance values can be calculated for any integrated peak of the loaded data including manually integrated peaks. The application calculates peak characteristics and displays them in the user interface.

The column parameters required for the performance calculations must be added to the processing method. The following parameters can be entered:

- Name
- Serial Number
- Length [m, cm or mm]
- Diameter [mm]
- Particle Size [user-defined unit]
- Dead Volume [mL]
- Void Time [min]

OpenLAB CDS provides the calculations for the system suitability parameters as defined by the US Pharmacopoeia (20th revision), the European Pharmacopoeia (7th edition), Japanese Pharmacopoeia (15th edition) and the Annual Book of ASTM Standards (Section E 685-93, Vol.14.01). The following list summarizes the available parameters in OpenLAB CDS. As some parameter names may differ in the given references, the items are sorted by the names used by the application, followed by the names used in the references.

- Tailing – USP Tailing factor, EP Symmetry or tailing factor, JP Symmetry factor
- Resolution USP – USP Resolution, ASTM Resolution
- Plates USP – USP Efficiency
- Plates JP – JP Efficiency (old)

1 Mandatory for column performance computation.
17.3.9 Custom Calculations

Custom calculations can be created with the Custom Calculation Editor which is launched from the Tools ribbon group in the Data Processing view. Custom calculations can be linked to or imported into a processing method to automatically apply them during reprocessing.

Custom Calculations provide access to results that are not calculated by OpenLAB CDS by default. The user-defined formulas are stored in Custom Calculation (.CC) files. Multiple formulas for several result calculations can be stored in one .CC file. Custom calculation files are either linked to or embedded in a processing method. Custom calculation results are visible in the Injection Results window after reprocessing - independent of any created reports.

The Custom Calculation formula language is based on Microsoft Visual Basic (VB.Net), extended by Language-Integrated Query (LINQ). In addition, some common pre-defined functions are accessible in the user interface of the Custom Calculation Editor. Users may write formulas using these functions and operators, or by creating own VB or LINQ expressions. Chemical constants may be stored in a separate file (Constants file) and pulled in from there when needed.

A “check file” routine optionally checks the syntax of a newly created or modified .CC file before using it in a processing method and computing results. It verifies the syntax of each calculation according to Microsoft Visual Basic standards and checks references to other files.

Custom Calculation (CC) results are always processed on a sequence (result set) level. With single injections the results are computed for each injection independently. With injections acquired within a result set, the results are computed at result set level when the complete result set is processed, reprocessed or requantified.

Custom Calculation results can be calculated and stored at 4 levels (“Scope”): Sequence, Injection, Signal, Peak or Group. When creating a new custom calculation the user first needs to define its name, scope and type. The type can be Integer, Double, Boolean or String. The scope functions give access to data on the scope level.

The following sets of operators, functions and variables are available for use in the Custom Calculations Editor:

- **Common functions** – any of the VB function, for example:
  - mathematical: Abs, log, log10, Exp, Round, Truncate
  - String manipulations: Str, Cstr, Trim, Len etc.
  - Program flow: If, Choose
  - Aggregate functions such as Average, Min, Max etc.

- **Operators** – any of the VB operators, for example:
  - Arithmetic: +, -, /, *
  - Logical: or, and, not, xor
  - Comparison: <, >, <=, >=, =, Like, <>
  - Concatenation: +, &
  - Enumerations

- **Fields, functions and custom calculations** – :
  - Fields give access to data calculated by the application.
  - Different functions are available at each level.
  - Custom calculations created in the .CC file are made available at the corresponding level.

Custom calculations may also include and further process results from other custom calculations. For more details please refer to the Custom Calculations User Guide (see chapter 24).

The CC file properties include the creator user name, the creation date, the last modification date, the name of the user who performed the last modification, and the version label. The custom calculation file audit trail provides a detailed list of modifications to a .CC file (for example, addition or deletion of custom calculations). It is not activated by default.
OpenLAB CDS automatically calculates and stores checksums for Custom Calculation files. If the checksum is wrong or missing, something may have been changed outside of OpenLAB. To avoid inconsistencies, OpenLAB CDS does not load such manipulated .CC files.

To include results from custom calculations in a report, they need to be added to the report template, as a single value, as part of a table or matrix, or in any expression. For details on report templates please refer to the chapter 18. Custom calculations (.CC) files can be saved in .pdf format and printed from there.

17.3.10 Method-based Reporting

In the processing method up to two report templates with different format and content can be defined for automatic injection report generation after processing. Reports can be printed using the windows default printer or saved to a file. If individual injection reports are not required, report printing can be disabled.

File-based reports are stored in the result set folder or the folder of the single run. One or more of the following file formats can be selected for printing: *.pdf, *.xls, *.doc, or *.txt. An additional copy of the generated report files can be saved to a different folder in the backend storage or on the Windows file system, for example for sharing reports with other users that don’t have access to the current project or to exchange data with another system. The destination is defined in the processing method.

For chromatogram outputs in reports users may specify a fixed chromatogram scaling in the processing method with a time and response range instead of automatic scaling.

If desired, a fixed chromatogram scaling can also apply to any manually generated reports, independent of the method linked to the reported injection.

17.4 UV Spectral Analysis

UV Spectral analysis processes spectral data acquired from a UV-visible diode-array detector or a fluorescence detector. There are different windows and functions specific to UV spectral analysis. To view those windows and access the functions, the focused injection must contain spectral data. There are two different processing method configurations designed for the qualitative and quantitative analysis of 3D UV data:

- **3D UV Quantitative** — General UV processing method used for the quantitation of specific compounds based on signals from an LC with an UV detector. This method configuration includes integration parameters, signal alignment, UV spectral extraction, compound identification, calibration parameters, spectral UV impurity check, UV spectral confirmation, system suitability calculations (for example, for noise determination), reporting, and if used, custom calculation results.

- **MS** — adds method sections related MS spectra extraction and MS Library Search

The UV spectral analysis provides additional quality criteria for routine analysis with the following applications:

- **Confirm the compound identity** — The application compares a UV spectrum with a specific UV reference spectrum stored in the method. A high match factor indicates that the compounds are probably identical.

- **Check for UV impurities** — The application compares all UV spectra of a peak with the apex spectrum. It calculates an overall match factor, the UV Purity value. A low UV Purity value indicates that there are co-eluted peaks with a significantly different UV spectrum.

The algorithm for the spectral comparison is identical in both cases. Please refer to the OpenLAB CDS Data Analysis reference guide for detailed information on the applied algorithm, see also chapter 23.

Both applications have related sections in the processing method specific to UV spectral analysis. These sections are:

- **Extraction section** — The Spectrum subset includes parameters for UV background subtraction. Users may define the background mode for apex spectra and arbitrary (non-peak) spectra and, if applicable, an external background time range. This time range is applied for the background mode "External time range", where the average UV spectrum of the given time range is used as the background spectrum.

- **Compound section** — The Spectra subset provides a compound table with the list of compounds, their order number, type (ISTD, ESTD, Time Reference, group compound), names, Purity Sensitivity value in percent (%) and an icon indicating the presence of a spectrum for UV Spectra Confirmation. In addition all parameters for UV Impurity Checking and UV Confirmation are set here.
17.4.1 UV Spectrum

The UV Spectrum window displays the extracted UV spectra of the focused injection. A spectrum can be extracted interactively in the Chromatograms window at a specific retention time or averaged over a time range. If multiple spectra are displayed in the spectrum window, the spectrum associated with the selected peak is highlighted. Extracted spectra also appear in the details area of the associated injection in the injection tree. To show or hide a specific spectrum the user can unselect it. Extracted spectra can be deleted or saved with the result set.

The way multiple spectra are displayed depends on the selected display mode. The UV Spectrum window displays the extracted UV spectra either overlaid or separated. There are further scaling options to adjust the display. These include the same scale globally for all spectra, individual scales per spectrum or normalized scales where each spectrum is displayed using its own signal maximum (100%).

Spectra can be easily zoomed in to reveal more details. For better overview a Zoom Overview Window can be enabled. This additional window will always display the entire spectrum with the zoomed section annotated as a red rectangle. It is shown in the upper right corner of the Spectrum graph. Further, the x- or y-axes or both can be linked across all panes. When zooming into one of several spectra, the zooming area will be applied to the other spectra as well.

A set of spectrum extraction tools help extracting spectra at the correct retention times. The behavior is configurable. For novice users hints for specific actions (e.g. extraction of background spectra) can be enabled. Snap tools help identifying apex and baseline points. Instead of extracting individual spectra, an average spectrum can be extracted from a time range by simply dragging the mouse over the required range. Alternatively the application automatically extracts the apex spectra for all peaks included in the time range.

If required, background correction can be enabled in the Extraction section of the processing method. The available background correction modes for apex spectra are:

- None,
- Spectrum at baseline start,
- Spectrum at baseline end,
- Spectrum at peak start and end, or
- External background time range.

For non-apex spectra the only available background subtraction mode is the external background time range.

17.4.2 Confirm Compound Identity with UV Spectra

For compound identity confirmation UV reference spectra can be stored per compound in the processing method. These spectra are typically obtained from one or more reference samples under well-defined chromatographic conditions. The identity of a compound is confirmed by comparing the current spectrum at the peak apex with the UV reference spectrum. The application calculates a match factor for the two spectra. Automatic background correction is optional and can be selected in the processing method.

For UV confirmation, the match factor must be greater than a given limit. The match factor limit is defined in the processing method. The UV confirmation results are shown in the injection results table and can be reported with the reporting engine. If the calculated match factor exceeds the given limit the cell is colored green in the injection results table, if not the cell showing the respective value is colored red.

UV confirmation is automatically performed if confirmation spectra are stored in the method. To turn it off the spectra have to be removed.
17.4.3 Check for UV Impurities

An impurity check assesses whether a peak is pure or contains impurities. This assessment is based on the comparison of spectra recorded during the elution of the peak. After applying a baseline correction, the spectrum at the peak apex is compared with all significant spectra recorded in the peak. The application calculates a match factor that characterizes the degree of similarity of the spectra.

The application performs a series of steps to evaluate UV impurities. For each peak it does:

- **Noise calculation** — Calculates the noise variance and the noise standard deviations from the spectra at baseline start and baseline end.
- **Determine significant spectra** — filters out spectra where the response range is too small; spectra are used for further calculations only if the response range is larger than 3 s, and larger than or equal to 10 % of the apex spectrum response range. The response range for each spectrum is calculated as max - min response.

