Spectroscopy + Lumetics LINK™

INTRODUCTION

LINK is the software solution for automated analytical data import, analysis, and reporting. LINK scans network locations for new measurement files, extracts all useful data, and copies this data directly to a centralized database. The powerful analysis user-interface allows datasets to be aggregated, grouped, and visualized in the form of charts/tables/images. User-customizable analysis templates deliver rapid and error-free data visualization, with the ability to be replicated across many studies and shared within your organization.

All instrument settings and parameters calculated by the instrument software are copied to the LINK database, including full underlying raw data curves. Sample metadata may be easily assigned and incorporated within the analysis to integrate various product/process variables. LINK has been demonstrated to deliver time savings more than 90% and provide a highly affordable fully automated data management and analysis solution.

LINK currently supports multiple instruments specific to Spectroscopy, including:

- CD Spectrometers – JASCO, Chirascan
- UV-Vis – Varioskan LUX, Agilent, Trinean, Shimadzhu UV-Vis, SpectraMax
- Slope Spectroscopy – SoloVPE
- FTIR – Bruker FT-IR, Antaris

SPECTROSCOPY DETAILS & APPLICATIONS

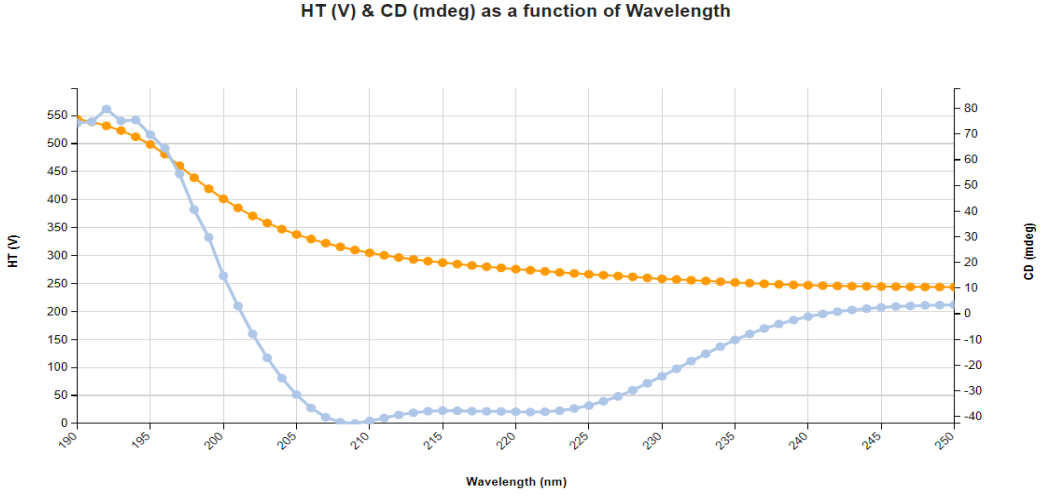
Spectroscopy is the study of light as a function of length of the wave that has been emitted, reflected, or shone through a solid, liquid, or gas. Therefore, spectroscopy is used to separate and measure the brightness of the different wavelengths. LINK may be utilized to assist directly in the following Spectroscopy application areas:

- Protein conformational studies
- Quantitative analysis of pharmaceuticals
- Formulation studies
- Protein folding and unfolding studies
- DNA/RNA interactions
- Enzyme kinetics
- Purity testing of optically active substances
- Natural products chemistry

