Separation Systems + 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 Separation, including:

- HPLC – Empower, ChemStation, ASTRA SEC-MALS, AKTA
- Electrophoresis – LabChip, iCE2/3 (via Empower), Maurice

SEPARATION SYSTEM DETAILS & APPLICATIONS

Separation is a unit operation that involves the separation of a mixture of various particles based on size by means of electrophoresis or Immunoaffinity capillary electrophoresis (ICE). Particle separation is a crucial step in the sample preparation process and particle/protein/antibody classification system. Separation is also utilized in the chromatography field to split a mixture of compounds for the purpose of identifying, quantifying, and purifying the individual components of the mixture.

Versatility for a Wide Range of Applications

- Protein & antibody characterization
- Post transitional modification characterization
- Quality Control
- Drug compound solubility
- Formulation development
- Stability studies
- Protein charge heterogeneity
- Sample preparation

INSTRUMENT SUPPORT DETAILS – CHROMATOGRAPHY

Empower Chromatography Data System from Waters is their flagship software to produce meaningful results and the ability to support multiple Waters instruments or advanced chromatographic techniques.

LINK supports Empower processed data sets for instrument/analysis settings, parameters, calculations, and raw data curves for Absorbance Units vs. Retention Time. PDF reports will be included as a series attachment within the LINK software. With a customizable import method, LINK includes setting a noise floor factor for removing small fluctuations below the noise floor and reducing the resulting size of the chromatogram's data set.

ChemStation/OpenLAB from Agilent is a software compatible with Agilent LC, GC, CE, CE/MS, and LC/MS instruments systems. Method Scouting Wizard creates a sample sequence containing all possible combinations of available columns, solvents, a set of predefined gradients and a set of predefined temperatures.

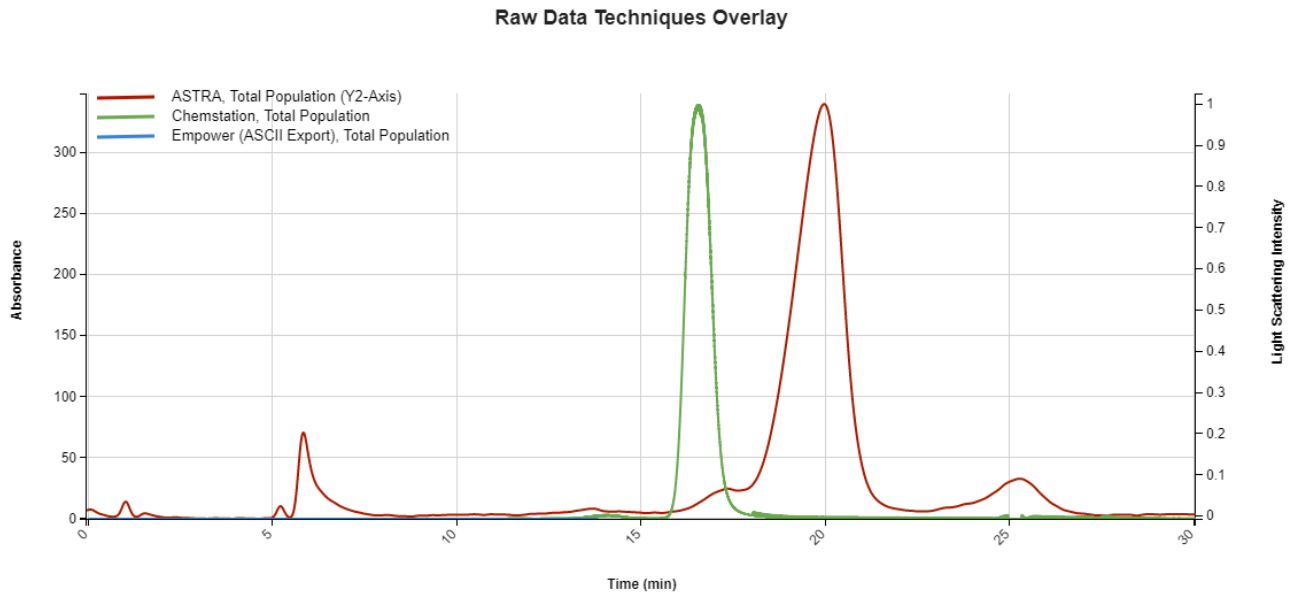
LINK supports ChemStation data sets for instrument/analysis settings, parameters, calculations, and raw data curves for Absorbance vs. Time.