For each spectrum of a peak the following calculations are done:

- **Background correction** — A linear interpolation of the two baseline spectra (the first spectrum before peak start and after peak end) is calculated. To correct each individual peak spectrum, the application subtracts the interpolation spectrum at the corresponding retention time.
- **Similarity calculation** — The application compares each of the remaining background-corrected peak spectra with the background-corrected apex spectrum. The match factor for each spectrum is a similarity value between 0 (no similarity) and 1000 (identical spectra).
- **Threshold calculation** — The application automatically calculates a threshold value for each spectrum of a peak, based on noise and variance of both spectra to be compared. The threshold value determines if a deviation from the apex spectrum is low enough to consider a spectrum as pure. A spectrum is classified as pure if the match factor is greater than or equal to the automatically calculated threshold value. The user can influence the level of the threshold value by changing the sensitivity in percent (%) in the processing method.

The calculations are summarized in the overall impurity evaluation. For each spectrum the application determines the purity ratio, a logarithmic ratio calculated from the sensitivity-corrected threshold value and the match factor.

The purity ratios for the single spectra of a peak are plotted as a purity ratio curve over the whole peak range in the lower part of the Peak Details window. The peak is annotated with the calculated UV purity value. The colored background of the purity ratio curve indicates the purity of a spectrum. It is considered pure (green background) if the purity ratio is greater than zero, that is, if the match factor is greater than the threshold value. The entire peak is considered pure if all single spectra are pure. As soon as one single spectrum is impure, the entire peak is considered impure, and the UV purity value is colored red in the injection results.

The UV purity value that is displayed in the Injection results table is calculated as an average of all match factors for the peak. The cell containing the UV purity value for a peak in the injection results is colored green or red accordingly to give a clear and fast indication of a peak’s purity. A purity indicator for each tested peak is shown in the Chromatograms window when this option is turned on in the properties.

When enabled in the processing method UV impurity checking is conducted either for all peaks or just for identified ones. By default the whole spectrum is used, but the spectral range can be limited in the method.
17.5 Mass Spectrometry

OpenLAB CDS can load, display and integrate Total Ion Chromatograms (TIC), Extracted Ion Chromatograms (EIC), and Selected Ion Monitoring (SIM) data. The data can be either acquired using a supported GC/MS or LC/MS instrument. There are different windows and functions specific to mass spectrometry. To view those windows and access the functions, the focused injection must contain MS data acquired using a LC/MS or GC/MS system.

Mass spectral analysis provides more selectivity and sensitivity for quantitative analysis, and more compound information for qualitative analysis. There are two different processing method configurations designed for the specific needs of:

- **MS Quantitation** — General MS processing method used for the quantitation of specific compounds based on signals from a GC/MS or LC/MS. This method configuration includes integration parameters, signal alignment, UV and MS spectral extraction, compound identification, calibration parameters, spectral UV impurity check, UV and MS spectral confirmation, system suitability calculations (for example, for noise determination), reporting, and if used, custom calculation results. MS library searching is available if NIST libraries are installed.

- **LC/MS Sample Purity** — Qualitative method specific to LC/MS, focused on sample purity confirmation. In addition to the parameters of the general MS method configuration, it contains MS sample purity calculations. In contrast to the general MS method, it does not contain calibration parameters, or system suitability calculations.

17.5.1 Processing MS Data

TIC and SIM chromatograms are signals that are stored in the data file, based on the acquisition method settings. The TIC is shown by default in the Chromatograms window. If several signals were acquired (for example, resulting from multi scan segments or SIM scans), these are shown as separate signals. The user can select or deselect signals in the signal selector.

Quantitation can be based on a TIC, EICs extracted per compound from the spectral matrix (single m/z value per compound), or SIM (acquired with single ion per chromatogram). For spectral confirmation a reference MS spectrum can be stored for each compound in the compound table similar to UV confirmation. The match score will be included in the injection results table.

Extracted Ion Chromatograms can be generated from scan runs, either automatically during reprocessing (for identified compounds) or interactively. Just by right-clicking the required ion in the mass spectrum of the peak of interest, users can generate an EIC from the related TIC. The EIC is extracted for the selected ion’s m/z value. It will be added to the list of signals and can be enabled or disabled the same way as other signals. In both extraction cases the m/z extraction range defined in the processing method determines the m/z interval used for the extraction. The interval can be symmetric or asymmetric. EIC and MS spectra cannot be extracted if no method is linked to the injection.

During quantitation or MS sample purity calculation, EICs for each identified compound are automatically extracted. To extract ion chromatograms over a time window around each peak rather than the entire run time an extraction retention time window can be specified in the processing method. With zero values for the time range, EICs are extracted over the full time range.

17.5.1.1 MS Library Searching

A prerequisite to performing MS Library searching is the installation of NIST MS Search and the required MS libraries, or the creation of the required user libraries using the NIST MS Search Program. One Library license is required per OpenLAB CDS workstation, AIC or client that will be performing MS library searching. The following MS libraries are supported:

- Agilent GC/MS libraries in NIST format,
- User-generated GC/MS or LC/MS libraries in NIST format,
- Newly generated user libraries from OpenLAB CDS data.

If an MS Library is installed, library searching can be enabled in the processing method. On reprocessing, all integrated TIC peaks will be automatically searched in the MS library. The MS spectra of these peaks are extracted according to the extraction parameters in the method, and will be listed for each individual injection in the injection tree when expanding the details. Users can define the following search parameters and filters in the method:

- Choose the MS Library to be used for searching from the installed libraries,
- Define the maximum number of search results to be displayed,
- Define the threshold for the match score. Only hits with a match score higher than the specified threshold are presented as search results.

The library search results can be reported using the customizable Library Search report template (see chapter 18 for more details).
17.5.1.2 Automatic Generation of Quantitative Methods

For integrated data the Data Analysis can automatically create (or update) a LC/MS or GC/MS quantitative processing method. With a single mouse-click on a standard injection in the tree the user launches this process:

For TIC data a wizard automatically extracts a spectrum for each peak and the most abundant ion from each spectrum to determine the correct EIC for each integrated peak. These extracted EICs for each m/z value are listed in the injection tree like any other signal. The EICs are used for quantitation. Optionally compound names can be assigned by best match in an MS spectrum library search. Likewise the automatic storage of peak spectra as reference spectra for compound confirmation can be enabled.

For SIM data the application automatically pulls compound names and their associated SIM ions from the acquisition method, if available. If a compound was designated as an ISTD in the acquisition method, this will transfer to quantitation method.

In a last step the levels and amounts for the calibrated compounds need to be specified by the user and the method is ready for use.

17.5.2 Confirm Compound Identify with MS Spectra

For compound identity confirmation MS reference spectra can be stored per compound in the processing method. For this purpose a spectrum for each identified peak can be extracted automatically from a chromatogram and stored in the processing method. Alternatively individual spectra can be selected interactively and added to the processing method.

The identity of a compound in a loaded chromatogram is confirmed by comparing the current spectrum at the peak apex with the MS reference spectrum stored in the processing method. The application calculates a match factor for the two spectra. Background correction is optional and can be enabled in the processing method.

For MS confirmation, the match factor must be greater than a given limit. The match factor limit is defined in the processing method. The MS confirmation results are shown in the injection results table and can be reported with the reporting engine. Color-coding reveals the outcome of MS confirmation at a glance. If the calculated match factor exceeds the given limit the respective cell in the injection results is colored green, if not the cell showing the respective value is colored red.

17.5.3 MS Sample Purity Calculation

With MS sample purity users can confirm that a target molecular weight is present and above a certain minimum purity limit. The underlying calculation assesses whether a sample is pure or contains impurities by comparing responses. On the one hand, there is the response of all compounds and fragment ions in a sample. On the other hand, there is the response caused by specific target ions. The sample purity is calculated as the ratio of both responses.

Up to five target ions for confirmation can be defined per sample during sample submission (single run or sequence) or during data processing in the injection list. The entry is either a molecular weight or molecular formula. If a formula is entered, the application automatically calculates the molecular weight from the formula. The values entered during Sample Submission can be replaced during data processing, for example to revise an incorrect formula. The applied algorithm can take polarity, common adducts, dimers or multiple charge states into account. More details are given below.

Users can enable the sample purity calculation in the MS Sample Purity section of the processing method. The following parameters need to be defined for the calculation:

- **Minimum purity limit** – threshold value for result flagging in the Sample Purity Results window.
- **Base signal** – any of the currently loaded signals can be selected as base signal for sample purity determination. It may be an MS signal or from another detector.
- **Calculation type** – either TIC% (area of corresponding peak in TIC relative to total area of peaks in TIC) or EIC/TIC% (area of peak in EIC relative to total area of peaks in TIC); the calculation type is only relevant if the base signal is an MS detector signal.

Adducts generated during ionization (that may attach to the target molecular ions) can be specified for positive or negative polarity. Users may select possible charge carriers and neutral losses from a customizable list, and enter the charge states of target ions and aggregates the ion may build. It is mandatory to select at least one adduct.

The settings are taken into account when the application looks for hits for the target ions. The application will extract as many EICs as are required to cover all possible hits for the targets. All EICs are shown in the Chromatograms window and are listed in the injection tree. In the course of the analysis the application checks for predefined target masses, applies adducts as specified, determines the retention time of the peak in the respective EIC and locates the matching peak in the chromatogram of the base signal. If a matching peak can be located, the target is marked as found.
For base signals other than MS the calculation is defined as the area of the corresponding peak in the signal relative to the total area of peaks in the signal.

In the Sample Purity Results window, a color code indicates whether all targets have been found and the overall sample is pure (the purity of the overall sample is above the specified purity limit). The window includes the detailed values for all targets in the selected injection. Purity values lower than the Minimum purity limit are colored red. As soon as one target has either not been found or has a purity value lower than the specified limit, the check is considered as failed and the columns representing the overall results (overall targets found and overall purity) for an injection are colored red.

The sample purity results can be reported using the customizable Sample Purity report template. Method parameters such as the sample purity threshold can be reported along with the results. More details about the reporting capabilities are outlined in the chapter 18.

