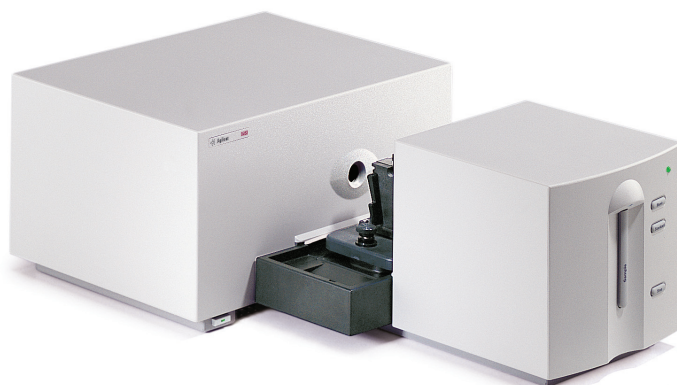# Agilent UV-Visible ChemStation for Spectroscopy Rev. B.05.01

Specifications

The Agilent ChemStation for UV-Visible spectroscopy provides instrument control, data acquisition, and data evaluation for the Agilent diode-array UV-Visible spectrophotometers for general purpose, dissolution, advanced, and biochemical analysis. Six software modules are available:

• General Purpose Software

• Advanced Software

• Biochemical Analysis Software

• Dissolution Testing UV-Visible ChemStation Software

• Security Pack for the UV-Visible ChemStation

• OpenLAB ECM Compliance Pack for the UV-Visible ChemStation (compatible with OpenLAB ECM version 3.4.1)

The UV-Vis ChemStation software is compatible with these Microsoft® Windows® operating systems:

• Windows 7 Professional 32-bit (SP 1) and 64-bit (SP 1)

• Windows Server 2003,

• Windows Server 2008 32-bit (SP 1).

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UV-Visible ChemStation Software Overview

General Purpose UV-Visible ChemStation Software (G1115AA)

The General Purpose software is the core component with instrument control, data acquisition, and standard data evaluation capabilities. The General Purpose software includes an additional mode that allows diagnosis and verification of the Agilent 8453 spectrophotometer. It is designed for ease of use in the routine laboratory or for the occasional user.

With the General Purpose software you can:

- Measure absorbance at up to six wavelengths simultaneously

- Measure spectra and automatically find peaks and valleys

- Use a user-definable equation for evaluation using up to six wavelengths, weight, and volume (for example, ratio at two wavelengths)

- Perform single component quantification

- Automate the measurement of standards, controls, and samples

Advanced UV-Visible ChemStation Software (G1116AA)

The Advanced ChemStation software adds extended spectral processing, advanced single and multi-component quantification capabilities to the General Purpose ChemStation software.

With the Advanced software you can:

- Perform extensive interactive mathematical operations with spectra

- Compare and compose spectra

- Define up to four equations simultaneously

- Perform up to four data analyses, or one main analysis and up to three confirmation analyses in parallel

- Perform multicomponent analysis with calibration based on pure or mixed standards

- Optimize the parameters for quantitative analysis with specific algorithms

- Configure reports

- Set up a complex sequence of automated analyses

Biochemical Analysis UV-Visible ChemStation Software (G1117AA)

The Biochemical Analysis ChemStation software adds single cell kinetics, multicell kinetics and thermal denaturation (DNA melt) capabilities to the general purpose software.

With the Kinetics software you can:

- Measure time traces at up to six wavelengths on one cell

- Measure time traces on up to seven cells in parallel (multicell option)

- Correct for background absorbance

- Evaluate the reaction rate

- Perform simple mathematical operations on time traces

With the Thermal Denaturation software you can:

- Measure temperature traces with user definable ramps (multiple up and down slopes)

- Determine transition temperatures (Tm) by first derivative or average absorbance methods

- Calculate a result by an equation based on Tm (for example, % GC)

- Correct for thermal expansion and molarity of the solvent

UV-Visible ChemStation Software Overview

Dissolution Testing UV-Visible ChemStation Software (G1118AA)

The Dissolution Testing ChemStation software adds single bath and multi bath dissolution testing capabilities to the General Purpose software.

With Dissolution Testing you can:

- Measure absorbance on up to 24 vessels offline

- Measure absorbance on up to six vessels, one blank and one control with an automated online sampling system including time control of the sampling

- Evaluate dissolution profiles

- Control and monitor dissolution baths (bath driver required)

- Set up complex pre-run and post-run sequences including operator guidance

- Use the data analysis features of the Advanced ChemStation software

- Correct results for volume changes

- Re-evaluate saved data

- Use four independent methods in case of multi-bath dissolution testing

- Configure customized reports

- Print combined reports on up to four dissolution runs (4 x 6 samples), including statistics according to the acceptance tables

Security Pack for the UV-Visible ChemStation Software (G1813AA)

The Security Pack is compatible with General Purpose, Advanced, Biochemical and Dissolution modes and supports the requirements for electronic records and signatures (21 CFR part 11). It extends the ChemStation to:

- Provide access control including user setup and password administration

- Prevent loss and unauthorized modification of raw data and metadata

- Add versioning on the ChemStation level to store all versions of a method to a new file

- Follow the detailed requirements for electronic records and passwords specified by the FDA 21 CFR, Part 11

- Allow the use of existing global groups and accounts for access control and user management

OpenLAB ECM Compliance Pack for the UV-Visible ChemStation Software (G5182AA)

UV-Visible ChemStation version B.05.01 is compatible with OpenLAB ECM version 3.4.1.