ASTRA SEC-MALS from Wyatt Technology is a luminary software for macromolecular and nanoparticle separation and characterization. The most powerful and versatile software available for the characterization of macromolecules and nanoparticles via multi-angle and dynamic light scattering.

LINK supports ASTRA data sets for instrument/analysis settings, parameters, calculations, and raw data curves for:

- Differential Refractive Index (RIU) vs. Time (min)
- Light Scattering Intensity (normalized) vs. Particle Size
- UV Absorbance vs. Time

Fig 8. Line Chart dashboard visualizing ASTRA, ChemStation, and Empower processed data plotting raw data curves for Absorbance (y1-axis) and Light Scattering Intensity (y2-axis) vs. Time.

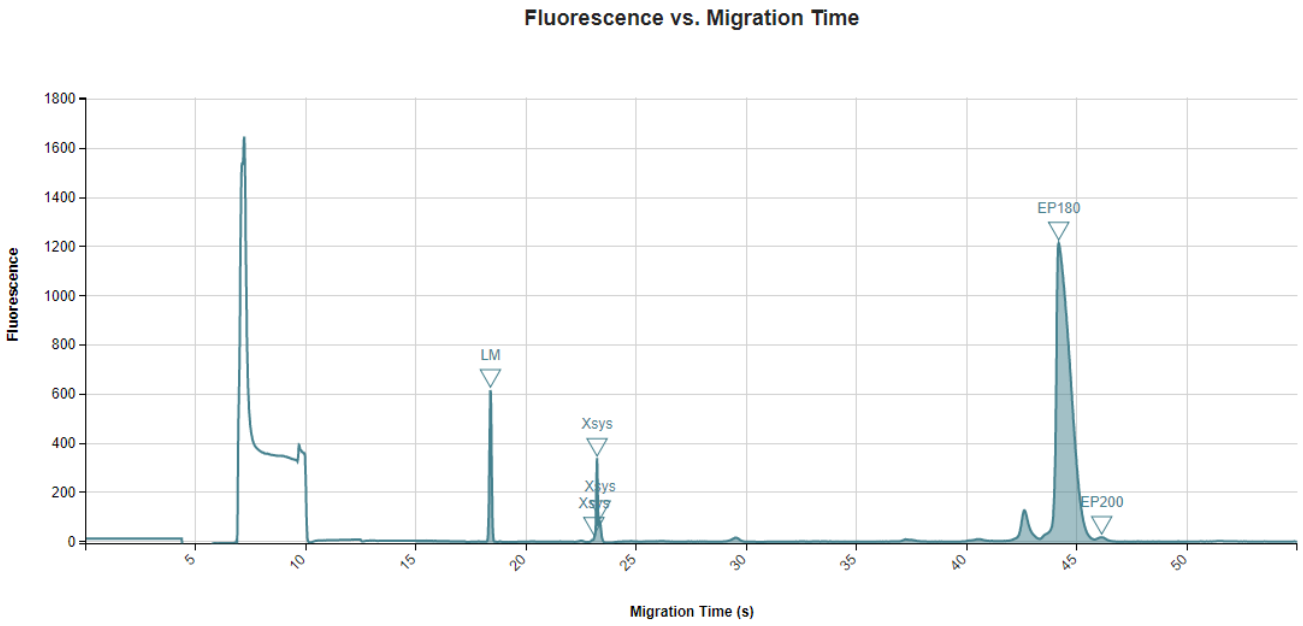


INSTRUMENT SUPPORT DETAILS – ELECTROPHORESIS

LabChip from PerkinElmer is an electrophoresis instrument that provides exact sizing and quantitation for RNA, DNA, and protein analysis. The process is based on traditional gel electrophoresis principles that have been transferred to a chip format. This protein characterization system provides the complete solution for reproducible quantitation, molecular weight sizing and percent purity analysis of protein samples.

LINK supports LabChip output data for instrument/analysis settings, parameters, calculations, and raw data curves for Fluorescence & Size vs Migration Time. With a customizable import method, LINK dynamically calculates LMWS and HMWS %Purities based on a specific size range. LINK dynamically measures all aspects of each peak (ie. purity, baseline, concentration, area, FWHM, height, peak index, peak number, signal noise, etc). Slope and other raw data calculations can be made, as well as metadata importation.