Please refer to the OpenLAB CDS Data Analysis reference guide for more detailed information, see also chapter 23.

17.5.4 MS Spectrum

The MS Spectrum window shows the extracted MS spectra of the focused injection. A spectrum can be extracted interactively in the Chromatograms window at a specific retention time or averaged over a time range. Extracted spectra automatically appear in the injection tree, in a list of Extracted Spectra of the associated injection. To show or hide a specific spectrum the user can select or unselect it in the tree. Extracted spectra can be deleted or saved with a result set.

A spectrum is always linked to other windows. For example, for a selected spectrum the corresponding chromatogram trace in the chromatograms window and the corresponding injection in the injection tree are highlighted. If multiple spectra are displayed in the spectrum window, the spectrum associated with a selected peak is highlighted.

The MS Spectrum window displays the extracted MS spectra in separate graphs. There are scaling options to adjust the display. These include the same scale globally for all spectra, individual scales per spectrum or normalized scales where each spectrum is displayed using its own signal maximum (100%).

Spectra can be easily zoomed in to reveal more details. For better overview a Zoom Overview Window can be enabled. This additional window will always display the entire spectrum with the zoomed section annotated as a red rectangle. It is shown in the upper right corner of the Spectrum graph. Further, the x- or y-axes or both can be linked across all panes. When zooming into one of several spectra, the zooming area will be applied to the other spectra as well.

Spectra can be extracted at specific times or peak-based. A set of spectrum extraction tools helps extracting spectra at the correct retention times. The behavior is configurable. Snap tools help to easily identify apex and baseline points. Instead of extracting individual spectra, an average spectrum can be extracted from across a peak (processing method parameter) or from a time range by simply dragging the mouse over the required range. Alternatively the application automatically extracts the apex spectra for all peaks included in the time range. For novice users hints for specific actions (e.g. extraction of background spectra) can be enabled.

Background correction is optional and can be enabled in the Extraction section of the processing method. The available background correction modes for apex spectra are:

- None,
- Spectrum at baseline start,
- Spectrum at baseline end,
- Spectrum at peak start and end, or
- External background time range.

For non-apex spectra the only available background subtraction mode is the external background time range.
18 Data Reporting

With OpenLAB CDS Reporting, the data loaded for analyzing and reprocessing is automatically available for reporting. To create new report templates, users can switch to the Reporting view and utilize the report template creation toolset of the Report Template Editor (RTE). It enables users to easily create report templates either by editing existing templates or creating new ones. New reports can be created without generating new result revisions because reports are entirely based on stored result values.

The report template audit trail logs all modifications done to a report template and can be reviewed using the Audit Trail Viewer. The Audit Trail Viewer is described in section 21.4.1. Usage of the RTE is limited to users or groups with a dedicated privilege.

The navigation pane hosts the Reporting tree, which enables navigation of all loaded injections, the available report items and stored reports templates. The Injection tree allows fast switching between loaded injections during report template development. The Report Items tree presents all available report elements sorted by different categories. The Report Template tree provides all report templates in the current project available for loading.

A key capability of the OpenLAB CDS Reporting is the ability to build reports on three different levels. A report can be based on a template presenting results

- from each injection within a result set (single sample reports),
- across an entire sequence of injections (sequence summary report), or
- from different sequences or result sets within the same project (cross-sequence summary report).

Template examples for each type of report are available as default templates and can be easily imported into the backend storage, if required.

For template editing RTE provides an easy-to-use interface that helps users to develop report templates using drag-and-drop of predefined report elements. Using report parameters provides even more flexibility compared to conventional reports. Users can easily create dynamic reports that contain data as chosen by the user, such as data limited to a specific time span. The time span is set by the user during report creation.

All report templates are based on the Report Definition Language (RDL), which is a standardized XML format provided by Microsoft®. The format is extended by typical features that scientists need on a daily basis. For example, the Report Template Editor (RTE) provides various preconfigured report items - also referred to as snippets - that users can employ to create new templates more quickly.

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

The Agilent Common Analytical Markup Language (ACAML) schema is a document format based on the XML (eXtensible Markup Language) standard using a patented schema. The approach is to define a technique- and application-independent unified language and schema. ACAML can be used to describe analytical data in a generic way, without any special aspects (e.g., result-centric viewpoint) starting from a single instrument or method up to a complex scenario with multiple instruments, methods, users and hundreds or thousands of samples. ACAML provides a common standard that allows seamless exchange of information between various platforms and applications. The current revision of ACAML supports chromatography data (LC, GC) and the MS specific data generated by MS detection (LC/MS, GC/MS).

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.
18.2 Creating Report Templates

The development of a new report template is started with a single mouse-click launching the New Template wizard. The wizard guides the user step-by-step through the complete task of developing a new template. As a first step the user has to choose the type of report his work will be based on:

- **Single injection** which will repeat for each injection in the selected data set (grouped by injection),
- **Single sequence summary** which include results for each injection within one result set in a single report (grouped by sequence), or
- **Cross-sequence summary** which can include results from multiple result sets (or single runs) within a single report (not automatically grouped).

Report templates can be developed in table or matrix format, on A4 or Letter paper format with adjustable left, right, top and bottom margins and portrait or landscape orientation. The area shown in the Editing Pane of the RTE considers the entered internal margins and the display will automatically adjust. For paper formats larger than A4 or Letter the dimensions for page height and width are extendable as required.

Experienced users can continue without using the wizard and work on individual report section as needed.

In the Reporting Tree, users can select the data, the report template, and the report items for creating a report. Elements or individual items are arranged in a WYSIWYG (“what you see is what you get”) workspace with extensive configurable properties.

While editing the template in the template editor pane, live data is being used. This enables a direct preview of the report item content during development without rendering the report using loaded data. Users can limit the number of records to be used for the preview.

RTE offers additional functions that are not available in the standard RDL report editors provided by Microsoft®, such as Microsoft® SQL Server Report Builder or Microsoft® Visual Studio.

These functions are for example:

- Display of scalable chromatograms and spectra (UV and MS)
- Usage of custom variables and aggregators for report based calculations

18.2.1 Report Items

The Report Items node in the Reporting Tree lists all items that can be added to a report template. The items are organized in folders that reflect the content. They 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 or composite groups. Each of these report items is commonly referred to as a snippet. New items are inserted by dragging and dropping a snippet into the report template, positioned, sized and if required, configured in the properties. Some of the items have no properties, but only fixed configurations.

The folders and subfolders, under which the snippets are located, are determined by the snippet itself and cannot be changed. Not all elements are always available. The availability of report items depends on the type of the current template, revision of OpenLAB CDS, and instrument module and driver versions. The set of report items is structured in the following categories:

- **Tables** – Preconfigured tables for various types of reports.
- **Matrices** – Preconfigured matrix report items.
- **Fields** – Tree of all available data fields (defined by type of report template).
- **Special Objects** – Generic report items such as graphics, lines, or blank text fields, page breaks or page numbers.
- **Instrument Information** – Report items for instrument information such as EMF counters or instrument modules.
- **Sequences** – Preconfigured composite groups containing a set of fields or tables related to sequence information, for example sequence overview or sequence and result set audit trails.
- **Samples** – Preconfigured composite groups containing a set of fields related to sample information, such as sample or column information, injection audit trail and e-signatures.
- **Method Information** – Information related to the used acquisition or processing methods such as the method audit trail, single method parameters or parameter tables, for example the table of initial integration events.
- **Calibration Curves** – Report items to display calibration curves.
- **Chromatograms** – Report items to display signals.
• **Spectra** – Report items to display spectra plots.

• **Charts** – Report items to display charts.

• **Composite Groups** – Contains the grouped report items that you saved as composite groups using the Report Template Editor. The Composite Groups folder is only displayed if a composite group has been saved in the past.

• **Text** – Report item to display a simple textbox.

For each item, and for many individual elements within each item, configuring the properties allows control of included data (peaks, compounds, signals, and injections) as appropriate. 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.

Some elements have specific properties such as scaling for graphic displays, legends for charts, or fields for peak labeling. A context-sensitive tabbed Properties dialog gives access to these functions. The Properties dialog is accessible from the context menu of the item or from the Report Editor Toolbar. To give an example, by enabling the display of history points for a calibration curve in the Properties dialog, markers will be printed in the calibration curve for all history points including disabled calibration points.

Composite groups can be stored centrally in the projects folder to make them available to other users for template development.

Fields can be selected and placed into the template for all result values, including custom calculations, generated by OpenLAB CDS during an acquisition and the subsequent data processing operations. Users may select and arrange the data fields in the report template according to the requirements, limited only by the structural relationships of the individual values.

The Report Template Editor provides three different types of fields:

• **Text fields** – textboxes that can contain either static text or dynamic expressions. Text fields are, for example, used to display static headlines in a report template.

• **Data fields** – field consisting of two parts, label and value. The label contains a static text; the value contains a dynamic expression. Data fields are typically used to show specific data, for example the sequence name or the sample name, or the content of sample or compound custom fields. Both, label and value are modifiable.

• **Custom fields** – sample or compound custom fields as configured in the OpenLAB Control Panel; custom fields are a sub-set of the data fields.

The availability of data fields depends on the selected report type. The data fields (contained in the folder Fields) are further arranged in the following categories (some examples for included fields are given):

• **Project** – project name.

• **Instrument** – ID and name.

• **Sequence** – information related to the sequence, for example, name, acquisition and modification information, sequence-level custom calculation results and result set version.

• **Sample** – sample-related information, such as sample name, type, vial, amount, calibration level, sample-level custom calculation results and custom fields.

• **Injection** – items related to the injection, for example, acquisition information, acquisition method, processing method, column information, injection volume and data file name.

• **Signal** – signal-related information such as detector type.

• **Compound** – compound-related information – names, amounts, concentrations, compound-level custom calculation results, compound custom fields and so on.

• **Peak** – peak-related items, such as area, height, retention time and performance factors.

• **Calibration Curve** – all calibration curve parameters, for example coefficients, curve type or origin usage.

For more flexibility user parameters can be defined within a report template. Parameters are given a variable name, the data type is selected and text for a user prompt can be defined. These parameters can be internal to the template, so no prompts are displayed, but the values defined in the template parameters can be set to adjust the behavior of the template for different reports. Multiple value parameters can be defined so the user selects from a list when the report is opened. Parameters always have default values so a defined value is available if the template is called through automation and the user cannot select or provide a value.
The RTE provides means for data protection. Individual report items may be locked to secure their definition in the report template. The privilege to lock or unlock items can be assigned to a user or a role. This allows validated calculations to be locked to prevent accidental or intentional modification while allowing users access to less critical elements in the report.

