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APPLICATION NOTE

Assessing PET Grade Through Molecular Weight Analysis Using the BeSEC

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Introduction

Polyethylene terephthalate (PET) is a versatile polyester widely used in fibers, films, bottles, and engineering materials. PET grades differ primarily by molecular weight.

Textile grade PET has a lower molecular weight, with intrinsic viscosity (IV) in the range of 0.64 to 0.68 dL/g, corresponding to approximately 20-30 kDa.

Bottle or chip grade PET has a higher molecular weight, with intrinsic viscosity (IV) between 0.7 and 1.0 dL/g and weight average molecular weight (Mw) typically 30 to 60 kDa or higher.

Molecular weight directly impacts both mechanical strength and processing behavior. While intrinsic viscosity provides an average value, it does not reveal the full molecular weight distribution. Combining Size Exclusion Chromatography (SEC) with light scattering detection enables direct measurement of absolute molecular weight and detailed distribution analysis, critical for process control and product optimization.

Advanced Light Scattering Detector BeSEC

Experimental Section

This study employed a SEC system with refractive index (RI) and light scattering (LS) detectors. The light scattering detector equipped in the BeSEC LS2 from Bettersize Instruments includes 90° and 7° angles. The BeSEC workstation integrates light scattering with RI or UV signals to calculate molecular weight averages (Mn, Mw and Mz) and distributions.

System Configuration:

- Detector: Light Scattering (LS) + Refractive Index (RI)
- Column: Shodex GPC KF-806M
- Mobile phase: Hexafluoroisopropanol (HFIP)
- Flow rate: 0.7 mL/min
- Injection volume: 100 µL
- Column temperature: 40 °C
- dn/dc: 0.296 mL/g

Sample Preparation:

Three PET samples were analyzed. Each powder was accurately weighed and dissolved in HFIP to a concentration of 2 to 7 mg/mL, stirred until clear, filtered through a 0.22 µm PTFE syringe filter, and transferred into vials for autosampler injection.

