Errors in Currently Employed Standardized Methods - Predicting the Fate of Polycyclic Aromatic Hydrocarbons and Polychlorinated Biphenyls in the Environment

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Alkylated polycyclic aromatic hydrocarbon (PAH) standardized methods mostly rely on gas chromatography/mass spectrometry operated in the selected ion monitoring (GC/MS-SIM). Most standardized methods are based on acquiring a given homologue's molecular ion (1-ion). Some methods include a second, confirming ion (2-ion) in the hopes of excluding non-target matrix ion signals from the total homologue peak area. Although all of the standardized methods use homologue-specific retention windows, these windows differ greatly among methods.

The objective of this study is to develop a method based on full scan TOF data that includes polychlorinated biphenyls (PCB). Our aim is to produce a method that results in accurate data without sacrificing detection limits and, at the same time, minimizes sample preparation. Errors in quantitation by employing currently used standardized methods based on NIST-certified Standard Reference Material (SRM), crude oil SRM 1582, or marine sediment SRM 1941b sample and by the method we developed will be presented. The method we developed relies on spectral deconvolution of three to five ions per PAH/PASH and as many fragmentation patterns as needed to correctly identify the C_1 to C_4 homologues (MFPPH).

Results will show that all of the currently employed standardized methods overestimate alkylated PAH homologues concentrations compared to MFPPH. Rather than straight-line integration of homologue peaks in retention window or recognizing peak patterns, the Ion Analytics data analysis software only integrates peaks that meet the compound identity criterion. In addition, automated production of component maps by two-dimensional gas chromatography/mass spectrometry physical property modeling will be discussed as a means of assessing pollutant weathering in the environment.