Templates are tamper-protected. If a report template that has been modified outside of OpenLAB CDS is loaded, it will be reported as "Uncontrolled Report Template" any time it is opened in the Report Template Editor. All reports generated with such a template will show a watermark with a corresponding warning symbol. An authorized user has to first validate the template with the Accept Template function before it will be available for unrestricted use. Once accepted, the warning message when loading the template and the watermark on printed reports will disappear.

More details on all available report items are documented in the OpenLAB CDS Online Help. Custom table report items can be created using the .NET Software Developers Kit (SDK). It can render data from any data source. Intelligent Reporting also supports external code references. This allows to extend reporting with custom .NET code (dll’s), create own complex calculations and read data from external files.

18.2.2 Expressions

In the Report Template Editor, expressions can be assigned to modify or create the contents of the report. Expressions can create or modify labels such as setting case for text, calculate values such as an impurity as a percent of a compound amount, or generate new values such as pass/fail indications based on a compound amount or any other calculation result. Expressions can be used for filtering data.

Users can store the values, calculations and statistical calculations as variables or arrays (aggregators) and access these variables or aggregated arrays from subsequent report items in the template. The Expression Editor helps create valid expressions by providing: direct field selection to make sure field names are correct, function selection to offer properly formatted function calls, and syntax checking for the complete expression to ensure expressions are not invalid. All expressions are based on Microsoft Visual Basic.

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

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

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

All capabilities and functions of the expression editor are described in detail in the Online Help System.

18.2.3 Charts

In the category Charts different types of report items are available providing for the graphical representation of data. As in tables or matrices, charts can also present aggregated data.

The following chart types can be integrated into a report template:

- **Line chart** – visualize categorized data using a direct line (optionally smoothed) to connect the values. The category values are used to label the x-axis, for example, categorize the data by the sample name, calibration level or compound name. Different series of data are shown as several lines in different colors. Line charts can be extrapolated to zero by adding a virtual data point at the origin of the coordinate system and extrapolate the lines to this virtual data point.
- **Column chart** – visualize categorized data using column bars. The category values are used to label the x-axis. Different series of data are shown as several bars in different colors. The columns can be displayed either stacked or unstacked.
- **Scatter chart** – the location of the data points is determined by x and y-values. The x-values are typically numeric values or date/time values. For example, a scatter chart can show the ratio of compound amount to peak area in an accuracy plot. Optionally the data points can be connected using a simple or smoothed line. A special case of a scatter charts is the Linearity Curve. With this function enabled, the correlation coefficient r and determination coefficient R2 values will be shown in the legend.
• **Bubble chart** – the location of the data points is determined by x and y-values. In addition, the size of the bubbles is determined by the variance in the value of a specific data field. The bubble size therefore adds a third dimension to the graph.

Further computations include the ability to display a line for the mean of all values in the chart, lines for the mean value plus and minus the standard deviation, or lines for the mean value plus and minus the relative standard deviation. Color and line styles are adjustable.

### 18.2.4 UV Data

With the available spectra snippets, users can create graphs for different scenarios where the combination of grouping and repeating enables more complex plot layouts:

• The **Spectra Plot snippet** contains a plot where all available spectra are shown in an overlaid format based on user-defined criteria. For example, the Spectra Plot snippet can show one graph for each peak, with overlaid spectra for all injections of the current sample.

• The **Spectra Plot All Peaks snippet** provides an output of plots with a single spectrum for each peak and signal.

• The **Spectra Plot Compounds snippet** prints one plot for each compound with the spectrum, the retention time and the compound.

• The **Spectra Plot per Peak snippet** is repeated by peak, that is, the entire report item is displayed once for each peak in the generated report. Multiple spectra selected from the same peak are shown in an overlaid graph.

### 18.2.5 Mass Spectrometry Report Items

The following report items and snippets related to mass spectrometry are available:

• Total Ion Chromatogram (TIC) and Extracted-Ion Chromatogram (EIC)
• MS Spectra Plots
• MS Sample Purity Results
• MS Library Search Results
• MS Spectra Confirmation Results

With the **MS Spectra Flow layout snippet** the MS spectra are embedded in a group that is repeated on signals and peaks.

The **MS Spectra Plot snippet** shows MS spectra of all integrated peaks in the TIC. The display can be adjusted based on filter conditions.

Additional snippets allow adding report items with MS Spectra confirmation results. Users can include MS Sample Purity Results as a predefined table with MS targets (names, masses and formulas), and the calculated purity values. The Target found and Target pure columns are automatically colored corresponding to the values and defined threshold values. The same color-coding can be used for peak filling in the chromatogram.

### 18.3 Automating Reports

OpenLAB CDS can be configured to automatically create injection reports after reprocessing each injection. This function is enabled in the processing method. Optionally users can configure a second injection report, which can have a different format and content. If reports are printed to files, the files are named automatically and stored in the data folder. Copies of the reports can be stored to an additional location in the backend storage or on the Windows file system, for example, to send reports to an external system such as a LIMS. The naming schema is `<datafile name>_01.<extension>` for the first report and `<datafile name>_02.<extension>` for the 2nd report, where the extension corresponds to *.pdf, *.xls, *.doc, or *.txt as defined in the processing method.

Sequence Summary and Cross-Sequence Summary reports can only be created interactively.

For unattended processing on client/server systems, hardcopy reports are always printed on the default printer configured on the AIC.
18.4 Default Templates

The OpenLAB CDS ships with a set of default report templates. These default templates provide similar content as the earlier classic reports but now in smaller, focused reports rather than one big report. Most reports are trimmed to fit on one page. The default templates can serve as a starting point for the development of own templates. The templates are not pre-installed but can be easily imported into the data backend with a single mouse-click.

After the import users will find the three categories of default templates added to the Report templates folder. Report templates have the extension *.rdl.

- **Single injection chromatography reports**
  - Short Area percent
  - Short ESTD results
  - Short ISTD results
  - Short Quant ESTD
  - Short Quant ISTD
  - Calibration
  - CSV export of results
  - Extended Performance
  - Performance and Noise
  - ISTD results with groups

- **Single Injection MS reports**
  - MS Library Search results
  - MS Library Search Cross Peak results
  - MS Library Search Long results
  - MS Library Search Short results
  - MS Sample Purity results

- **Method Report**
  - Method report

- **Chromatography Summary Reports**
  - Replicate Injections report
  - Extended Sequence Summary report
  - Short Sequence Summary report

18.5 Report Template Documentation Tool

OpenLAB Reporting includes a Report Template Documentation Tool. This tool is a standalone application installed with OpenLAB CDS to view the description of the RTE supported report templates. The description of the report template includes layout of report items along with their parameter details, such as calculation variables, report parameters, expressions used, filter condition, sorting condition, audit trail and so on. Users may save this description in PDF format for documentation purposes.
19 Data and Method Compatibility

Data acquired with OpenLAB CDS, OpenLAB CDS ChemStation Edition or EZChrom Edition, Multi-technique ChemStation for GC, LC, LC/MS and A/D, and EZChrom Elite can be reviewed and reprocessed. OpenLAB CDS evaluates the raw data and, if available, the ACAML (Agilent Common Analytical Markup Language) files generated by OpenLAB CDS A.01.01 or higher.

Acquisition and data analysis methods from earlier revision of OpenLAB CDS can be partially reused by importing them.

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

Sequences can be imported in *.CSV format.

This chapter provides an overview of the available import functions. More details on preparing a migration are provided in a separate document. See chapter 24.3.

19.1 Method Migration

OpenLAB CDS ChemStation or EZChrom Edition acquisition methods can be imported under certain preconditions. For Data analysis methods an import function transfers compound information into OpenLAB CDS processing methods.

19.1.1 Acquisition Methods

OpenLAB CDS ChemStation or EZChrom Edition LC and GC acquisition methods can be reused if they were created using OpenLAB CDS drivers based on the RC.NET architecture. Converted methods may contain new parameters not available in earlier revisions of the OpenLAB CDS Rev-A Editions. These parameters will contain default values after the conversion, so it is always recommended to review the content of converted methods before using them for new data acquisitions. The corresponding import functions are available in the acquisition client.

Classic ChemStation Edition methods first need to be migrated to RC.Net. Please refer to the section 19.5.

19.1.2 Data Analysis Methods

The data analysis method compatibility is limited to peak identification – compounds can be imported from existing ChemStation and EZChrom methods.

Users can create a new processing method with a compound table that uses a ChemStation method created with the Multi-technique ChemStation B.01.01 or higher as a starting point. The following parameters of the ChemStation method are loaded into a new processing method:

• Compound name
• Signal name
• Expected retention time
• Retention time window
• Flag if a compound is an internal standard (ISTD)
• Associated ISTD that a compound refers to
  o If there is only one ISTD, it is the associated ISTD of all other compounds.
  o ISTDs with an empty name are ignored.
  o Groups that are used as ISTD are ignored.

ISTD amounts are not imported. A warning is displayed if there is an ISTD compound without an ISTD amount.
Users can create a new processing method with a compound table that uses an EZChrom method created with EZChrom A.04.01 or higher as a starting point. EZChrom Elite methods are not supported. The following parameters of the EZChrom method are loaded into a new processing method:

- Signal name
- Compound name
- Expected retention time
- Retention time window
- Flag if a compound is an internal standard (ISTD)
- Associated ISTD that a compound refers to
  - If there is only one ISTD, it is the associated ISTD of all other compounds.
  - ISTDs with an empty name are ignored.
  - Groups that are used as ISTD are ignored.

ISTD amounts are not imported. A warning is displayed if there is an ISTD compound without an ISTD amount.

### 19.2 Data Import

The data analysis subsystem can directly read the data and results that were acquired and calculated with the following OpenLAB CDS versions:

- OpenLAB CDS A.01.01 or higher, consisting of
  - OpenLAB CDS ChemStation Edition revision C.01.01 or higher,
  - OpenLAB CDS EZChrom Edition revision A.04.01 or higher,
- OpenLAB CDS 2.0 or higher

The data analysis can further import raw data originating from

- Multi-technique ChemStation B.01.01 or higher, and
- EZChrom Elite 3.3.2 or higher.