The Compliance Pack is compatible with General Purpose, Advanced, Biochemical and Dissolution modes and supports the requirements for electronic records and signatures (21 CFR Part 11).

The Compliance Pack provides a secure link to OpenLAB ECM allowing centralized control and administration of user privileges, system audit logs and electronic records storage. New features for this release include customizable UV ChemStation-specific user roles and user privileges. In addition it provides:

- Access control to ChemStation through mandatory login

- Use of existing global groups and accounts for user management, including password administration

- Customizable user roles and user privileges applied within ChemStation

- OpenLAB ECM file versioning for ChemStation files

- Full data security in the OpenLAB ECM database, including system audit trails

- A single comprehensive audit trail in the ChemStation application containing a record of all changes to data files

- Compliance with the detailed requirements for electronic records and passwords given by the FDA 21 CFR, Part 11

Common ChemStation Software Features

System Configuration

The instrument system is configured with the Configuration Editor program for instruments and controlled through a GPIB (Agilent 8453 spectrophotometer and Agilent 89090A Peltier temperature controller) or a LAN (Agilent 8453). Users can specify the connected instruments, the GPIB addresses, the directories for data, methods and automation files, and the color definitions for the ChemStation. Other accessories, which are controlled through the GPIO interface of the Agilent 8453, are configured from within the ChemStation software.

Networking

The software has been successfully tested for compatibility with the standard networking components of the Microsoft Windows environment. The offline version of the ChemStation is ideally suited to work on a networked PC enabling a user in an office to reprocess data at leisure without impacting the efficiency of the laboratory instrumentation.

Analytical Instrumentation

The ChemStation software controls and acquires data from Agilent 8453 spectrophotometers and the Agilent 89090A Peltier temperature controller. All control and data acquisition for these instruments is performed through the GPIB interface system (IEEE-488) or through a LAN (8453 only). The 89068C/D sipper and sampler accessories are controlled through the general purpose GPIO interface of the Agilent 8453.

The Agilent G1120A multicell transport accessory uses a dedicated interface on the Agilent 8453.

Data Analysis — Graphic

Data is displayed in graphic windows together with information about the samples in table windows. A combination of windows is called a view. In a view the windows are linked so that a change in one window automatically updates the other windows. 'Zoom', 'cursor', and 'tabulate data' functions are all available through point and mouse click.

The Microsoft Windows features of 'cut', 'copy' and 'paste' can be used to move data within the application or transfer data to other applications.

Data Analysis — Reporting

A variety of reporting options are provided from simple copies of windows to a fully detailed GLP-compatible report.

Printing Windows — any graphic or tabular window can be selected and printed. The hard copy includes a header with date, time, and number/title of the window printed.

Reports — all reports include a header on each page, which identifies the report by time, date page number, and a single line for a user-defined constant text. A print preview is available for all reports.

The report device and output format for a file may also be specified. When a file is specified as the destination, the software supports ASCII and Windows metafile (WMF) output formats. The ASCII files may be used by word-processing software and can be parsed into spreadsheet software. The WMF format is useful for transferring graphic information into word-processing software.

Methods

The analytical method, which is stored in a single file on disk, fully describes how a particular analysis is performed. It contains all the parameters for sampling system, instrument control, task selection, data acquisition, and data analysis.

Instrument Control and Data Acquisition

The integration times of the Agilent 8453 spectrophotometers can be varied from 0.1–25.5 seconds. Full or partial spectra can be acquired as single measurements.

Full diagnostics and verification of an Agilent 8453 can be performed. All features of the Agilent 89090A Peltier

temperature controller can be set from the software. They include setting the temperature, turning the stirrer on and off, adjusting the stirring speed, and selecting the temperature units (C,F,K). Data that is read from the Peltier includes actual temperature and external sensor temperature. If a Peltier is configured, the temperature information is automatically appended to each measured spectrum.

The status of all instruments is continually monitored and can be displayed in the status windows. On acquisition, spectra are automatically labeled with all information that is directly available to the system, including the data, time, operator name, Agilent 8453 serial number, cell path length, and temperature if the Agilent 89090A Peltier is being used. Additional information such as sample name, comment and sample properties such as component names or concentrations may be entered by the user as required. All this information is automatically stored with the spectra when they are saved to disk.

Computer

To operate correctly, the UV-Visible ChemStation software requires a PC with the following minimum specifications:

- 1 GHz 32-bit (x86) processor

- Microsoft Windows operating system: Windows 7 Professional 32-bit (SP 1) or Windows Server 2003

- At least 2 GB for Windows 7

- Hard disk drive with at least 40 GB free

- DVD drive

- Super VGA color monitor

- 256 colors and 1 MB video RAM. Small fonts are recommended

- A LAN interface or an appropriate GPIB interface

The UV-Visible ChemStation software has been tested on Hewlett-Packard PCs that meet the above specifications. Although the software is designed to be compatible with other PCs, Agilent Technologies will not necessarily accept responsibility for defects reported on such hardware.

Printers

The ChemStation software operates with any Microsoft Windows compatible printer directly connected to the PC or a Microsoft Windows compatible printer connected through a Local Area Network (LAN). Printer performance enhancement hardware should operate correctly with the system but is neither supported nor recommended.

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