INSTRUMENT SUPPORT DETAILS – CD SPECTROPOLARIMETERS

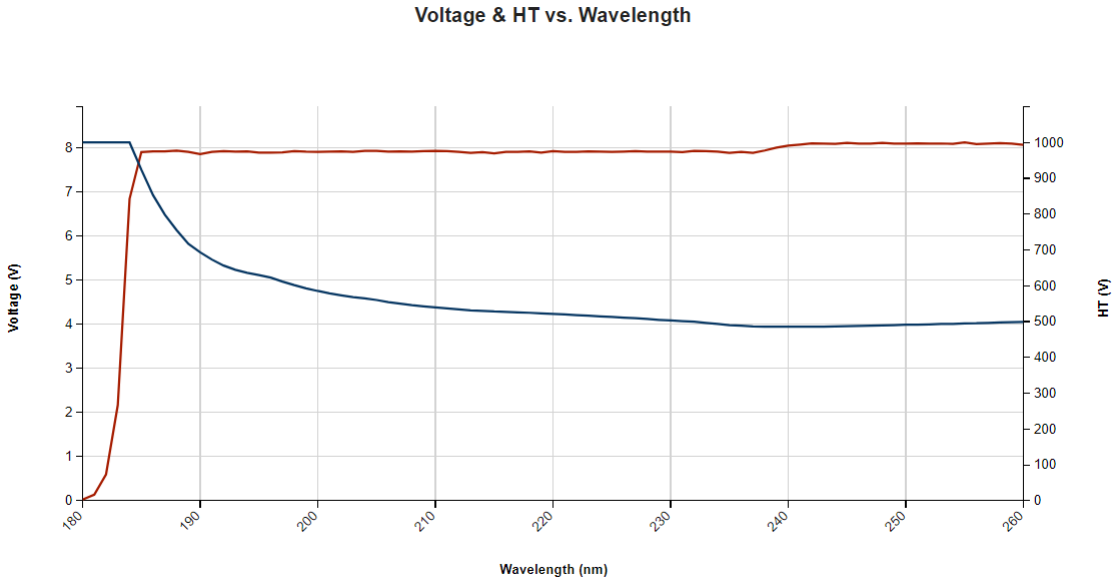
The **J-1000 Series** Circular Dichroism spectrophotometers from JASCO are designed for high sensitivity measurements in the near- and far-UV regions. The J-1000 Series use high dynamic range detectors to obtain high quality spectra of samples with excellent signal-to-noise. LINK supports the JASCO multi-channel instrument for both far-UV or near-UV data sets while importing the raw data curves of CD vs. wavelength and curve subtraction. With a customizable import method, LINK provides flexibility to include dynamic calculations for HT (V) acceptance range over which valid CD and HT raw data will be imported.

Fig 1. Column Chart dashboard visualizing JASCO measurement files plotting raw data curves with visualization settings for 'line + marker".



Chirascan from Applied PhotoPhysics a CD system for analyzing biomolecules of all types and sizes. Chirascan data contributes to a deeper understanding of biomolecular characteristics, mechanisms, and interactions. This system analyses more than α-helix and β sheet but determining the structural and thermodynamic properties of chiral molecules of all shapes and sizes. LINK supports Chirascan output data for instrument/analysis settings, parameters, calculations, and raw data curves for wavelength vs. voltage, temperature, HT, count, and CD. The dynamic properties of Chirascan are supported through multiple visualization preferences and internal LINK calculations options.

Fig 2. Line Chart dashboard visualizing Chirascan measurement files plotting raw data curves for Voltage & HT vs. Wavelength.



INSTRUMENT SUPPORT DETAILS – UV-VIS SPECTROSCOPY

Agilent 8453 is a UV-Visible Spectroscopy System with diode-array technology. LINK supports Agilent data sets for instrument/analysis settings, parameters, calculations, and raw data curves for Absorbance vs. Wavelength.

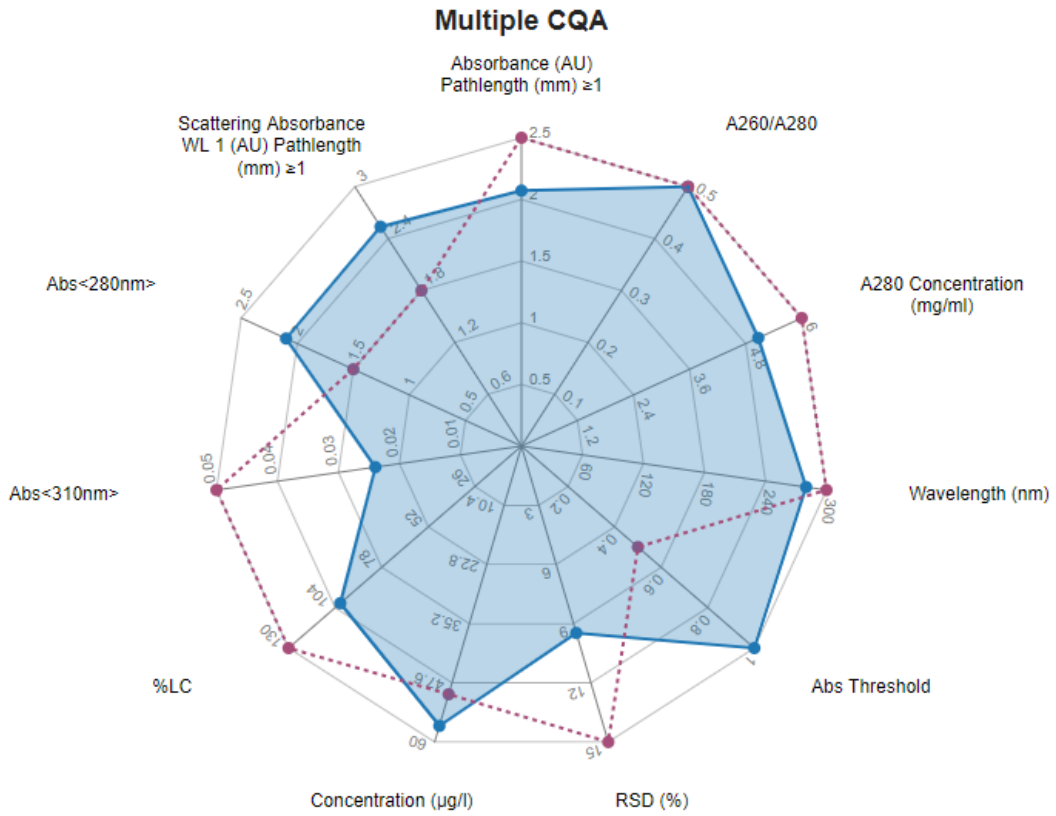
The **S2 PICOFOX** from Bruker is the first portable benchtop spectrometer for fast quantitative and semi-quantitative multi-element microanalysis of liquids, suspensions, solids and contaminations using the principle of total reflection X-ray fluorescence spectroscopy (TXRF).