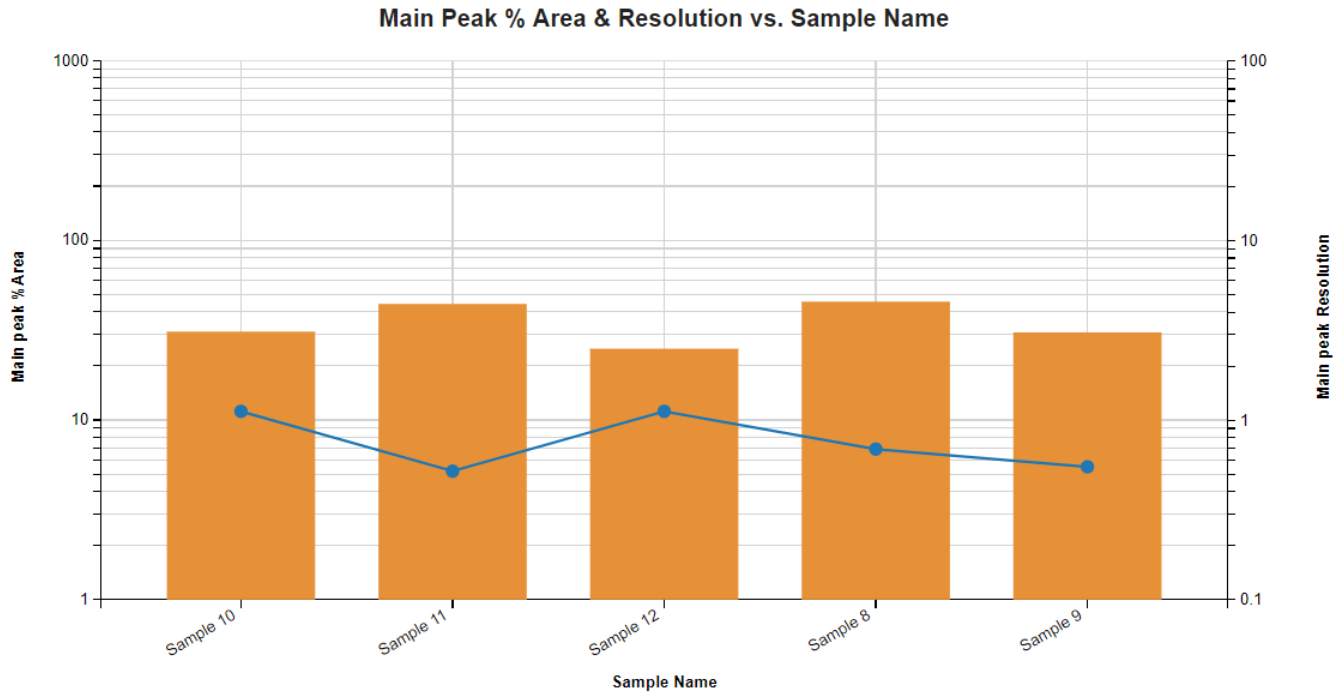
Fig 1. Line Chart dashboard visualizing LabChip measurement files plotting raw data curves for Fluorescence vs. Migration Time. Dynamic calculations specific to LabChip data are utilized as LINKdb Field Markers and fill regions along the x-axis.



Maurice from ProteinSimple innovates the conventional capillary electrophoresis technology to automate protein profiling either by size or charge. Maurice provides a reproducible, quantitative analysis of identity, purity, and heterogeneity profiles for therapeutic proteins & monoclonal antibodies.

LINK supports Maurice output data from PDF reports for instrument/analysis settings, parameters, and calculations. The full PDF from which the data was extracted is also imported as a series attachment within the LINK software.

