

Agilent ChemStation for UV-Visible Spectroscopy: Advanced Software

Specifications

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Common Features

Agilent 8453 UV-visible spectroscopy systems are based on a PC-controlled spectrophotometer and a range of software products, each with features that meet the needs of specific user groups. Agilent 8453 UV-visible spectroscopy systems include:

- · Agilent 8453 spectrophotometer
- Agilent ChemStation general purpose software for UV-Visible spectroscopy*
- · PC with monitor
- Microsoft[®] Windows[®] 7 Professional 32-bit operating system
- · HP Office Inkjet printer
- 1-cm quartz cell and check-out sample
- * Additional software products are available for advanced tasks, kinetic measurements, thermal denaturation, dissolution testing, ECM access or compliance with 21 CFR Part 11 (Security Pack).

Ease of Use

Agilent 8453 spectroscopy systems use symbolic graphics to:

- · make the system intuitive
- provide confirmation of the current status at a glance
- · provide visual confirmation of actions
- provide fast access to frequently performed activities

Stored methods include all necessary parameters to immediately start measurements after loading.

Regulatory Compliance

The built-in features of the Agilent 8453 spectrophotometer combine with Agilent ChemStation to make it easy to comply with all of today's regulatory requirements, including 21 CFR Part 11.

- A validation program which covers requirements for design qualification, installation qualification and operational qualification.
- The Agilent 8453 fulfils all requirements of the European Pharmacopoeia (EP) and United States Pharmacopeia (USP).
- Built-in tools for performance verification (EP and USP tests) and software validation.
- OQ/PV standards kit which meets the needs of both EP and USP for convenience and time saving.
- Compliance services are available for software and hardware with documentation created individuallually for the target configuration.

Productivity

The Agilent 8453 system with manual sampling is already a highly productive UV-visible spectroscopy system. For example, the setup of an automated analysis is done in a single dialog box. You can use automation to guide an operator through a series of manual measurements, or combine it without changes with sampling accessories to provide semi- or fullyautomated analysis. Automation controls the following sampling systems:

- the Agilent sipper system
- the Agilent XY autosampler
- · the Agilent multicell transport

Spectral Acquisition

All measurements contain full spectra, which allows:

- change parameters like wavelength, background correction or even data type without remeasuring
- change the data analysis mode without remeasuring, for example, quantification instead of an equation
- use the spectral information for identification, peak/valley find, or to diagnose measurement problems



Agilent Technologies

Flexibility

The Agilent ChemStation software is modular to provide the functionality required for different tasks. To meet these requirements, six additional software modules are available.

- General purpose software including verification and diagnostics, for standard applications.
- Advanced software for more capabilities in data evaluation, method development and automation.
- Biochemical analysis software, including kinetics and thermal denaturation.
- Dissolution testing software for single and multibath dissolution testing.
- * Access software module to the Agilent OpenLAB Enterprise Content Manager (ECM)
- Security Pack for compliance with FDA 21 CFR Part 11 (advanced and dissolution testing software only).

Agilent ChemStation for UV-Visible Spectroscopy: General Purpose Software

General Description

The general purpose software for Agilent ChemStation is the core software with instrument control, data acquisition, and a mode for standard data evaluation capabilities. A separate mode allows diagnostic and verification of the Agilent 8453 spectrophotometer.

The general purpose software is specially designed for ease of use in routine labs or for occasional users. It allows the following data types to be used:

- absorbance
- transmittance
- · first to fourth derivative

An Execute Advanced Method mode allows execution of any method that was developed using the advanced software for Agilent ChemStation.

Data Analysis Tasks

Fixed Wavelength(s)

- Data at up to six wavelengths can be extracted from the spectrum
- Different types of background corrections can be applied

Spectrum/Peaks

- Finds up to specified number of peaks and/or valleys in spectrum
- The last measured spectrum is annotated with peaks and valleys
- The found peaks of all spectra are displayed in a results window

Ratio/Equation

The Equation mode allows the user to enter an equation for the evaluation of data. The variables which have been entered for the samples are:

- Up to six specified wavelength values, weight and volume
- Mathematical functions include +, -, ×, /, log, ln, exp, sqr, sqrt

Results are displayed in a window with the values at the specified wavelengths and the equation results. The results are automatically corrected for the pathlength of the cell and the dilution factor.

Quantification

- A virtually unlimited number of standards can be used for the calibration. The only limit is the memory of the PC.
- Concentration of Standards can be entered directly by the user or calculated from the given weight, volume, and purity from the software.
- Four calibration curves are available: linear, forced zero (Beer-Lambert's law); linear; second order, forced zero; and second order.
- Calibration diagnostics include a plot of the processed spectra, a plot of each data point and the fitted calibration curve.
- Calibration curve statistics are the standard deviation for each calibration coefficient, the standard deviation of calibration, and the correlation coefficient.

Automation

Automation comprises an automation table which consists of:

- up to three standards (only for quantification)
- two controls
- a user-defined number of samples (only limited by sampling device)

The automatically-generated result report can include statistics on the samples (average, standard deviation, % RSD, minimum and maximum value). Automation normally, but not necessarily, involves automated sample introduction as well as measurement and evaluation.