Trinean from Unchained Labs develops and produces a new approach for high throughput full scan UV-VIS spectral analysis of microliter droplets of DNA/RNA, protein or small compounds.

UV-1900i from Shimadzu provides measurement modes include photometric, spectrum, quantitation, kinetics, time course and bio-methods.

SpectraMax from Molecular Devices is a multi-mode microplate reader for triple-mode cuvette ports, validation tools, and compliance software.

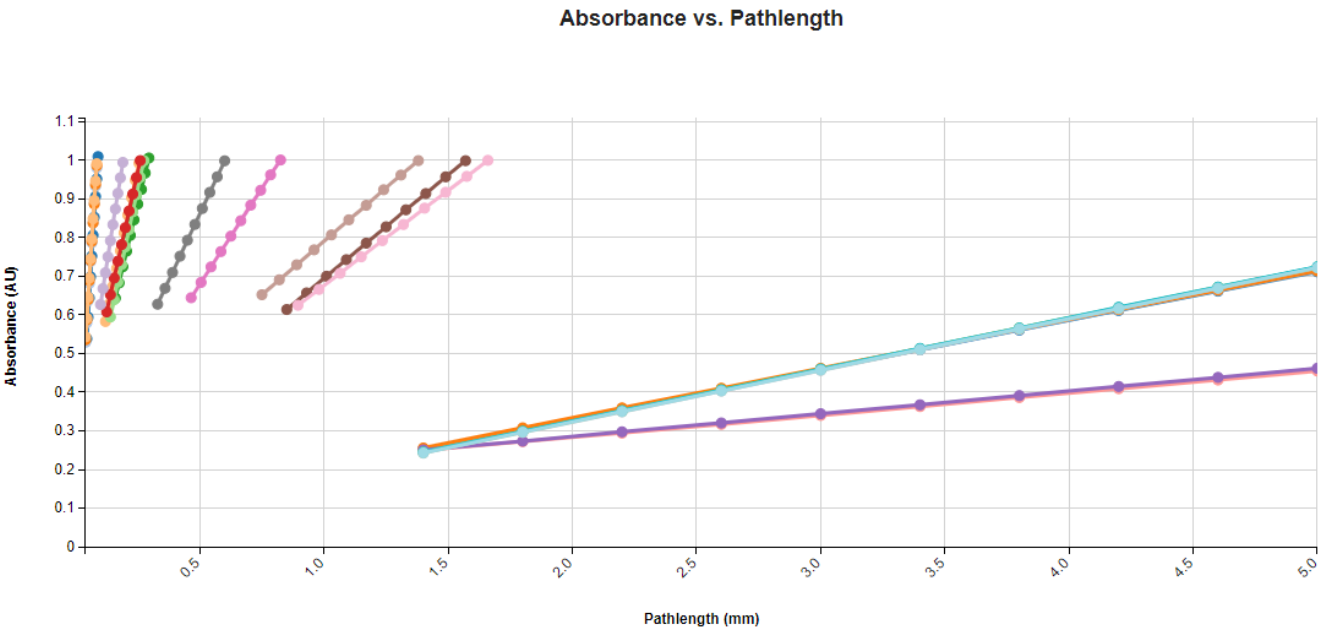
Fig 3. Radar Chart dashboard visualizing UV-Vis data plotting many critical quality attributes with limit lines.