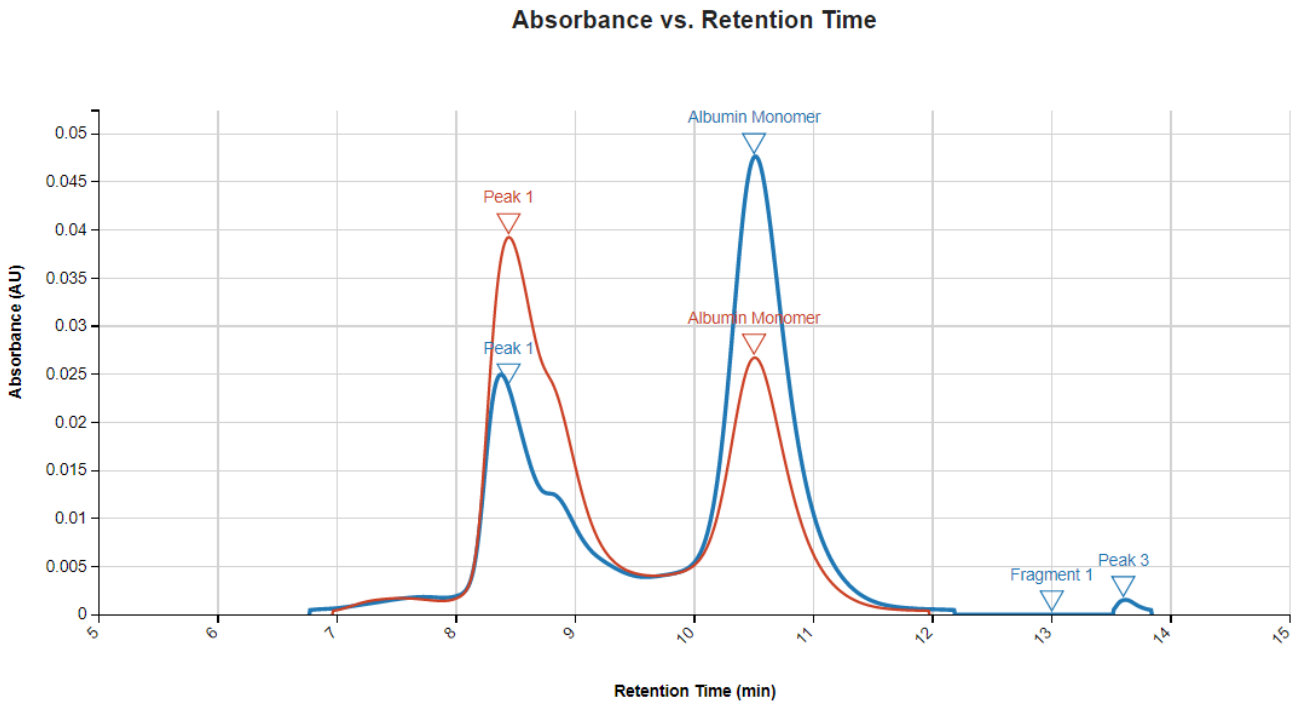
Fig 2. Colum Chart dashboard visualizing Maurice measurement files plotting Main Peak %Area (y-1 axis) & Main Peak Resolution (y-2 axis) vs. Sample Name.



iCE2/3 from Waters provides a customized technique that tailors the capillary to capture the analytes of interest. iCE™ platforms provide reproducible, quantitative analysis of identity, purity, and heterogeneity profiles for therapeutic proteins & monoclonal antibodies. The iCE output data is processed using Empower chromatography data software (CDS) and imported into LINK with a specific export method.

LINK supports Empower processed data sets for instrument/analysis settings, parameters, calculations, and raw data curves for Absorbance Units vs. Retention Time. PDF reports will be included as a series attachment within the LINK software. With a customizable import method, LINK includes setting a noise floor factor for removing small fluctuations below the noise floor and reducing the resulting size of the chromatogram's data set.

Fig 3. Line Chart dashboard visualizing Empower processed raw data curves for Absorbance vs. Retention Time. Dynamic calculations specific to Empower data, are utilized as LINKdb Field Markers along the x-axis.



VISUALIZATIONS – LINK ANALYSIS

LINK's dynamic analytical suite will aggregate data and provide visualization tools to suit your specific needs. Imported Separation Systems 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. Separation data can be visualized separately, as well as overlaid in the same chart and tables.