During processing, OpenLAB CDS Data Analysis does not alter any ChemStation or EZChrom raw data or methods, but only writes new results to the ACAML results.

#### 19.2.1 Multi-technique ChemStation B.01.01 or higher

Only injection parameters and raw data will be imported. Imported injection parameters include, if available:

- Sample name
- Vial number
- Replicate number
- Operator
- Instrument name
- Injection date and time
- Acquisition method name
19.2.2 EZChrom 3.3.2 or higher

Only injection parameters and raw data will be imported. Imported injection parameters include, if available:

- Sample name
- Vial number
- Operator
- Acquisition date and time
- Acquisition volume
- Acquisition method name

19.3 Data Export

OpenLAB CDS provides functionality to copy OpenLAB data to the local file system as an OpenLAB archive (*.olax) from the data analysis client. The archive will either contain the result set or all single injections from the folder selected for export.

The OpenLAB archives (*.olax files) cannot be read by other applications than OpenLAB CDS. During import of an archive from the local file system into OpenLAB CDS, the data contained in the archive is imported into the secure data storage with its original name into the selected folder. If data with the same name already exists, a number will be appended.

The export and import are logged in the System Activity Log (see section 21.5.1).

19.4 Importing Report Templates

The Reporting is based on OpenLAB Intelligent Reporting which was already integrated in OpenLAB CDS ChemStation and EZChrom Edition. Existing report templates originating from previous versions of OpenLAB CDS can be imported.

Since a new version may contain new parameters not available in earlier revisions it is always recommended to review the report content, thoroughly test it and, if needed, revalidate before use.

19.5 Transitioning from previous Agilent data systems

Migration is the process of moving methods, sequences, and data to the new OpenLAB CDS. Several administration guides are available, outlining the migration workflow for workstation and client/server systems. Users will find instructions for the following tasks: planning the migration, copying data, migrating methods, migrating raw and result data, recreating sequences. Further, the guides provide information on differences between old and new data system and the acquisition method conversion from classic to RC.Net methods. For information on the available guides and publication numbers please refer to section 24.5.
20 Data Storage

Central as well as local data storage is provided by OpenLAB Data Store. Data Store is a dedicated laboratory data management solution. Data Store is available as a workstation, a single server solution for small to medium sized laboratories, and as a multi-server configuration for larger laboratories.

Data Store allows users to easily collect, organize, search, and review all of their OpenLAB CDS data. It automatically extracts searchable metadata from files, and provides powerful search capabilities.

Client machines that access the OpenLAB Data Store server make use of the following components:

- **OpenLAB Data Store web interface** – OpenLAB Data Store provides a thin client web based user interface that can be accessed using a web browser. The web interface provides access to the OpenLAB Data Store folders and files.
- **OpenLAB Control Panel** – The Control Panel is the user interface that provides access to administrative functions used for managing the OpenLAB Server.

In this document, the terms „central data storage“ or „central repository“ refer to instances of OpenLAB Data Store.

For more details please refer to the *Data Store Administration Guide* (see section 24.2).

20.1 OpenLAB CDS File Types in the Data Storage

Data is organized in projects (see section 12.2) as the top-most hierarchical element. And each project is assigned a folder in Data Store for the storage of the analytical data. Upon project creation the following sub folders are created by default in the project folder:

- **Methods** – see below.
- **Report Templates** – storage location for *.rdi files
- **Results** – see below, section 20.1.2.
- **Sequences** – storage location for sequences that were saved for further use
- **Sequence Templates** – storage location for sequence templates

OpenLAB Data Store provides a multi-level folder storage model. The number of levels is not limited, and data can be stored in any folder level.

20.1.1 Methods

All master methods and custom calculation files are stored in the methods folder and can be optionally structured in subfolders as defined by the user:

- **Acquisition Methods** (*.amx)
- **Sample Prep methods** (*.smx)
- **Processing methods** (*.pmx)
- **Custom Calculation files** (*.ccf)
20.1.2 Results

OpenLAB CDS data is stored in the central data storage as files in the Results folder:

- Single runs are stored in Single Sample Result (*.SiRslt) folders,
- Result sets are stored in Result Set (*.Rslt) folders.

Both contain all or some of the following files:

- Acquisition Methods (*.amx)
- Sample Prep methods (*.smx)
- Processing methods (*.pmx)
- Sequence (*.sqx)
- Raw Data files (*.dx and *.ms)
- Report templates (*.rdl)
- Reports (*.pdf, *.xls, *.doc, or *.txt)
- Injection Results (*.rx)
- Sequence results (*.acaml)
- Manifest file (.mfx)

21 Compliance

21.1 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. For details please refer to section 12.3.3.

21.2 Data Security

The OpenLAB Control Panel functionality related to security includes the following

- System Activity Log (see section 21.5.1)
- Selection of authentication provider (see section 12.3.3.1)
- Management of users, groups, roles, and privileges (see section 12.3.5, 12.3.6 and 12.3.7)
- Security Policy (see section 12.3.4)

21.3 Data Integrity and Traceability

OpenLAB CDS stores data in a manner that ensures compliance with 21 CFR Part 11. It provides secure data storage with access control and an audit trail. Data files are versioned to ensure data integrity and traceability. In addition, OpenLAB CDS provides electronic signatures allowing users to sign off on data.
21.4 Audit Trails

Besides the [System Activity Log](see section 21.5.1) maintained by the OpenLAB Control Panel and the audit trail of the optional data backend (see section 21.4.3), OpenLAB CDS provides the following audit trails documenting all changes to the analytical data:

**Acquisition:**
- Acquisition method audit trail — a record of changes made to the acquisition method,
- Sample preparation method audit trail — a record of changes made to the sample preparation method,
- Sequence audit trail — a record of changes made to the sequence in the acquisition client, including sequence table entries such as vial locations, sample types, or sample amounts.

**Processing:**
- Processing method audit trail — provides a detailed list of modifications of the processing method (e.g. compound identification, integration parameters, or reporting parameters).
- Injection audit trail — lists modifications such as method linking, reprocessing, or manual compound identification. Also manual integration activities or calibration curve modifications are recorded here.
- Result set audit trail — a superset of all injection audit trails that are contained in the result set.

**Reporting:**
- Report template audit trail

Each time a user saves a modified item, the changes are logged in the corresponding audit trail. The Save event itself is not logged, unless the item is saved without any modifications.

When saving methods, sequences or results (also automatic saving during reprocessing), users are asked to enter a reason, if this option was enabled for the project.

The injection audit trail and result set audit trail are enabled by default. The Method Audit Trail and Sequence Audit Trail must be activated for a project before they start recording. Once enabled, an audit trail cannot be disabled.

The behavior of audit trails in general and the sequence, method or results audit trail in particular depend on the project settings defined in OpenLAB Control Panel (see section 12.2.2.3).

21.4.1 Audit Trail Viewer

All audit trails can be inspected in an Audit Trail Viewer window. By default, a summary view is displayed, which shows all entries for an injection, result set, sequence, method or report template grouped by version and category. Users can switch to the Detail view, which shows all entries for an item listed by date with the newest entry first. The Detail view provides means to filter or search the audit trail. Entries are displayed in Summary or Detail View and can be filtered by date or searched by a keyword. Authorized users may also add Manual Entries to the audit trail, and print the displayed information or export it to a PDF-File.

In the acquisition client, the audit trail viewer is launched from the respective method or sequence panel. In the data analysis client, it is opened from the Audit/E-sign ribbon tab or the context menu of an item in the navigation tree. The sequence audit trail can be reviewed in the acquisition and the data analysis client.
Each audit trail entry includes:

- **State of the entry** – annotates new entries, that were not yet saved and manual audit entries
- **User name** – full name, if configured in the OpenLAB Control Panel, otherwise the login name,
- **Date and time stamp of the change,**
- **Detailed description of the change,**
- **Host name of the PC** the software client was launched from when the change was done,
- **Reviewer name / date of review** – populated when the audit trail is reviewed and saved,
- **Reason of change** – if enabled for the project (see below),
- **Category** of the audit trail entry – for example: new, method linking, reprocessing, manual entry, audit trail review, saving, affected instrument module etc.,
- **Sample and data file name** of the injection (result set audit trail only).

Users may also add Manual Entries, such as user comments, to the audit trail, and print the displayed information or export it to a PDF-File.

### 21.4.2 Audit Trail Review

The Review function facilitates a review as mandated by the regulations. It enables a frequent and documented review. Records that have not yet been reviewed are clearly marked.

As long as an audit trail has not been reviewed, the entries are shown with a purple (magenta) background. Reviewed entries are shown with a grey background. During the review, an authorized user can inspect all new entries. If required, the user will need to scroll down until the last not reviewed entry at the bottom of the list is visible. By clicking the Review button the user completes the review. The Review button is active only after the user has scrolled down to the last new entry. The background color changes from magenta to grey. Two new entries are added to the audit trail, documenting that it has been reviewed:

- the recording of the review action and,
- that all reviewed entries are marked as such.

The action is completed by saving the data. Once the user has saved the data, the changed audit trail will be saved along with it.

### 21.4.3 Activity Log of Data Storage

The Activity Log of the data storage system is a record showing who accessed the system and when, and what operations he or she performed during a given period of time. The log contains file-related, system administration and folder administration entries. Each transaction is documented with the identity of the operator, the dataset and a date and timestamp. For example, administrators can see when a file was added and who added it. For each operation, the central data storage system asks the user for a reason. This reason is also shown in the Activity Log. For automatic uploads there are default reasons given by the system.

In OpenLAB Data Store the Activity Log is always enabled.
21.5 Log Files

21.5.1 System Activity Log

The System Activity Log contains detailed information on the various events associated with the OpenLAB Server or with specific instruments. It is a centralized view of the audit logs and can access all entries. Users 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.

Event messages can originate from different components, for example user management or instruments. The following types of events (subsystems) are recorded and reflect the origin of the message:

- System
- Instrument Management
- Instrument
- Project Management
- Instrument Controller
- User
- Group
- Role
- Security
- Printer
- License
- Data Processing

Events can include system messages, warnings and errors. The System Activity Log records these events irrespective of whether the user has been alerted by the system or not. For each entry there is a one-line overview with date/time stamp, affected user and short description in the Activity Log Viewer. The entry can be expanded to reveal more information such as type, affected subsystem, source PC and detailed description.