Interactive Spectral Processing

Spectra may be interactively processed by the user with the following functions:

- absorbance transmittance
- scalar add and multiply
- spectral add and subtract
- calculation of derivatives
- interpolation of data points by a spline algorithm

Verification and Diagnostics

The general purpose software includes a Verification and Diagnostic mode to allow the user to verify and diagnose the correct operation of Agilent 8453 spectrophotometers. It allows the following tests to be performed:

- · spectrophotometer self test
- performance verification checks such as photometric and wavelength accuracy
- wavelength reproducibility
- stray light

- noise
- baseline flatness
- drift (1 hour, optional)
- performance verification, including all tests required by the European Pharmacopoeia and United States Pharmacopeia

The diagnostics allows the user to:

- · check the lamp intensities
- · check the lamp stability
- · check the dark current
- check the pump time for a sipper/autosampler system with a flow test

PC Requirements

To operate properly, the Agilent ChemStation software requires a PC with:

- 1 GHz 32-bit (x86) processor (3 GHz for Windows Vista or Windows 7)
- Microsoft Windows operating system:
- Windows XP Professional 32-bit (SP 2 or 3),
- Windows Vista Professional 32-bit (SP 1 or 2),
- Windows 7 Professional 32-bit (SP 1),
- Windows Server 2003, or
- Windows Server 2008 32-bit (SP 1)
- At least 1 GB RAM (2 GB for Windows Vista and Windows 7)
- · Hard disk drive with at least 40 GB free
- CD-ROM drive
- SVGA graphics (1280x1024)

Instrument control is done through GPIB or LAN with the Agilent 8453.

Agilent 8453 UV-Visible Spectrophotometer

General Description

The Agilent 8453 offers the latest in diode-array technology.

- Compliance with all requirements of the European Pharmacopoeia (EP) and United States Pharmacopeia (USP)
- · Small footprint to save bench space
- Prealigned deuterium and tungsten lamp light sources for trouble-free maintenance
- Built-in buttons to measure sample, standard, and blank for convenient measurements even with gloves
- Thermally-stable ceramic spectrograph for a wide operating temperature range
- Communication through GPIB or LAN for dedicated or networked PC control
- Firmware upgrade from PC for easy participation in future developments
- Built-in GPIO interface for control of accessories

Regulatory Compliance

The Agilent 8453 supports compliance with GLP regulations.

- Serial number and firmware revision held in non-volatile memory
- Own clock for time and date stamps
 of the spectra
- Extensive self-test procedures that check the electronics and key optical to ensure consistent performance between validation
- Built-in electronic logbooks which contain the results of selftests, notes on instrument maintenance, events and errors

Diode-Array Advantages

Backed by almost two decades of experience in the development and manufacture of diode-array spectrophotometers, the Agilent 8453 gives you clear advantages.

- Fast spectral scanning for complete spectral information and multiwavelength applications such as user-defined equations
- Open sample area for convenient sample handling
- High throughput optics guarantees excellent signal-to-noise for high sensitivity
- Virtually absolute wavelength resettability allows selection of optimum wavelength and use of electronic standards
- · Exceptional ruggedness and reliability

Optical Specifications

Wavelength range	190–1100 nm	
Slit width	1 nm	
EP resolution test	>1.6	spectrum of a 0.02% v/v solution of toluene in hexane, ratio absorbance at 269 nm/266 nm
Stray light	<0.03%	at 340 nm (NaNO ₂ , ASTM)
	<0.05%	at 220 nm (Nal, ASTM)
	<1%	at 198 nm (KCI, EP)
Wavelength accuracy	<±0.5 nm	(NIST 2034)*
	<±0.2 nm	at 486.0 and 656.1 nm
Wavelength reproducibility	<±0.02 nm	ten consecutive scans (NIST 2034)
Photometric accuracy	<±0.005 A	at 1 A (NIST 930e)
	<±0.01A	potassium dichromate, EP method
Photometric noise	<0.0002 A	sixty 0.5-s scans at 0 A, 500 nm, rms
Photometric stability	<0.001 A/h	at 0 A, 340 nm, after 1-hour warmup, measured over 1 h, every 5 s, constant ambient temperature
Baseline flatness	<0.001 A	0.5-s blank, 0.5-s scan, rms
Typical scan time	1.5 s	full range
Physical Dimensions		
Height × width × depth	185 × 344 × 560 mm (7.3 × 13.5 × 22.0 in)	
Weight	16.5 kg (36.3 lb)	
Power Requirements		
Line voltage	90–264 V AC	
Line frequency	47–63 Hz	
Power consumption	70 VA typical	
Environmental Conditions		
Operating temperature	0-50 °C (32-122 °F)	
Non-operating temperature	-40-70 °C (-458 °F)	
Humidity	<95 %, at 25–40 °C (77–104 °F)	

* The methods used are application-relevant, for example, the wavelength accuracy specification is given for the complete wavelength range and not just for a single wavelength.

The ceramic chassis used in the Agilent 8453 spectrophotometer is manufactured under licence from Carl Zeiss.

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