New Software for the Agilent UV-VIS Spectrophotometer

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Topics

Introduction to Agilent’s UV-visible history and offerings
Instrument Technology and Software architecture
UV-visible Applications
Demo of Agilent’s UV-visible ChemStation Software
Questions and Answers
Agilent (HP) UV-Visible Spectroscopy Systems Spectrophotometer History

8450
Introduced 1979

8451
Introduced 1984

8452A
Introduced 1986

8453
Introduced 1995
Product Offerings to Customers Solutions

- Working and fully tested system
- Instrument and accessories
- PC hardware and software
- Instrument communication
- Compliances Services for IQ/OQ/PV
- Accessories and supplies for UV-visible Spectroscopy
**Agilent UV-Visible Spectroscopy Systems**

**The 8453 Spectrophotometer**

**Agilent 8453 UV-Vis Spectrophotometer**
- 190-1100nm Wavelength Range
- 1nm Slit Width, 1nm Sampling Interval
- 0.1 second Full Spectrum Scan
- Fully EP & USP compliant
  -> improved Resolution, lower Stray Light
- Instrument logbooks
  -> GLP
Spectrophotometer Instrument Design

Conventional Single-beam Spectrophotometer

1. Light source
2. Entrance slit
3. Dispersion element
4. Sample
5. Exit slit
6. Monochromator
7. Detector

Diode Array Spectrophotometer

1. Light source
2. Entrance slit
3. Sample
4. Dispersion element
5. Polychromator
6. Detector
Diode-Array Advantages

The diode array advantages are resulting from the different design of diode array instruments

• Simple mechanical and optical design
• Open sample area
• Fixed arrangement of grating and detectors
• Fast acquisition of complete spectra
• Statistics
Open Sample Area

Reversed Optics

Room light cannot reach detectors
  – Narrow “acceptance angle” after sample
  – Geometry of spectrograph

Easy and convenient access
  – Better productivity
  – Less error prone

Easy installation of accessories
  – Room light is not a problem
  – Simple installation of accessories
Agilent UV-Visible Spectroscopy Systems
The ChemStation Software Mode Structure

- **Dissolution Testing**
  - Dissolution Testing
  - Multibath Dissolution Testing
  - Combined Reports

- **Advanced**
  - Advanced
    - (Deletes Execute Advanced Method)

- **Biochemical Analysis**
  - Kinetics
  - Thermal Denaturation

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**General Purpose**
- Standard
- Execute Advanced
- Verification & Diagnostics
Common Features to all Applications

Universal data structure for Spectra

Common Basic features for
- Instrument control
- Accessory configuration and handling
- Method handling
- Raw data storage, retrieval and export

Application / context switch in a running ChemStation

Views of different types on raw data and results
- Graphical windows
- Table windows

Extensive on-line Help

New: Access to Agilent’s OpenLAB Enterprise Content Manager (ECM)

Lots of common functionality for ease of learning and ease of use
General Purpose UV-Visible ChemStation
Software Key Features - An Overview

Graphical User Interface (GUI) with Integrated Status Display
Includes all Common Application Tasks
Single Dialog Box for Method Setup
Easy Automation
One-page Report
Verification & Diagnostics
Execute Advanced Methods capability
Developed on ChemStation Platform for Analytical Applications
General Purpose UV-Visible ChemStation Software
Common Application Tasks

- Fixed Wavelengths
- Ration/Equation
- Spectrum/Peaks
- Quantification
Advanced UV-Visible ChemStation Software
Key Features - An Overview

Flexible Method Setup
Time Based Measurements
Multiple Data Analysis / Confirmation Analysis
Single Component Analysis SCA & Multi Component Analysis MCA
Sophisticated Automation
Method Development Tasks
Sophisticated Interactive Mathematical Functions
Sophisticated Result Statistics
Custom Report Generator
Customization / Macro Programming
Advanced UV-Visible ChemStation Software
Data Analysis

- Three-step Data Analysis
- The result of each processing step can be displayed
- Separation of raw spectra into Samples and Standards
Advanced Mode - Automation
Setup Automation Table

Sequential list of actions to be performed:
Advanced Mode – Report Style Editor
Customizing Reports
Advanced Mode - Macro Programming Documentation and Tools

Macro Programming Guide

- Available On ChemStation CD-Rom under \Manuals\Understanding\UV-Visible Systems

Commands Reference

- Online Help/Commands

Debugging tools

- List Messages Window (lms, setverbose)
- Tool for examining the register structure
- Tool for editing and creation of display description tables (DDT).
- Available on ChemStation CD-Rom under \Ucl\Uv-ucl\Utility

Macro Tools

- Available on ChemStation CD-Rom under \Ucl\Uv-ucl\Macros
Dissolution UV-Visible ChemStation Software
Key Features - An Overview

Rich Data Analysis features
– Full Spectral Acquisition support
– Match Factor for Sample Integrity checking
– Multi-ingredient Formulation Analysis
– Excipient Corrections

On-line Control and Monitoring
– Open System Architecture via bath driver

Flexibility and Scalability
– Sampling System independent Method

Dissolution Testing Mode
Main Screen
Kinetics UV-Visible ChemStation Software
Key Features - An Overview

Real-time display of spectra and time traces
Rate calculation (initial rate, zero order, first order, difference)
Export of rate data to *.CSV or *.DIF files
Gain settings independent from reference measurement

Single Cell Measurements
• On-line time traces at up to 6 wavelengths
• Full spectra acquisition at 0.1 s

Multi Cell Measurements
• Up to 8 cells in a single run
• Zero cells compensation
• Configurable cell setup for use as Blank, Sample
• On-line time trace for each sample
Kinetics UV-Visible ChemStation Software
On-line Monitoring
Thermal Denaturation UV-Visible ChemStation Software

Key Features - An Overview

Software control of Peltier Accessory
  - Multiple heating/cooling ramps and rates.

Real-time status display of melting curve

Full spectrum acquisition
  - Internal reference or three-point drop-line for background correction.

Automatic $T_m$ (melting temperature) calculation
  - Absorbance mean or first derivative methods.

User defined equations
  - For calculation of % GC or other result
  - For correction for thermal expansion of the solvent.
Thermal Denaturation UV-Visible ChemStation Software
Data Evaluation View

- The image shows a screenshot of the software interface for analyzing thermal denaturation data.
- The interface includes a graph for Interpolated Heating Trace and a graph for First Derivative of Heating Trace.
- The graph shows the relationship between temperature and absorbance, typically used to determine the melting point of DNA.
- The software interface includes options for calculation setup, sampling, and thermal measurement.

Additional Information:
- The software is designed for the Agilent UV-Vis Spectrophotometer.
- The eSeminar for this software was held in December 2008.
- Agilent Technologies is the manufacturer of this software.
Agilent UV-Visible ChemStation Software
Summary

Application focus for ease of use
Large shared set of common features
Full spectral acquisition with sophisticated recalculation features
Data import and export functionality
Link into ECM for data exchange and archiving
Customization features including macro programming

Now supported on Windows XP and Windows VISTA