The system activity log can be exported, printed and selections can be copied to the clipboard. The output is provided in two formats – summary and detailed.

21.5.2 Instrument Activity Log

The Instrument Activity log is a simplified view of the System Activity Log that is accessed from the instrument panels. 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 Instrument Activity Log. The logbook records these events irrespective of whether the Activity Log window is displayed or not. The information is shown in tabular format and can be filtered by user, description and date. The following information is logged for each event:

- Date and time stamp of the message,
- User name – full name, if configured in the OpenLAB Control Panel, otherwise the login name,
- Description of the event,
- Details on the activity, for example, run and injection information upon the start of a single sample analysis.

The Activity Log displays the last 1000 records of Acquisition activity. The Log Viewer Window provides means to filter or search by user, description, and date range.
Events automatically added to the log include:

- Submission of a single run or sequence,
- Addition of an item to the run queue,
- Start of a run in the run queue,
- Start or end of an injection, and
- Submission of an item for processing.

The instrument conditions, such as flow, temperature, pressure and solvent composition for liquid chromatographs may be continuously recorded and stored with each data file as instrument curves. 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.

21.5.3 Processing Log

The processing log shows the errors, warnings, or success messages that occurred during the most recent reprocessing. These messages are indicated by a symbol in the injection tree and can be also viewed in a tooltip by hovering over the symbol.

There are two types of processing log files:

- The result set log contains all messages for the entire result set.
- The injection log contains only the messages for the selected injection.

The processing log files can be inspected in the Log Viewer window. By default, a summary view is displayed, which shows all the entries grouped by category. The detail view shows all entries listed by date with the newest entry first.

Each processing log file entry includes:

- State of the entry – annotates whether it is an error, warning or success message.
- Category of the entry, for example processing error,
- Message content,
- Sample and data file name of the injection (result set log only),
- Date and time stamp of the message,
- User name – full name, if configured in the OpenLAB Control Panel, otherwise the login name.

Users may print the displayed information or export it to a PDF-File.
22 Instrument Control

Instrument drivers provide the functionality and user interface for the instrument setup and configuration, instrument control, acquisition method parameter setup and modification, and instrument status monitoring.

Agilent developed the RapidControl.NET Instrument Control Standard (RC.NET standard) for direct instrument control. This standard is also open to other analytical device manufacturers and enables them to develop their own drivers for OpenLAB CDS. All drivers supported in OpenLAB CDS are based on this standard.

The drivers are seamlessly embedded in OpenLAB CDS. OpenLAB Control Panel is used for the setup and configuration of instruments (see section 12.1). The acquisition client hosts the user interface for managing acquisition methods as well as the instrument dashboard (see chapter 16).

Instrument driver packages can be deployed independently from OpenLAB CDS, which means adding a new instrument to the system does not affect or alter the installed CDS software. Therefore adding a new instrument driver has a very limited impact on the system.

The instrument control capabilities are documented in the following sections, each relating to a specific technique.

The supported instruments and firmware are further detailed in the OpenLAB CDS Requirements Guide (see section 24.4). For more details on the instrument capabilities please refer to the corresponding hardware manuals (see section 24.3).

22.1 Gas Chromatography

22.1.1 Instruments

The OpenLAB CDS combines instrument control, data acquisition, and data analysis for the Agilent 7890 series, 7820, 6890 series, and 6850 Series gas chromatographs (GC), the Agilent 490 Micro GC and the 35900E series dual channel interfaces.

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

When interfaced to an Agilent gas chromatograph, the Agilent OpenLAB CDS 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; please refer to the instrument’s user manual for a full list of parameters. OpenLAB CDS can display graphically the oven temperature, inlet temperature, inlet pressure, auxiliary channel pressure, and column flow programs. OpenLAB CDS also can control, through a timetable, valves or relays for gas sampling and other applications.

22.1.2 Sampling Systems

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

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

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

The Agilent 7697A or G1888 Headspace Samplers and the Agilent 78xx and 68xx GCs can be added to the system and controlled within the OpenLAB CDS.

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

22.1.2.1 Barcode Reading

The 7693 series ALS 150 vial tray with optional bar code reading and heating can be used to help build automation sequences and verify that the identity of the injected sample matches the name in the sequence table at injection time. The instrument has to be configured for Sample Identification. See also sections 16.4.2 and 17.2.5.
22.1.3 Method Resolution

When loading a method, the system automatically verifies that method and current instrument configuration are consistent. It alerts the operator of potential issues by displaying the differences in a method resolution report. For example, it will detect if a method was created on a different GC system or if the instrument configuration has changed.

The system checks the following for hardware consistency (depends on GC system type):

- Autosampler: front ALS presence, back ALS presence and tray presence
- Inlet presence, type and cryo type
- Detector presence and type
- Thermal Aux presence
- Pressure Aux presence, type and PCM channel B control mode
- Valve Box presence

The method resolution process tries to fix the method in a consecutive step. During the review of the changed method in the method resolution editor the user has the following two options:

- **Resolve the changed method** - Review all method parameters and fix as needed.
- **Cancel** – the system does not update the method or GC. The user can load a different method or view the method parameters. The method resolution process is terminated.

After the method has loaded, the operator has to verify all parameters, including maximum oven temperature, review the Events table and update it to match the new configuration, if necessary. Finally the resolved method is saved.

22.1.4 Maintenance

The GC Maintenance panel can be accessed from the Control Ribbon Tab. It consists of three tabs – Early Maintenance Feedback Counters, Maintenance Log and Maintenance Actions.

The availability of Early Maintenance Feedback (EMF) depends on the GC type. Early Maintenance Feedback tracks the GC’s consumable resource and part usage, and alerts users before they need to be replaced or serviced. User can configure two limits (Warning and Service due) for each consumable resource or part. For details about the EMF counters for any instrument, refer to its operating manuals.

Maintenance events, the time, and any associated messages are tracked in a Maintenance Log.

Maintenance actions include the import of EMF limits from a file, or the export of the current limits to a file, synchronization of GC and PC clock and other configuration-specific tasks.

22.2 Liquid Chromatography

OpenLAB CDS controls and acquires data from the Agilent InfinityLab LC Series, the Agilent 1200 Infinity Series, the Agilent 1200 Series and the Agilent 1100 Series. They include modules for solvent delivery (pumps and degassers), sample injection and column thermostats, valve solutions, detectors and many others. Instrument control is provided through module drivers.

For all modules the user may set a stop time and optionally post-run time, for example for column equilibration. Typically the stop time is set for one module, the pump or the injector, and other modules are set to “As Pump/Injector” for the stop time. However, depending on the application, individual times may be defined. A new run can be started as soon as all modules have completed the previous run including the post time. If no stop time is set, the instrument will continue until it is stopped manually. An automatic module turn-on time (date and time) can be set for each module, for example to allow for sufficient equilibration time in the morning before the operator comes in and submits the first sequence of the day.

For a detailed and current list of all supported modules please refer to the OpenLAB CDS Requirements Guide (see chapter 24) and the driver release notes delivered with each new version of the Agilent instrument drivers (included on the driver DVD).
22.2.1 **Solvent Delivery Systems**

All solvent delivery systems offer parameters for solvents, the solvent composition, the flow rate and pressure limits. A time-table can be used for defining composition gradients and modifying other parameters like flow rate and pressure limit over time. These parameters can be viewed graphically.

OpenLAB CDS supports an extensive list of solvent delivery systems that include isocratic, binary and quaternary pumps.

22.2.2 **Sampling Systems**

The injection systems may be manual or automated with an autosampler, well-plate sampler or a multisampler. All automatic injectors may be programmed for different injection volumes, the speed of injection and the injector wash procedure (e.g. needle wash, needle seat flush). The user may also use a complete injector program for sample dilution, standard addition or sample derivatization.

22.2.3 **Column Compartments**

The following Agilent column compartment types are supported:

- Multicolumn Thermostats (MCT),
- Thermostatted Column Compartments (TCC) and
- Integrated Column Compartments (ICC)

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

Valve-Thermostat-Clusters (VTC) allow the combination of multiple internal and external valves and temperature zones in column thermostats for switching between up to 32 columns and sophisticated temperature control.

22.2.4 **Valves**

For a detailed and current list of all supported valves please refer to the *OpenLAB CDS Requirements Guide* (see section 24.4).

22.2.5 **Detectors**

OpenLAB CDS supports multiple UV/Vis based detector types such as Diode Array Detectors (DAD), Variable Wavelength Detectors (VWD), Multiple Wavelength Detectors (MWD) and Fluorescence Detectors (FLD). In addition OpenLAB CDS provides control of special detectors, such as Evaporative Light-Scattering Detectors (ELSD) and Refractive Index Detectors (RID). Mass-based detectors are covered in section 22.3.

22.2.5.1 **UV Detection**

UV detection comprises the following detectors:

- Variable Wavelength Detectors
- Multiple Wavelength Detectors
- Diode Array Detectors

The Agilent OpenLAB CDS software can simultaneously acquire multiple chromatographic and reference signals each with an independent bandwidth. The data and spectra acquisition rate and the maximum number of signals depend on the capabilities of the individual detector in use. Spectral data from all DADs may be acquired in a peak-controlled or full acquisition mode. Depending on the detector model up to 8 different spectra acquisition modes are available:

- **None** — No spectra are taken.
- **Apex** — A spectrum is taken at the apex of the peak.
- **Apex + Baselines** — Spectra are taken at the apex, and baselines of the peak.
- **Apex + Slopes** — Spectra are taken at the apex, upslope, and downslope of the peak.
- **Apex + Slopes + Baselines** — Spectra are taken at the apex, baselines, upslope, and downslope of the peak.
• **All in Peak** – All spectra within the peak are taken.

• **Every 2nd spectrum** – Spectra are taken continuously, but only every second spectrum is stored; other spectra are discarded. This reduces the amount of data storage necessary.

• **All** – Spectra are taken continuously depending on the setting of the peakwidth. Eight spectra are acquired per peakwidth.

