Agilent ChemStation for UV-visible Spectroscopy: Advanced Software

Specifications

General Description

The advanced software for Agilent ChemStation adds extended spectral processing, advanced single and multicomponent quantification and automation capabilities to the general purpose software.

Data Analysis

The advanced software allows:

- extensive interactive mathematical operations with spectra
- to compare spectra using regression or normalization algorithms as well as to compose spectra
- to define up to four equations for evaluation of data—in addition to the values at specific wavelengths other information such as dilution or weight can be used
- to use extensive diagnostic tools for single component calibration
- do multicomponent analysis with calibration based on pure or mixed standards
- multiple analyses—up to four equivalent data analyses can be performed in parallel (data analysis can comprise spectral processing, wavelength value extraction, and evaluation steps)
- confirmation analysis—up to three confirmation analyses can be specified in addition to the main analytical analysis
- to create customized reports based on modules from predefined reports or user-defined templates

Method Development

Four special utilities are provided to assist the user in developing the best parameters for quantitative analysis.

Evaluate Standards for linearity— performs a single component calibration at each wavelength over a user specified wavelength. It determines the correlation coefficient and uncertainty at each wavelength.

Compare Calibrations—puts the results from two independent calibrations side by side on the screen for comparison.

Optimize Wavelength for selectivity and accuracy—quantifies a user-selected sample at all wavelengths and plots the quantification results against wavelength.

Test Method for precision—calculates the average and standard deviation of multiple analyses of an identical sample.

21 CFR Part 11

The optional Security Pack software can be added for full support of compliance with 21 CFR Part 11.

- Provides access control, including user setup and password adminstration based on Microsoft Windows without using a relational database.
- Locks sessions during automated data acquisition.
- Prevents loss of raw and meta data and their unauthorized modification.
- Stores deleted spectra together with results for review during an audit, or even for restoring.
- Adds versioning at the ChemStation level to store reprocessed versions.
- Supports the detailed requirements for electronic records and passwords as specified by 21 CFR Part 11.
- Sequence control based on an analysis stage concept to avoid operational errors and to assure storage of the data created.

Automation

Automation is set up by entering an automation table as a sequential list of the actions to be performed. Information about samples and standards being measured can be entered in the sample table. An automation table can be combined with any sampling system from manual to fully automated.

Customizing

The advanced software can be customized using a powerful command set, including Microsoft Windows dynamic data exchange (DDE).

PC Requirements

To operate properly the Agilent ChemStation software requires the following:

- IBM-compatible PC with 1 GHz 32-bit (x86) or 64-bit (x64) processor
- Windows XP or Windows VISTA operating system
- 1 GB RAM
- CD-ROM drive
- SVGA graphics

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

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Published December 28, 2009
Publication Number 5989-6970EN

Agilent Technologies