Fig 4. Critical Quality Attribute vs. Sample Metadata

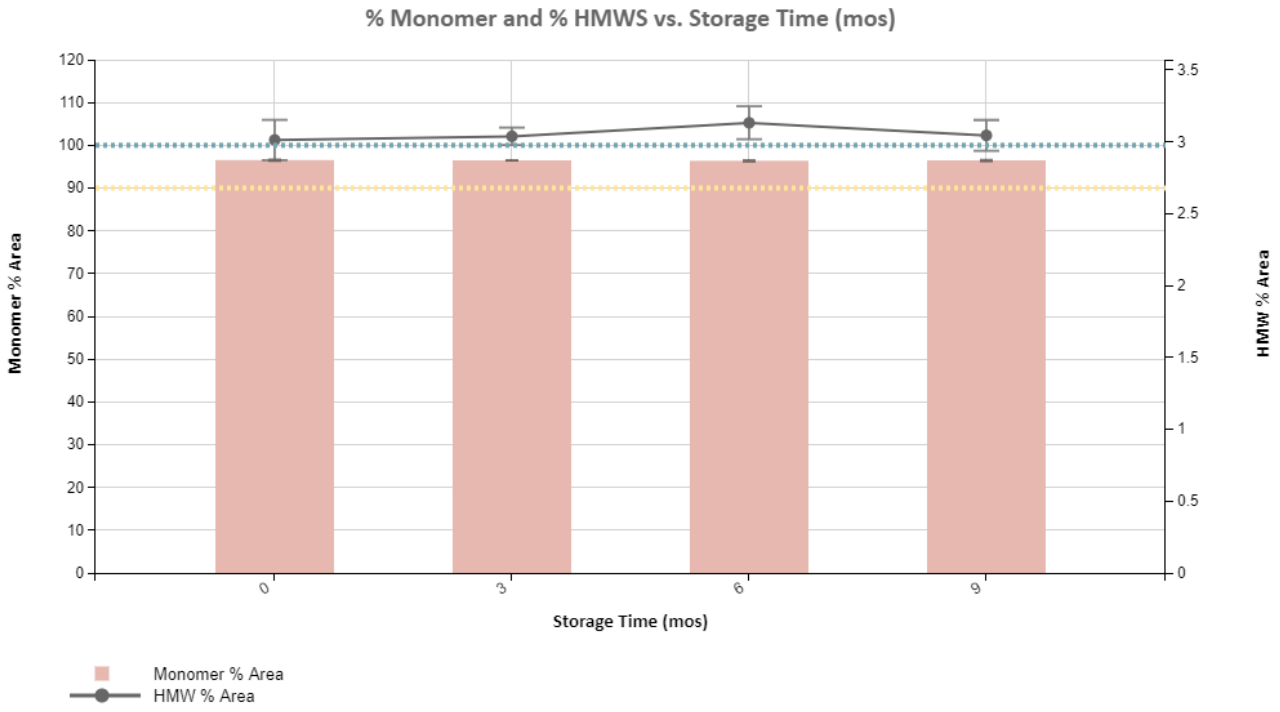


Fig 5. Multiple Critical Quality Attribute Visualization

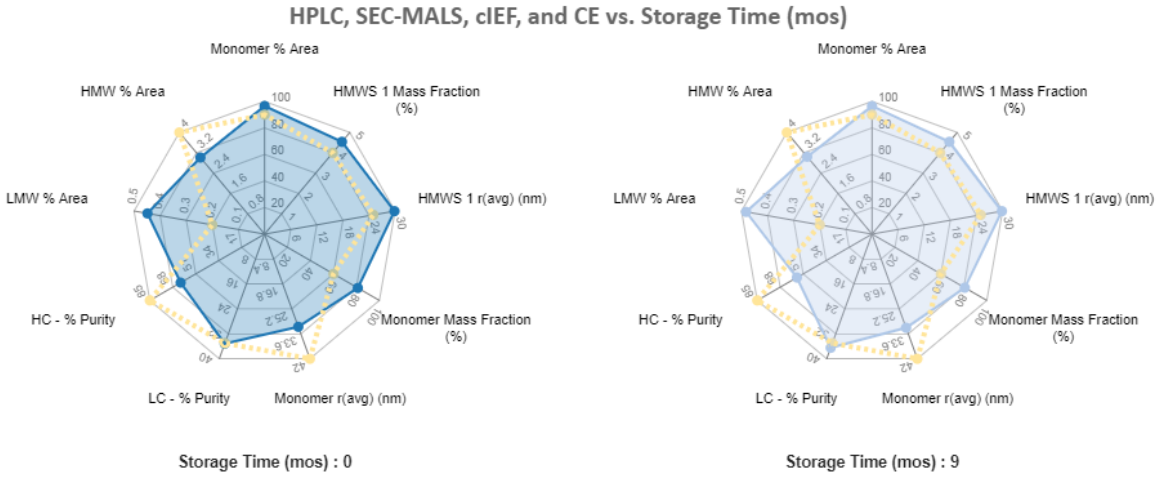


Fig 6. Multi-Factor Visualization

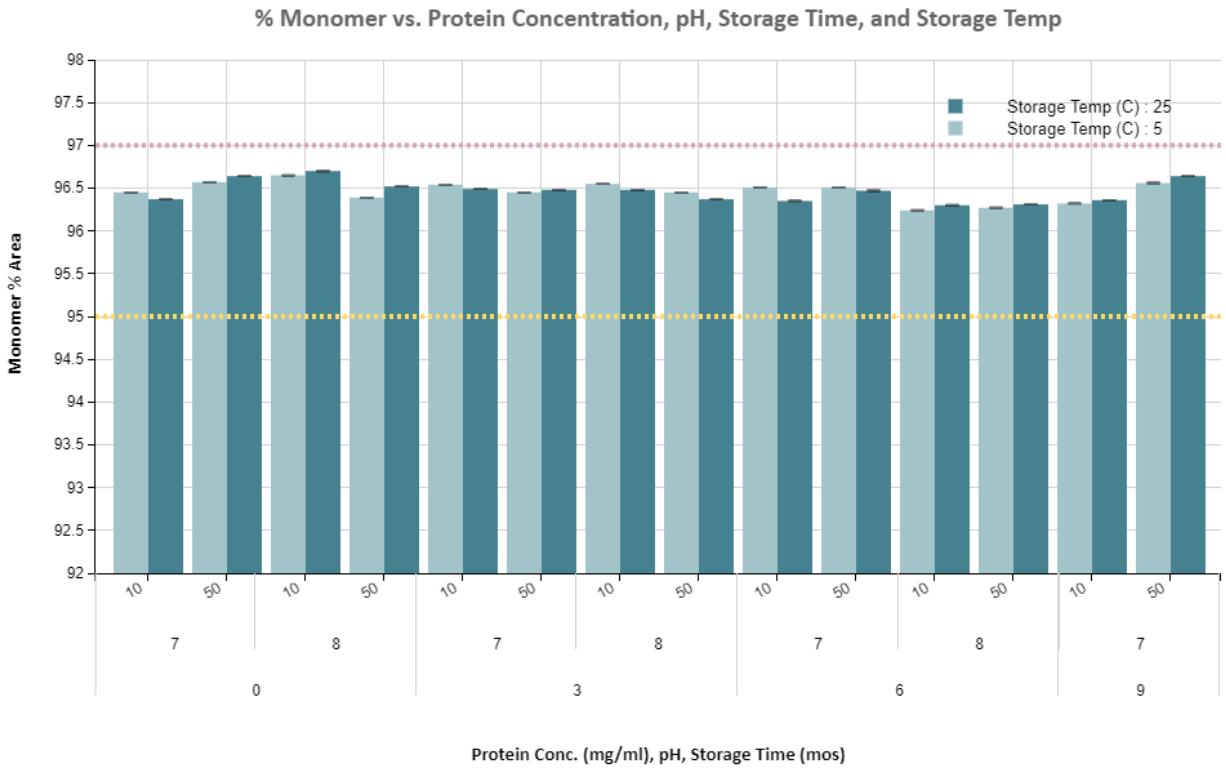


Fig 7. Raw Curve Data - Chromatograms

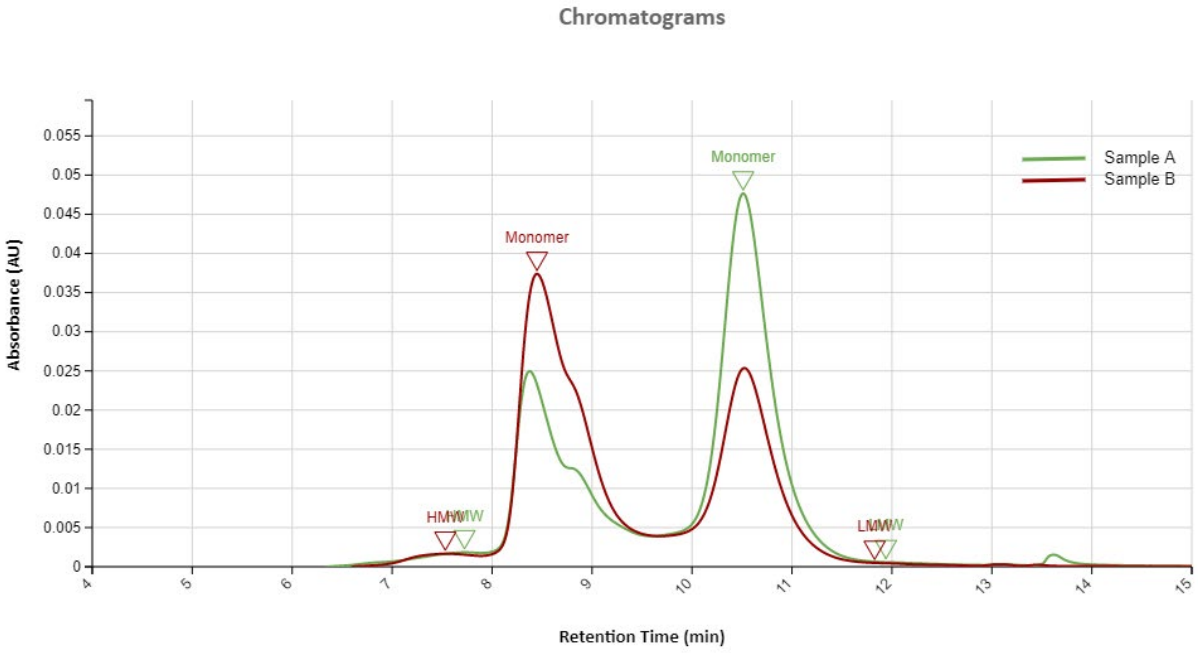


Fig 8. Raw Curve Data – Electropherograms

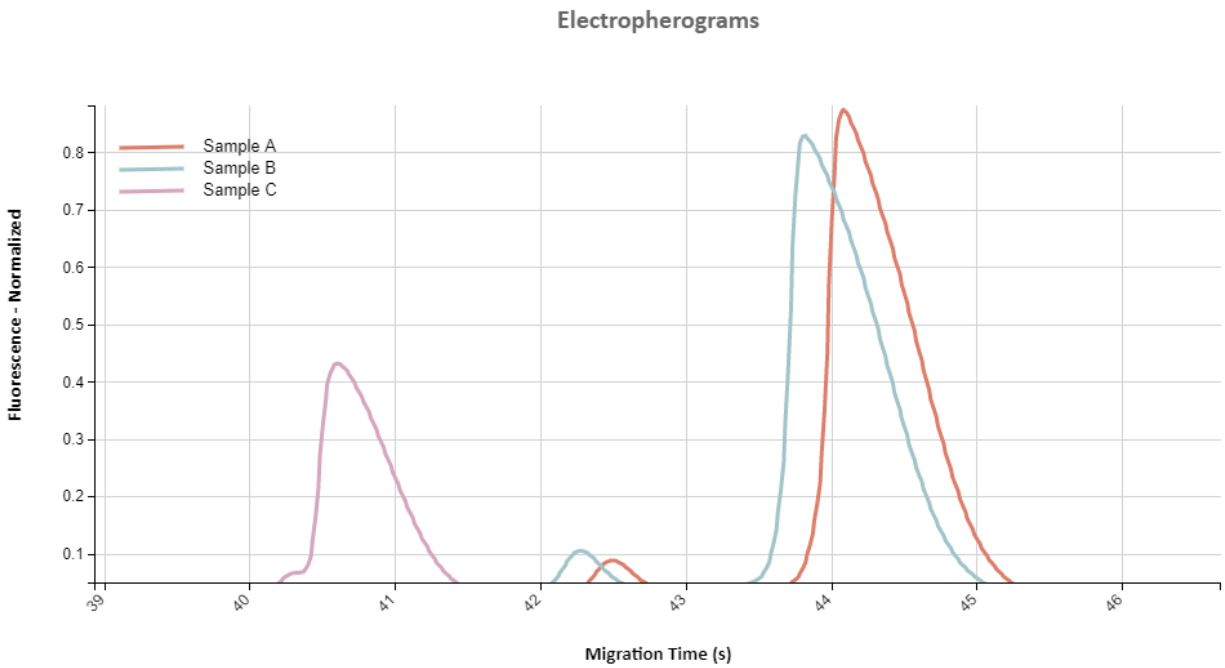


Fig 9. Complimentary Techniques Comparison