Results and Discussion

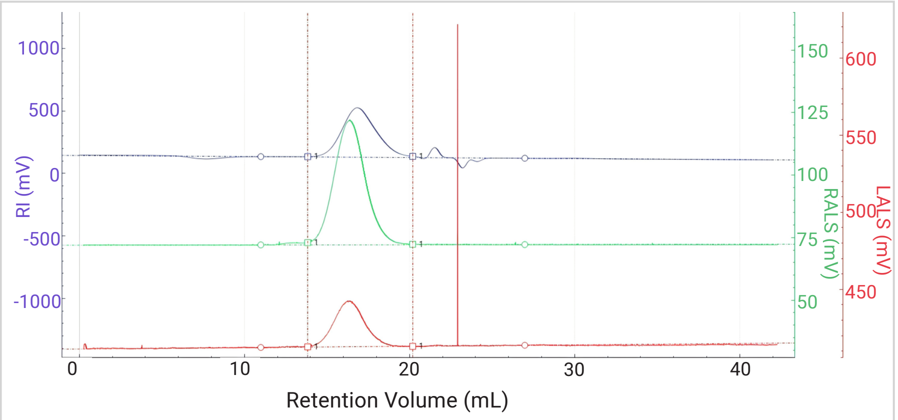

Figure 1. Elution profiles of the multi-detector signals for Sample A

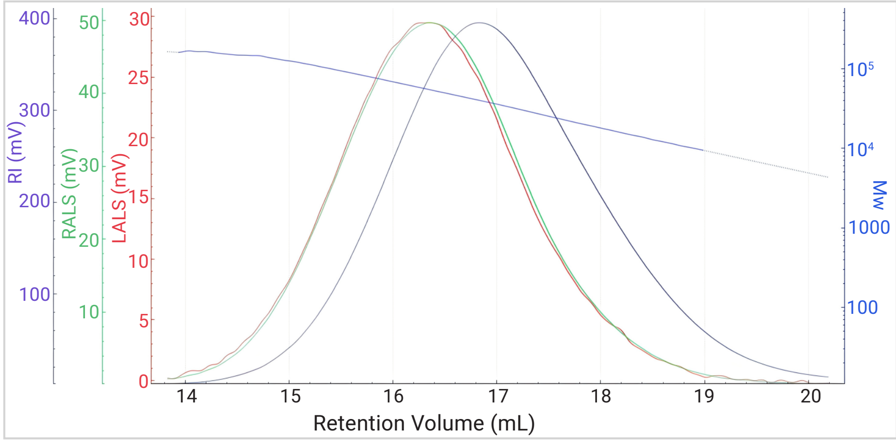

Figure 2. Elution profile of the molecular weight for Sample A

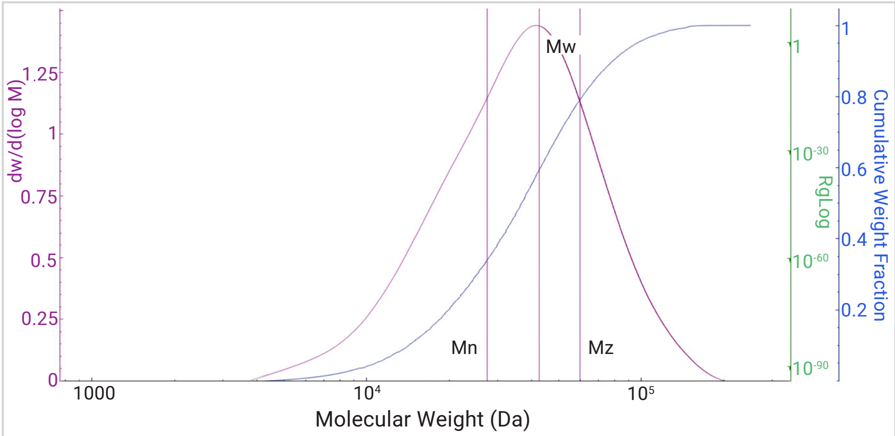

Figure 3. Molecular weight distribution of Sample A

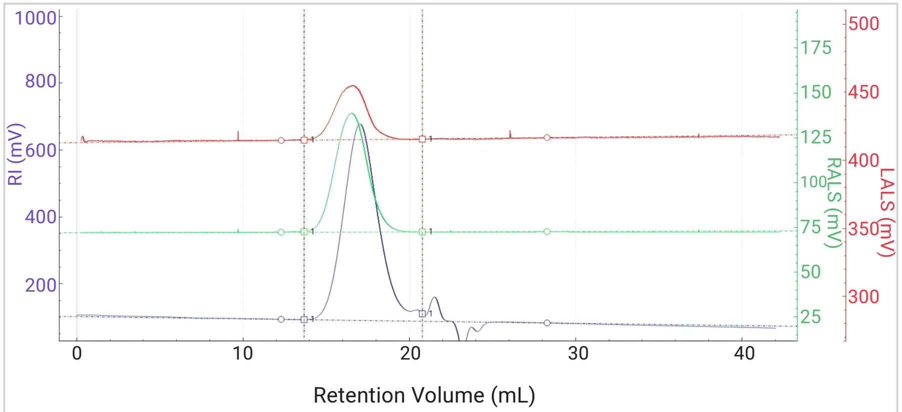

Figure 4. Elution profiles of the multi-detector signals for Sample B

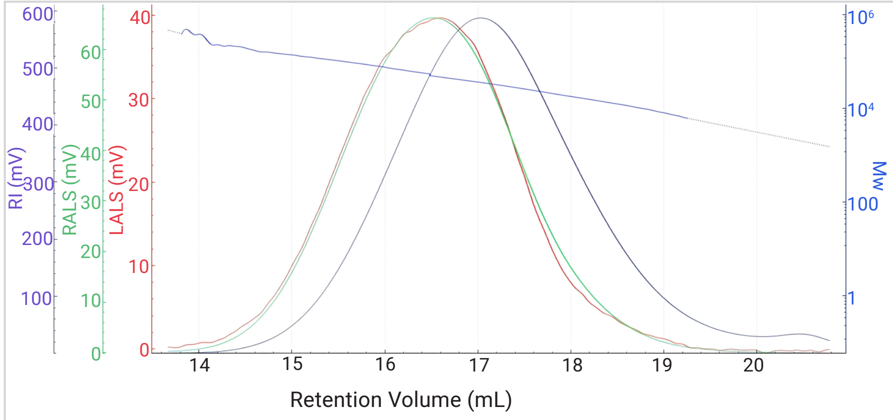

Figure 5. Elution profile of the molecular weight for Sample B

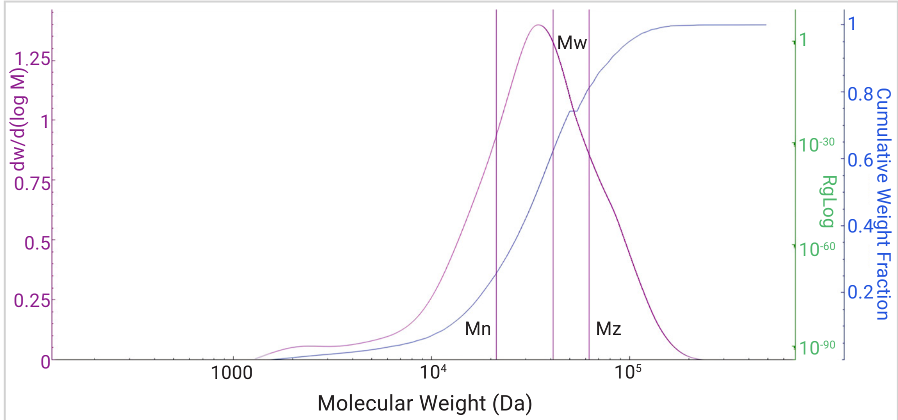

Figure 6. Molecular weight distribution of Sample B

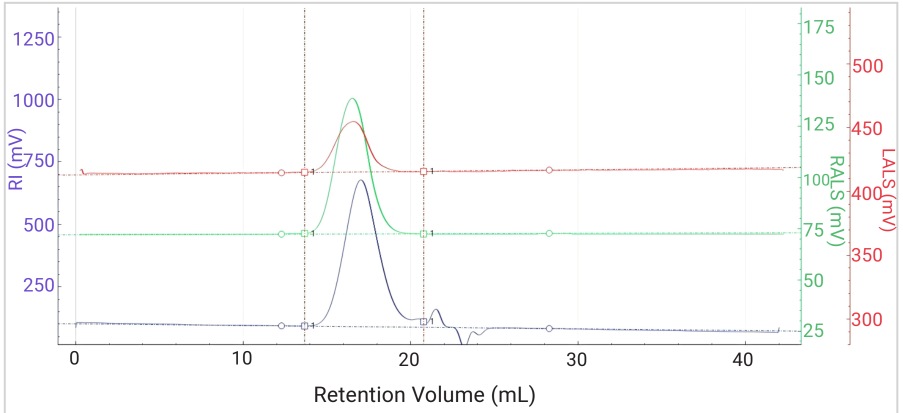

Figure 7. Elution profiles of the multi-detector signals for Sample C

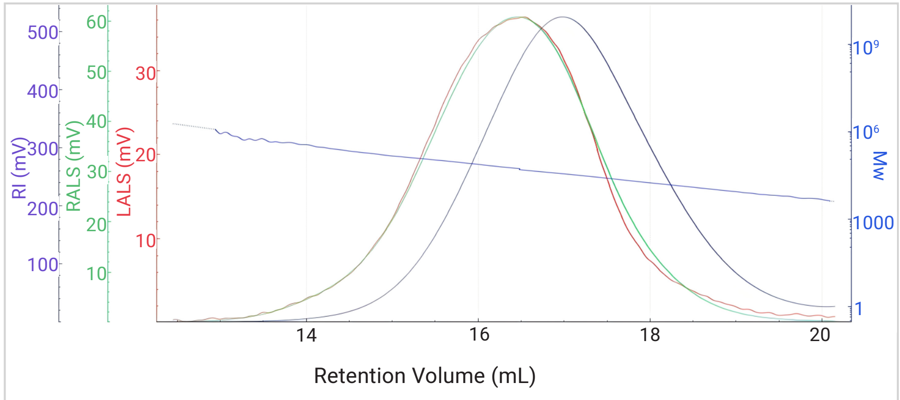

Figure 8. Elution profile of the molecular weight for Sample C

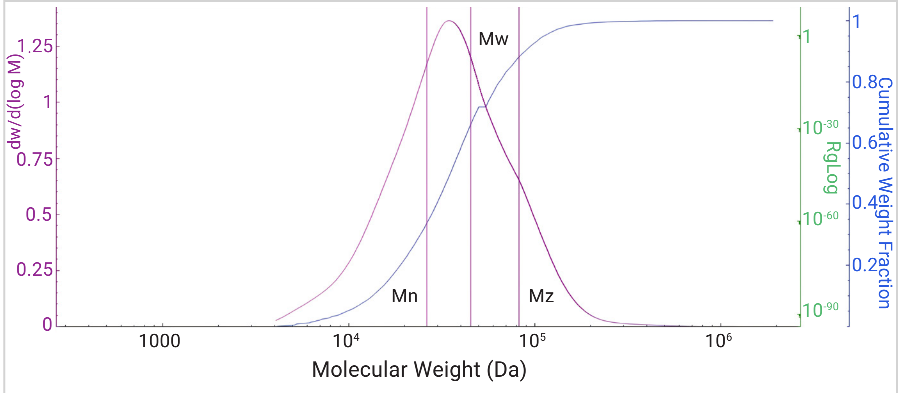

