PW23 Quantitative LC-MS of Polymers: determining accurate molecular weight distributions by combined size exclusion chromatography and electrospray mass spectrometry with maximum entropy data processing

Till Gründling[1,2], Michael Guilhaus[1] and Christopher Barner-Kowollik[2]

1. Bioanalytical Mass Spectrometry Facility, Analytical Centre, The University of New South Wales, Sydney 2052
2. Preparative Macromolecular Chemistry, Institut für Technische Chemie and Polymerchemie, Universität Karlsruhe (TH), Engesserstr. 18, 76128 Karlsruhe, Germany

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SEC-LC and MS data are combined to measure polymer MW distributions accurately.

Size exclusion chromatography (SEC) combined with refractive index (RI) and electrospray ionisation (ESI) MS detection to determe accurate molecular weight distributions (MWDs) of synthetic polymers corrected for chromatographic band broadening. The method exploits the ability of the MS to accurately depict peak profiles and retention volumes of individual oligomers as they separate while quantitative information on absolute concentration of oligomers (not accurately available from ESI MS) is obtained from the RI detector only[1].
A computational method based on the maximum entropy principle reconciles the data from both detectors into an accurate MWD. Poly(methyl methacrylate) standards with MW to 10 kDa are used as model compounds. MWDs thus determined are compared to MWDs calculated with conventional calibration of the SEC retention time axis with data from the MS[2]. Distributions <7 kDa were weakly influenced by band broadening. The maximum entropy algorithm successfully corrected the MWD of a 10 kDa standard for band broadening effects. MW averages were between 5 and 14% lower than those specified by the manufacturer from methods based on classical polymer mass measurements. The method has the unique and significant advantage of simultaneously obtaining accurate MWDs for polymers in heterogeneous mixtures (e.g., distribution with differing monomer or end-groups). It is also consistent approach for analysing data obtained by coupling MS and concentration sensitive detectors to polymer liquid chromatography.

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