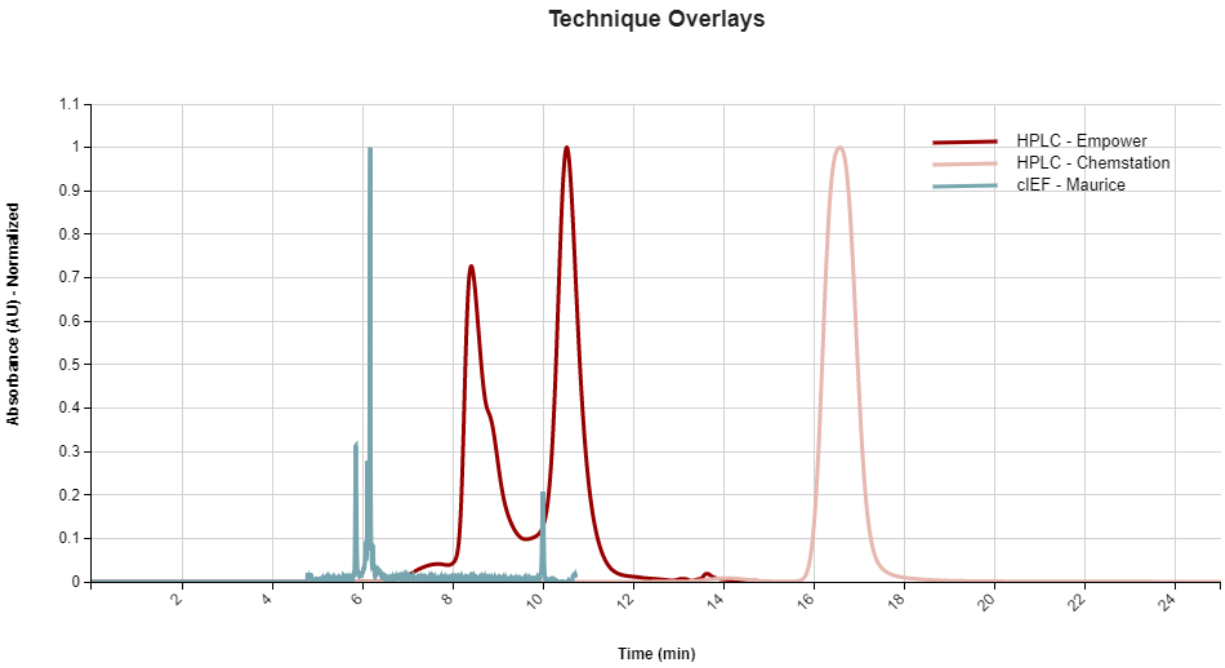


Fig 10. Tabular summaries

Measurement Summary Table – Measurement Results

Sample Name	SEC MALS - Monomer r (nm)	SEC MALS - Monomer Mass (µg)	SEC MALS - Monomer Mass Fraction (%)	SEC MALS - HMWS r (nm)	SEC MALS - HMWS Mass (µg)	SEC MALS - HMWS Mass Fraction (%)	HPLC - Monomer % Area	HPLC - HMWS % Area	HPLC - LMWS % Area	CE - HC % Purity	CE - HC Size (kDa)	CE - LC % Purity	CE - LC Size (kDa)	cIEF - Main Peak % Area	cIEF - Post Main % Area	cIEF - Pre Main % Area
Sample A	31.89	8.38	80.43	29.85	0.47	4.54	96.44	3.07	0.49	54.64	60.43	36.46	31.98	48.03	7.64	31.61
Sample B	31.23	8.12	81.23	29.85	0.47	4.54	96.48	3.05	0.47	63.26	60.46	33.96	30.76	24.03	2.06	32.09
Sample C	31.23	8.12	81.23	29.85	0.47	4.54	96.47	3.05	0.48	60.74	59.38	36.38	31.95	53.59	10.41	34.09

DASHBOARD DOWNLOADS

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

- LabChip Dashboards: http://lumetics.com/dashboards/LabChip/LabChip.zip
- Maurice Dashboards: http://lumetics.com/dashboards/Maurice/Maurice.zip
- Empower Processed Data: http://lumetics.com/dashboards/Empower/Empower.zip
- ChemStation/OpenLAB Dashboards: http://lumetics.com/dashboards/ChemStation/ChemStation.zip
- ASTRA Dashboards: http://lumetics.com/dashboards/ASTRA/ASTRA.zip

CONTACT LUMETICS

For direct assistance, please contact Lumetics LINK™ Support:

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Website: http://lumetics.com/