Figure 9. Molecular weight distribution of Sample C

Figures 1 to 9 present chromatograms, molecular weight elution profiles, and distribution plots for the three PET samples. In Figures 1, 4 and 7, the blue trace is the RI signal, the green trace is the right-angle light scattering (RALS) signal and the red trace is the low-angle light scattering (LALS) signal. Figures 2, 5 and 8 present chromatograms with molecular weight profiles, where the blue line shows the molecular weight as a function of elution time. Figures 3, 6 and 9 display the differential and cumulative molecular weight distributions.

The chromatograms exhibit clean baselines with minimal noise, and strong signal-to-noise ratios. Molecular weight profiles decrease steadily with elution volume, consistent with SEC principles, larger chains elute first, followed by smaller ones. Scattering peaks show no tailing and molecular weight curves remain stable at the end, confirming effective size-based separation.

Table 1. Molecular weight results of PET samples

Sample	Mn (Da)	Mw (Da)	Mz (Da)	Mw/Mn
Sample A	27594	42463	59631	1.53
Sample B	21274	41191	62620	1.93
Sample C	26112	42411	68615	1.62

Table 1 summarizes the molecular weight data. All three samples exhibit weight-average molecular weights above 40 kDa, meeting bottle-grade PET requirements. Notably, Sample B displays a broader distribution (Mw/Mn ≈ 2) indicating a higher proportion of low molecular weight species.

Conclusion

The BeSEC LS2 with light scattering detection provides accurate molecular weight characterization for PET samples. All three samples meet bottle-grade specifications, with clean, stable chromatographic profiles and well-aligned detector signals. The ability to resolve molecular weight distribution offers valuable insight for quality control and grade selection.

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