INSTRUMENT SUPPORT DETAILS – SLOPE SPECTROSCOPY

SoloVPE System from C Technologies expanded the mature UV-Vis technique from a 2-dimensional to a 3-dimensional science. LINK supports SoloVPE data sets for instrument/analysis settings, parameters, calculations, and raw data curves for Baseline Absorbance & Scattered Channel Absorbance vs. Pathlength

Fig 4. Line Chart plotting raw data curves for Absorbance vs. Pathlength



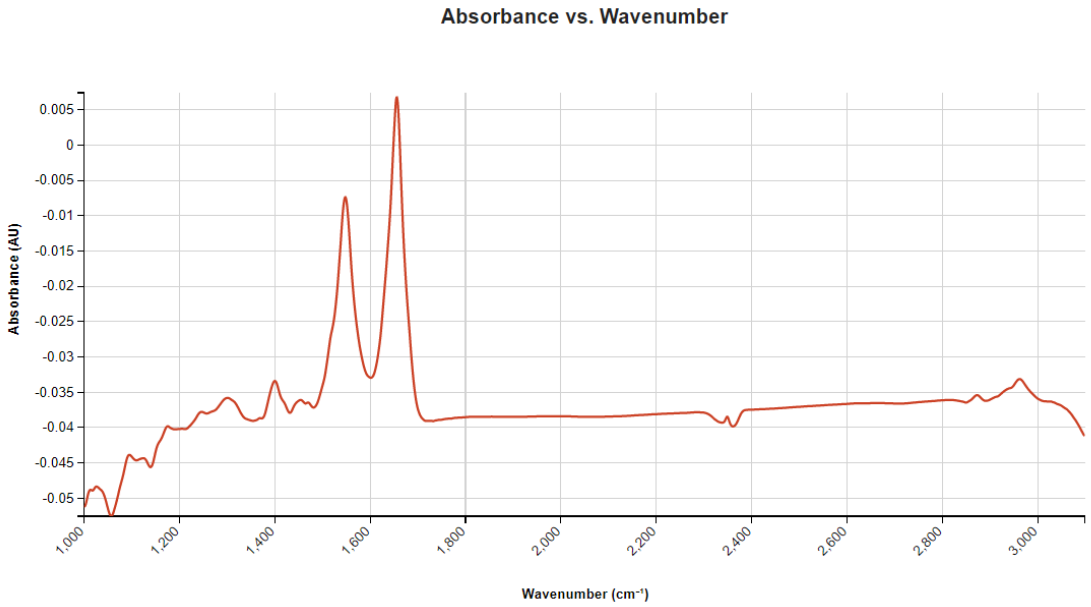
INSTRUMENT SUPPORT DETAILS – FT-IR

Fourier-transform infrared spectroscopy (FTIR) is a technique used to obtain an infrared spectrum of absorption or emission of a solid, liquid or gas. An FTIR spectrometer simultaneously collects high-spectral-resolution data over a wide spectral range.

Bruker FT-IR Spectrometers are intelligent systems for analytical and demanding R&D. LINK supports FT-IR data sets for instrument/analysis settings, parameters, calculations, and raw data curves for Absorbance vs. Wavenumber (cm^{-1})

Antaris FT-NIR Analyzer from Thermo Fisher Scientific provides robust and reliable data collection for at-line, online and in-line analysis.

Fig 5. Line Chart dashboard visualizing FT-IR spectrometer raw data curves for Absorbance vs. Wavenumber (cm^{-1}).



VISUALIZATIONS – LINK ANALYSIS

LINK's dynamic analytical suite will aggregate data and provide visualization tools to suit your specific needs. Imported spectroscopy measurement data can be analyzed using the LINK platform's customizable charts, tables, calculations, images etc. User-customized analysis templates deliver rapid and error-free data visualization with the ability to be exported as a word report to share across your organization. Spectroscopy data can be visualized separately, as well as overlaid in the same chart and tables.