The wavelength range for spectra storage can be set by the user as well as the spectral resolution. A threshold value defines the height of the smallest expected peak. Smaller peaks will be ignored by the peak detector and peak spectra will not be saved. The spectral resolution can be influenced by the slit width. The possible values depend on the detector hardware.

All Detectors may have the initial parameters changed during a run by a time-based program.

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

22.2.5.2 Special Detection

Special detection summarizes the following detectors:

• Fluorescence Detectors (FLD)
• Refractive Index Detectors (RID)
• Evaporative Light Scattering Detectors (ELSD)

The Agilent FLDs may be programmed for single wavelength or simultaneous multiple wavelength detection and spectra acquisition. Up to four signals at different excitation or different emission wavelengths may be obtained. Within a timetable initial excitation or emission wavelengths, response time, PMT Gain and baseline behavior as well as spectral parameters may be changed. Excitation or emission spectra can be watched online and stored. Spectral data from capable FLDs may be acquired in a peak-controlled or full acquisition mode. The available spectra modes are:

• **None** – No spectra are taken.
• **Apex** – A spectrum is acquired at the apex of the peak.
• **All in Peak** – All spectra within the peak are acquired.
• **All w/o signal** – All flashes are used for spectra acquisition. The mean value of all measured wavelengths is shown on channel A. This setting is useful for unknown spectra. Spectra are acquired continuously.

The wavelength range for spectra storage can be set by the user as well as the spectral resolution. A threshold value defines the height of the smallest expected peak. Smaller peaks will be ignored by the peak detector and peak spectra will not be saved. Optionally the spectral range can be adjusted so that there is always a difference of at least 25 nm between the excitation wavelength and emission wavelength.

Depending on the model the Agilent RID provides maximum signal acquisition rates of more than 100 Hz and an electronically maintained steady optical unit temperature. During the course of an analysis the RID can be programmed with a timetable to change polarity and peakwidth of the acquired chromatographic signal.

The Agilent ELSDs deliver evaporation down to 10 °C and up to 120°C. The available temperature range varies by product. Initial parameters include a digital filter, which can be set to optimize signal-to-noise ratio and peak shape, gain and signal offset. Some initial parameters including the temperature can be changed during a run using a time table.

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

22.2.5.3 HDR Cluster

A cluster allows combining several modules into one logical unit. Such a cluster is shown as a single instrument module in the OpenLAB CDS. The 1290 Infinity and Infinity II HDR Clusters consist of two DADs, one with a long flow cell (for example, 60 mm), the other with a short flow cell (for example, 10 mm). The signals from the two DADs are combined to produce a high-dynamic-range signal, which allows detecting compounds with very low concentration (e.g. impurities) next to high concentration compounds (target substance).
22.2.6 Maintenance and Diagnostics

The Agilent Lab Advisor is a maintenance, diagnostics and calibration software toolset that can be added for maintaining and diagnosing the Agilent LC systems. It is independent of OpenLAB CDS and provides full diagnostic and maintenance capabilities including an extended list of tests and calibration procedures. For more information please refer to section 24.3.

22.3 Mass Spectrometry

22.3.1 Instruments

22.3.1.1 GC/MS

OpenLAB CDS controls and acquires data from all current Agilent 5975 and 5977 GC/MS Single Quadrupole (SQ) systems (with the exception of the integrated 5975T GC/MSD), in Electron Ionization mode only. The GC/MS system can be used with any of the Agilent GC and Sampling System hardware supported by OpenLAB CDS.

22.3.1.2 LC/MS

The OpenLAB CDS provides instrument control, data acquisition, and data analysis for the current 6100 Series LC/MS Single Quadrupoles (SQ) systems, namely the G6120C and G6130C LC/MS SQ systems. The supported sources include Electrospray (ESI), APCI, APPI, Agilent Jet Stream ESI, and Multimode Source. The LC/MS system can be combined and used with the Agilent 1100 and Agilent 1200 Infinity Series modules and systems for LC supported by OpenLAB CDS.

22.3.2 MS Tuning and Calibration

When the MS is used as a detector for chromatography, a mass spectrum is associated with each data point in the chromatogram. To obtain high quality, accurate mass spectra, the MS must be optimized to

- Maximize sensitivity
- Maintain acceptable resolution
- Ensure accurate mass assignments.

Tuning is the process of adjusting MS parameters to achieve these goals.

The software provides two ways to tune the MS:

- **Autotune** is an automated tuning algorithm that tunes the MS for good performance over the entire mass range.
- **Manual Tune** allows the advanced user to adjust MS parameters to meet user-defined criteria. Manual tuning is an iterative process of maximizing sensitivity while maintaining acceptable resolution, ensuring accurate mass assignment, and providing the desired relative abundance across the spectrum. It is most often used when maximum sensitivity is required, when a restricted mass range is to be targeted, or when a tuning compound other than the standard calibrant is needed.

Both LC/MS and GC/MS can be tuned through the OpenLAB CDS by the automated introduction of a calibrant and tuning for adjusting signal intensity, mass transmission, resolution and mass accuracy.

The tuning operations further include a **Checktune (LC/MS)** or **Tune Evaluation (GC/MS)** functionality, where a calibrant is introduced and a report is generated, but no parameters are changed.

Multiple tune files can be stored in the OpenLAB CDS. Each MS acquisition method is linked to a corresponding tune file. Most recent tune reports are stored with all acquired data.

All tune operations are protected by user permissions which are configurable in the OpenLAB CDS Control Panel.

22.3.3 Instrument Control (Acquisition)

Data from an LC/MS or GC/MS is acquired using either Selected Ion Monitoring (SIM) or Scan mode, or a combination of both (GC/MS only).

SIM ions and Scan parameters can be time programmed. The MS method can have different time segments. Each time segment can have different values for the MS parameters and the acquisition type (LC/MS only). The user interface changes depending on which Scan Type is selected.

For both, LC/MS and GC/MS, the MS parameters are set as part of the acquisition method in the same way that the GC and LC parameters are set. The parameters for the MS are stored in the same method as the LC or GC parameters.
22.3.3.1 LC/MS Acquisition Method
The MS acquisition parameters include: the ion source, the stop time (typically determined by the LC pump) and the tune file to be used. The fast electronics of the LC/MS enable ultra-fast scan speeds and rapid polarity switching for certain models.

In Scan mode the following parameters are entered for time-programming:

• Start time (min) of the time segment
• Segment name
• Start Mass (m/z) of the mass range over which to scan
• End Mass (m/z) of the mass range
• Scan Time (ms)
• Fragmentor (V) – controls the applied voltage
• Polarity

The scan speed (u/sec) is not set directly; it is calculated based on the start and end mass, and the scan time. Users may optionally change the values of the scan time (ms) manually. A threshold value determines how large a signal must be for it to be saved.

In SIM Mode the following parameters are entered per time segment:

• Start time (min)
• Compound Name
• ISTD – whether or not the compound is the internal standard
• Ion mass(es) (m/z)
• Dwell time (ms) – length of time for the detector to count the ions
• Fragmentor (V)
• Polarity

The cycle time is calculated automatically using the number of masses in the table and the dwell time.

Scan data can be saved in the data file as centroid or profile data. With centroid storage the m/z values and the abundance are recorded at the mathematical center of mass of the analog data. Centroid MS data shows discrete m/z values. A single m/z and abundance data point is recorded. The file size is significantly smaller with centroid data. Profile MS data shows a collection of signals over multiple scans.

Chromatograms for online display can be defined separately. Available choices are the Total Ion Chromatogram (TIC), Channel TIC (TIC per segment), Extracted Ion Chromatograms (EIC) and a Base Peak Chromatogram (BPC) which allows setting masses or mass ranges to be excluded. The real-time chromatograms are not permanently stored.

The data storage mode is set in the Tune user interface, where the scan type can be set as:

• MS Scan – centroid MS data
• MS SIM
• MS Profile – profile MS data

LC/MS has a divert valve that is time programmed to allow switching the LC to waste at specified times during the run.

22.3.3.2 GC/MS Acquisition Method
The GC/MS acquisition parameters defined in the method include run time (typically determined by the GC oven), solvent delay, Electron Multiplier (EM) mode (Gain Factor, EM Volts or Delta EM Volts), tune file to be used, and acquisition type - besides SIM and Scan mode, the GC/MS provides a simultaneous SIM/Scan mode.

In Scan mode (centroid) the following parameters are entered for time-programming:

• Start time (min)
• Start mass (m/z)
• End mass (m/z)
• Scan speed (u/sec)
• Threshold
In SIM mode the following parameters are entered for time-programming:

- **Start Time (min)**
- **Group Name** – a descriptive name for this SIM time segment.
- **Ion Count** – the calculated number of SIM ions defined for this time segment (read only).
- **Total Dwell Time (ms)** – the calculated sum of all dwell values for each ion specified for this time segment (read only).
- **Cycle Time (ms)** – calculated from the scan speed, mass range, and step size (read only).
- **Resolution** – high or low resolution.
- **EM Mode** – depending on the selected mode for acquisition the value for gain factor, EMV or Delta EMV can be specified per time segment.
- **Applied EM Volts** – automatically populated based on EM settings.

The corresponding SIM ions for each time segment are defined in the SIM Ion Table. Users may enter:

- **Compound name for the SIM ion**
- **Ion mass(es) (m/z)**
- **Dwell time (ms)**
- **Plot ion** – select ion signal for real time display during the run.
- **Create Signal Data** – select ion signal for permanent storage as 2D signal (without MS spectra) as part of the MS data set. These signals can be used for processing in a 2D method mode.

There is a maximum of three scan time segments allowed. For SIM/Scan operation, only one scan time segment is allowed. The values for frequency, cycle time, and step size are calculated by the system and displayed for each time segment. The maximum number of SIM time segments allowed is one hundred. Up to 60 ions for each SIM time segment can be set in the SIM ion table.

Under Chromatograms, the user can select what signals to plot in the real time display, and optionally select that these signals be saved as ‘chromatographic’ signals in addition to the 3D-MS data.

With Timed Events the acquisition parameters can be modified during a run. The EM parameters available in the Timed Events panel of the method editor dynamically change depending on the initial setpoints defined in the detector settings of the acquisition parameter panel. The user enters a time when the event is to be triggered, the event type that is changing, and, if required, the new value.