Fig 6. Critical Quality Attribute vs. Formulation

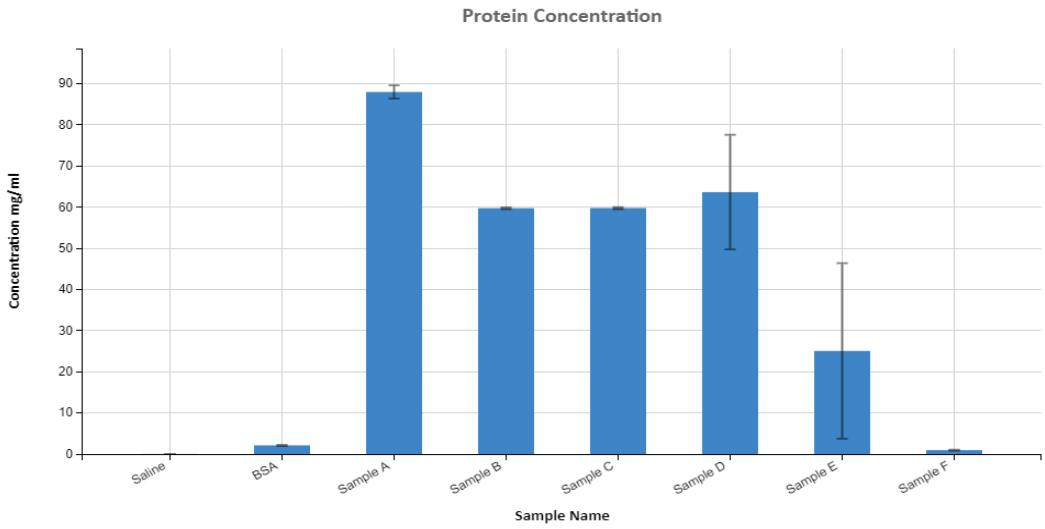


Fig 7. Critical Quality Attribute vs. Process Variable

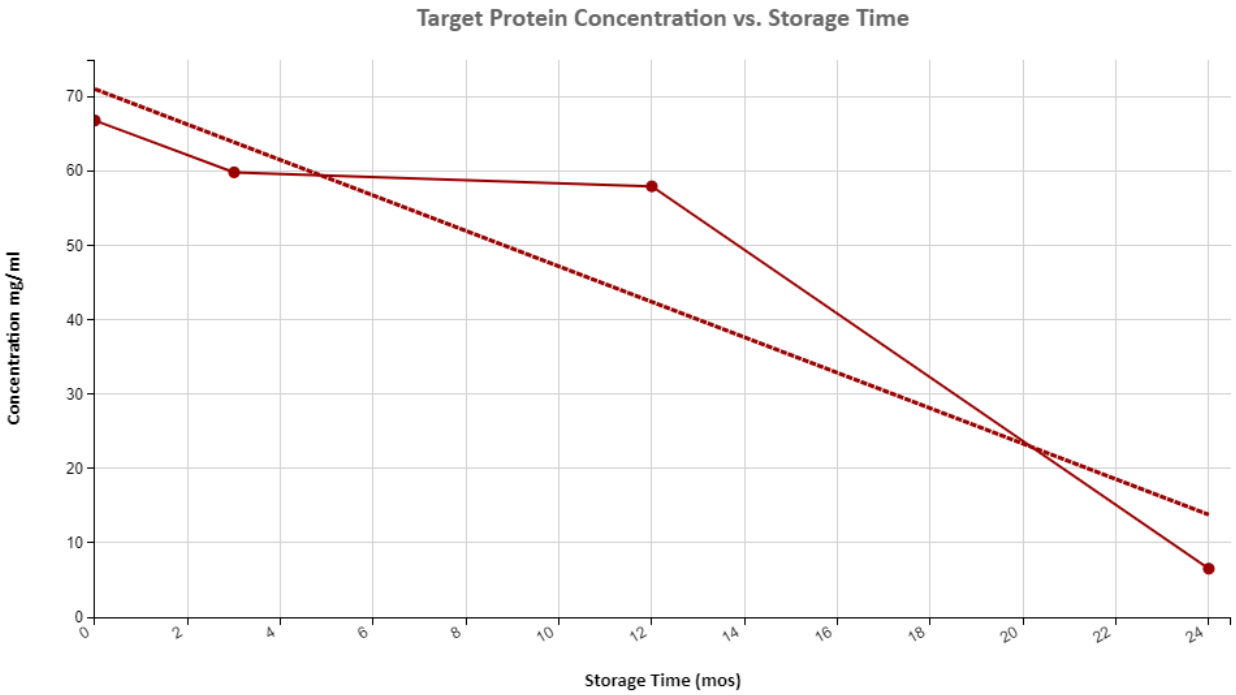


Fig 8. Multiple Critical Quality Attribute Visualization

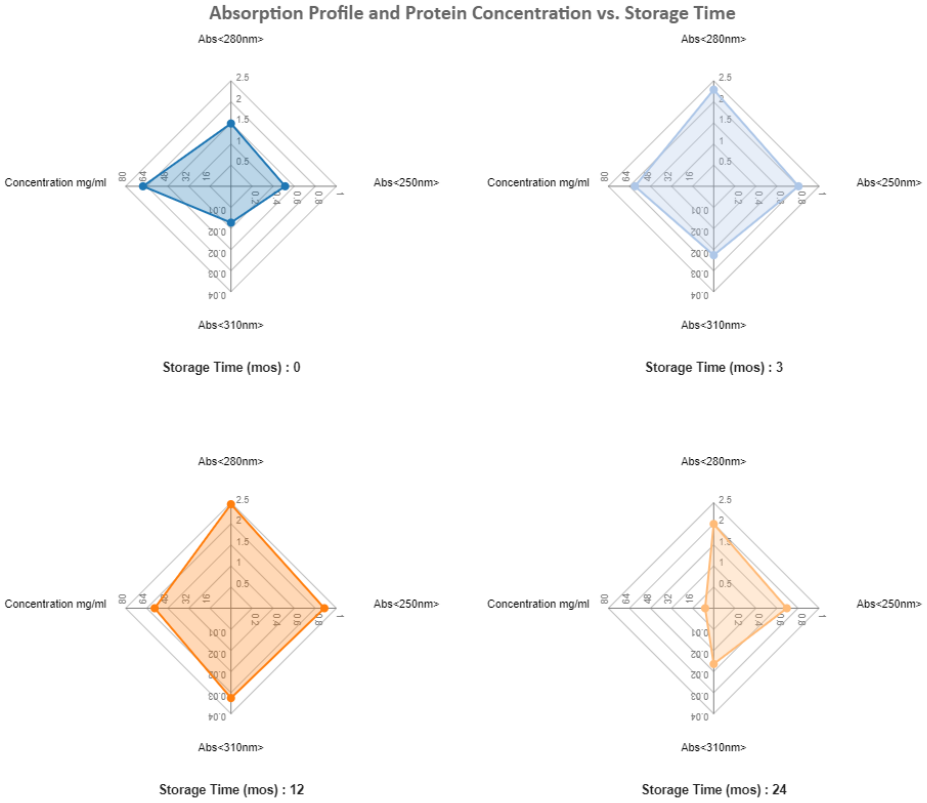


Fig 9. Multi-Factor Visualization

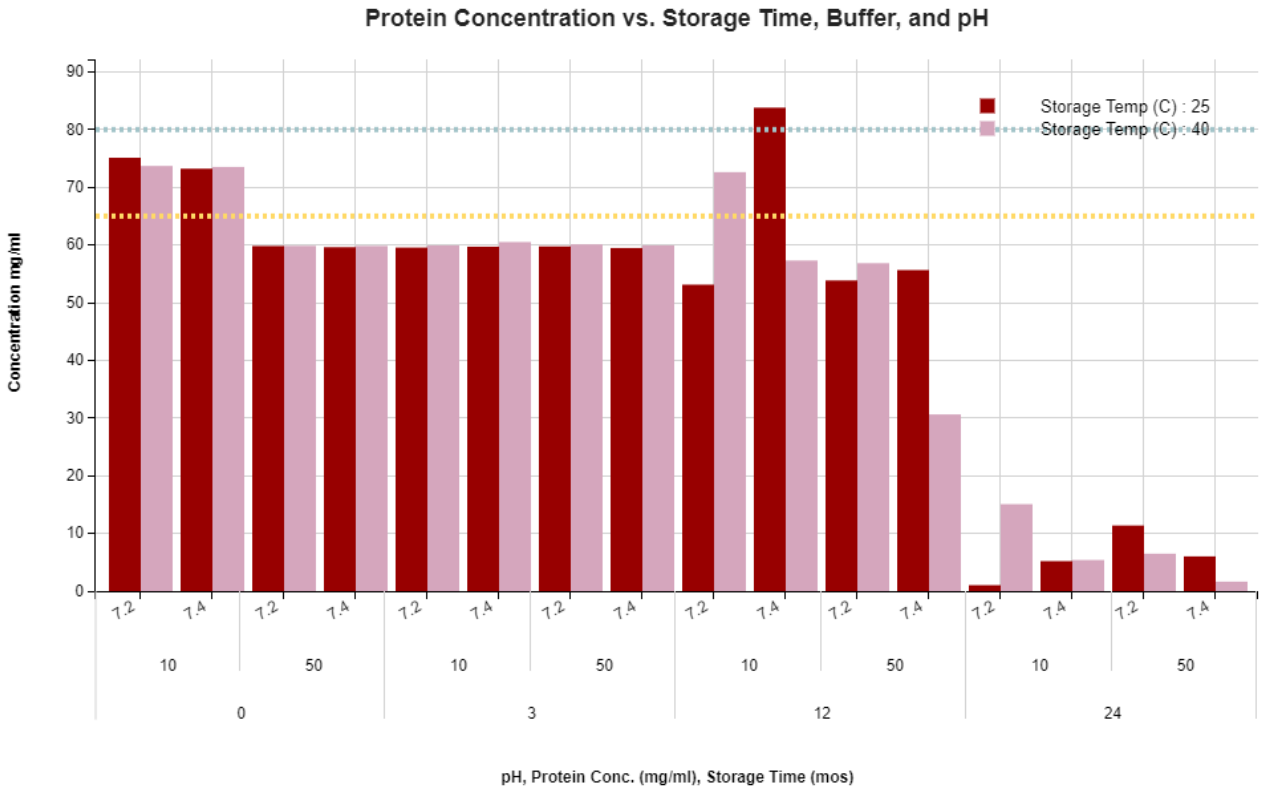


Fig 10. Raw Curve Data – Absorbance Spectra

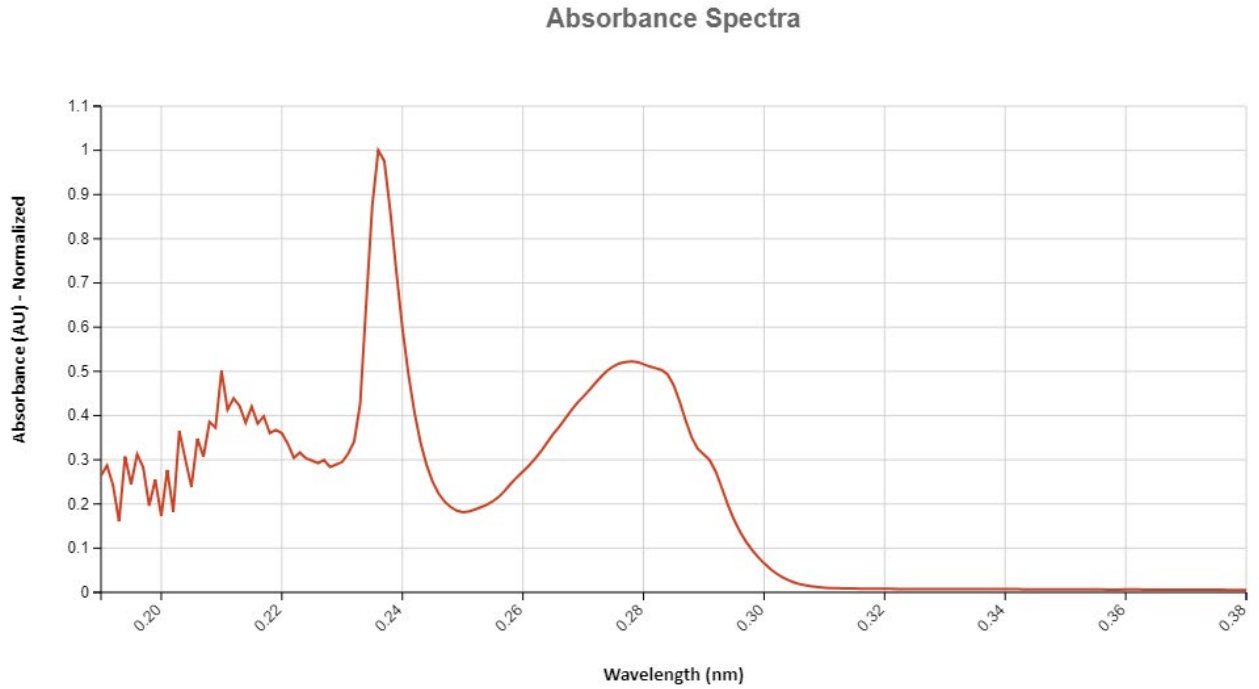


Fig 11. Raw Curve Data – CD Spectra

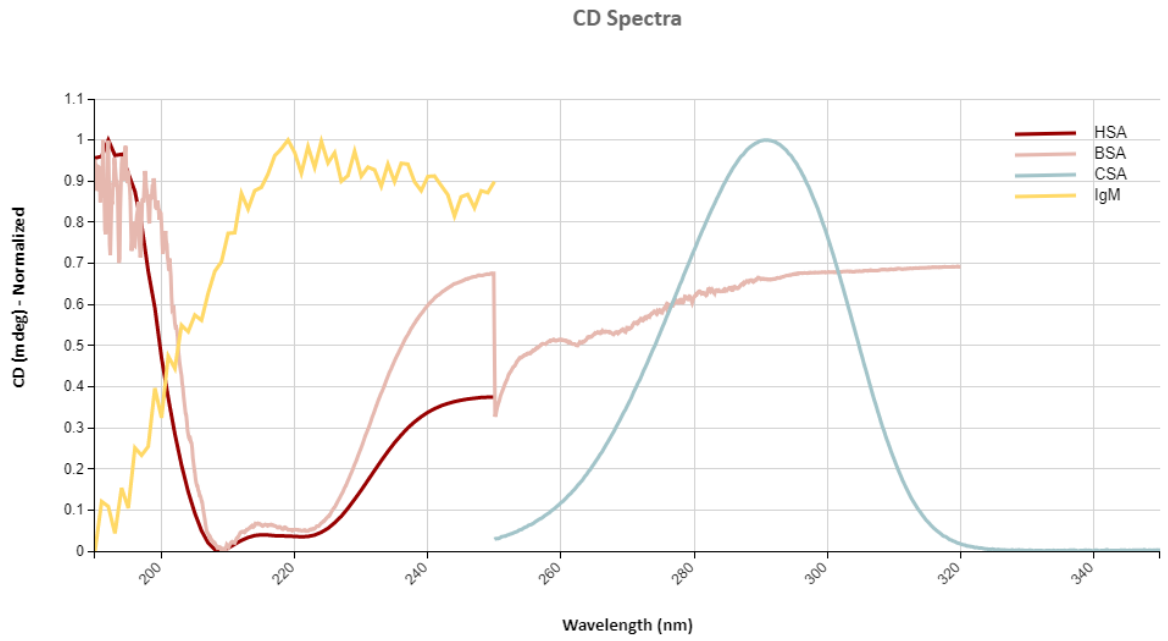


Fig 5. Tabular summaries

Measurement Summary Table – Measurement Results

Sample Name	Abs<250nm> - AVG	Abs<280nm> - AVG	Abs<310nm> - AVG	Concentration mg/ml - AVG	Secondary Peak - Area (Gaussian Fit)	Secondary Peak - % Area (Gaussian Fit)
Sample A	0.67	1.91	0.02	88.01	18.44	43.08
Sample B	0.83	2.35	0.03	59.76		
Sample C	0.73	2.10	0.02	59.81		

DASHBOARD DOWNLOADS

These downloadable Analysis Dashboards are tailored to meet the most common needs of scientists using spectroscopy applications. If assistance is required, please contact LINK experts to assist in dashboard modifications or development of new dashboards of interest.

- JASCO Dashboards: http://lumetics.com/dashboards/JASCO/JASCO.zip
- Chirascan Dashboards: http://lumetics.com/dashboards/Chirascan/Chirascan.zip
- Agilent 8453 Dashboards: http://lumetics.com/dashboards/Agilent/Agilent.zip
- S2 PICOFOX Dashboards: http://lumetics.com/dashboards/S2PICOFOX/S2PICOFOX.zip
- Trinean Dashboards: http://lumetics.com/dashboards/Trinean/Trinean.zip
- Shimadzu Dashboards: http://lumetics.com/dashboards/Shimadzu/Shimadzu.zip
- SoloVPE Dashboards: http://lumetics.com/dashboards/SoloVPE/SoloVPE.zip
- Bruker FT-IR Dashboards: http://lumetics.com/dashboards/BrukerFTIR/BrukerFTIR.zip
- Antaris Dashboards: http://lumetics.com/dashboards/Antaris/Antaris.zip

CONTACT LUMETICS

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