### 22.3.4 Maintenance and Diagnostics

Common instrument diagnostics and maintenance functions for the GC/MS detector, including Venting, are collected under Maintenance and Diagnostics. These functions are used by users and trained Agilent service personnel to troubleshoot the GC/MS operation. Details on each function are available in the user documentation.
22.4 3rd Party Instrument Control

Due to the standardized interface definition of the RC.NET instrument control standard, instrument drivers for advanced control of instruments not only from Agilent Technologies but also from other vendors can be deployed. This standard is open to other analytical device manufacturers and enables them to develop their own drivers.

The list of supported instruments continues to expand. As a result the following information is only an excerpt of what may be currently available, so please ask your Agilent Sales representative for the full list of supported instruments.

22.4.1 Waters Acquity LC

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

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

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

For more details, please refer to the full documentation set shipped with each driver on the 3rd Party Instrument Media kit.
22.5 A/D Converters

An A/D converter allows the system to acquire data from an instrument or detector that is not directly interfaced for data acquisition; for example, an instrument that cannot be connected using LAN, or a third party instrument, which does not come with an RC.Net driver for OpenLAB CDS.

An A/D converter can be configured as a generic module for all instrument types in OpenLAB Control Panel. It either connects an independent instrument or attaches a detector to an existing LC or GC instrument.

22.5.1 35900E Series Dual Channel Interface

The Agilent 35900E dual channel interface allows configuring one or two analog signals per instrument; 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. During configuration a TTL I/O state can be assigned to a selectable action in the method editor event table. Only configured events can be selected in a method.

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

22.5.2 SS420x Analog/ Digital Converter

The SS420x is an intelligent 24-bit analog to digital conversion module that provides remote acquisition for up to 4 channels of data. The channels can be started or stopped independently for up to four instruments or detectors. It supports data acquisition rates of up to 120 Hz depending on the used base frequency. The user can configure the base frequency of the SS420x and, for each channel, the gain range, channel name and, Y-axis unit and multiplier.

The SS420x has four built in triggers and eight relay outputs for programmable switching applications. The eight relay outputs allow the selection from three possible states: Open, Closed, Last State. The four run trigger inputs allow the selection from two possible states: Open, Closed.

For the acquisition the user can enable up to four channels, select the sampling rate per channel and enter an individual acquisition delay time, if needed.

The following event types can be configured for external event control for each channel:

• Trigger signal – input from an external device to initiate the start of a run.
• Ready signal – output to external device to indicate “device is ready for injection”.
• Valve / external event – output to external device.

The configured event types can be time-programmed during a run.

For most current information and more details on the instrument capabilities please refer to the corresponding user manual.
23 OpenLAB Help and Learning System

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

- **Getting Started** facilitating an easy learning experience for basic operation and familiarization with the principles of the software,
- **Context Sensitive Online Help** covering usage of the individual CDS components, and
- **User documentation** covering installation, set-up and administration.

The Agilent OpenLAB CDS software is provided on a read-only USB stick containing all required installation files and documentation. The Help and Learning Platform is installed as part of the Software installation, alternatively it can be installed standalone, on computers where the OpenLAB CDS software is not installed.

The entire user information can be accessed via a searchable common platform called “OpenLAB Help and Learning”. It includes all user assistance material available for the OpenLAB CDS (including system setup and maintenance), complemented by the instrument driver help for the installed drivers as well as selected instrument guides.

The OpenLAB Help and Learning system is accessible in different ways:

- Via a desktop shortcut,
- By clicking the “?” icon on the top right of any OpenLAB CDS software panel, or
- From the OpenLAB CDS software user interface, via specific Help Topics, that open context sensitively with the F1 key.

In addition to the electronic files installed with the software as part of the Help & Learning system, all documents are provided as *.PDF files in the doc folder on the installation USB stick (see section 24.4 for more details).

### 23.1 OpenLAB CDS Getting Started

The powerful new Getting Started Modules helps users to easily learn the new functionality and main aspects of OpenLAB CDS at their own pace, whenever they need it. The modules walk users through detailed steps of using the OpenLAB CDS software. A specific module is dedicated to each instrument control technique, covering LC, GC, LC/MS or GC/MS control.

The on-demand eLearning materials give users a new experience where they not only learn the concepts, but are learning through task-based software simulations. This allows users to get the experience of using OpenLAB CDS software even without an installation of the software.

OpenLAB CDS Getting Started Modules are available in English, Japanese, Chinese and Brazilian Portuguese, and are continuously updated to cover new software functionality introduced by new releases.

### 23.2 OpenLAB CDS Help (How To)

OpenLAB CDS includes comprehensive, HTML5-based, context sensitive and indexed online help. The detailed explanations are backed up by graphics where appropriate, and may be printed, or copied to the Windows clipboard for incorporation in the user’s own documentation.

Context sensitive Help is available for the following components:

- Control Panel
- Acquisition
- Data Analysis
- Reporting
- Custom Calculations Editor
- Instrument Drivers
23.3 OpenLAB CDS System Setup and Maintenance

The OpenLAB CDS software product comes with a series of installation manuals that cover the prerequisites for the installation, the installation and the configuration as well as the technical transition from earlier versions of the OpenLAB CDS, ChemStation, EZChrom Elite or ICM:

1. Hardware, software and network requirements, and supported instruments:
   ○ OpenLAB CDS Requirements Guide

2. Technical Transition:
   ○ Technical Transition to OpenLAB CDS (multiple documents), see section 24.5 for details

3. Installation, system setup and maintenance procedures specific to the purchased configuration:
   ○ OpenLAB CDS Workstation Guide
   ○ OpenLAB CDS Client/Server Guide

24 Further OpenLAB CDS Documentation

Further documentation is available on the Agilent Website:

• Information specific to Central Data Storage (OpenLAB Data Store),
• Technical Notes with further information not covered by the user documentation listed in chapter 23, and
• Hardware Manuals not included with the OpenLAB CDS Help and Learning System.

24.1 Understanding and Customizing OpenLAB CDS

A set of reference and user manuals are electronically provided with the OpenLAB CDS product:

1. Reference information on the principles of calculations and data analysis algorithms for advanced users:
   ○ OpenLAB CDS Data Analysis Reference Guide

2. How to create custom calculations with examples and references:
   ○ Custom Calculator User Guide

As part of the user-contributed library, this manual covers the customization capabilities of the OpenLAB CDS Data Analysis:

• Data Analysis Customization Guide
24.2 OpenLAB Data Store

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

- OpenLAB Data Store Hardware and Software Requirements Guide
- OpenLAB Data Store Installation Guide
- OpenLAB Data Store Administration Guide

Additional “How To” Information is given in the OpenLAB Data Store Online Help system, which is accessible from the Data Store user interface.

24.3 Technical Notes, User Manuals and other References

Technical notes, user manuals and further publications are available from Agilent website. The following items were referenced in this document:

- OpenLAB CDS 2.0 Workstation Site Preparation Checklist:
- Agilent Original Bundle PC (Technical Note, 5990-7990EN)
- Agilent Lab Advisor software web page:
- Support for Title 21 CFR Part 11 and Annex 11 compliance: Agilent OpenLAB CDS version 2.0 (White Paper, 5991-6492EN)
- Agilent CrossLab Compliance - Document Approval web page:
- Equipment Qualification Plan (EQP) Review Documents for Hardware and Software:
- Standard EQP Review Document for Software (includes detailed description of complete Software OQ Test Suite):

For recent user manuals (for example hardware manuals) please refer to the Agilent website:

Enter the product number of the instrument in the search field to retrieve the related user manuals.
## 24.4 Documentation and Manuals on the OpenLAB CDS USB Stick

The following manuals and documents are included on the OpenLAB CDS USB stick; some of them are also installed with the Help and Learning System:

<table>
<thead>
<tr>
<th>Document Title</th>
<th>Target User Group</th>
<th>Part Number</th>
<th>File Name</th>
</tr>
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<tbody>
<tr>
<td>End User License Agreement</td>
<td>Administrator</td>
<td>M8410-90100</td>
<td>OpenLAB_license_terms.pdf</td>
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<tr>
<td>OpenLAB CDS Requirements Guide</td>
<td>Administrator</td>
<td>M8410-90020</td>
<td>OpenLABRequirements2.0.pdf</td>
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<tr>
<td>OpenLAB CDS Quick Reference Sheet</td>
<td>Analyst</td>
<td>M8418-90060</td>
<td>OpenLABCDS.pdf</td>
</tr>
<tr>
<td>OpenLAB CDS Data Analysis Reference Guide</td>
<td>Scientist, Analyst</td>
<td>M8410-90030</td>
<td>DataAnalysisReference2.0.pdf</td>
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<td>Data Analysis Customization</td>
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<td>M8410-90090</td>
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<td>License Generation Form</td>
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<td>M8410-90070</td>
<td>CDS_LicenseGenerationForm.pdf</td>
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<td>Record of Agilent OpenLAB CDS License Change</td>
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<td>OpenLAB CDS Declaration of Software Quality</td>
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<tr>
<td>OpenLAB Data Store Release Notes</td>
<td>Administrator</td>
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<tr>
<td>OpenLAB Data Store Hardware and Software Requirements Guide</td>
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<tr>
<td>Agilent 6100 Series Single Quadrupole LC/MS Systems Installation Guide</td>
<td>Administrator</td>
<td>G19660-90088</td>
<td>LCMS_Quad_Installation.pdf</td>
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</table>

Note: For all documents with the exception of the Declaration of Software Quality documents there are also localized versions available (Japanese, Chinese and Brazilian Portuguese).

Drivers and documentation for 3rd Party Instrument Control are contained on a separate 3rd Party Instrument USB stick.
### 24.5 Transition Guides

The following migration guides are available in the Help & Learning Platform, or from the Agilent website.

<table>
<thead>
<tr>
<th>Document Title</th>
<th>Target User Group</th>
<th>Part Number</th>
<th>File Name</th>
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<tr>
<td>Transitioning from OpenLAB CDS ChemStation Edition to OpenLAB CDS 2.0 - Workstation to Workstation</td>
<td>Administrator</td>
<td>M8420-90050</td>
<td>MigrationGuide__OpenLABCDSChemStnToCDS2.0.pdf</td>
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<tr>
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<td>M8420-90070</td>
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<td>M8420-90080</td>
<td>MigrationGuide_EZChromEliteToCDS2.0.pdf</td>
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