

Identifying Linear and Branched Isomers from Standard PFAS Analysis for Source Delineation

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Background/Objectives. As more and more poly- and perfluoroalkyl substances (PFAS) sites are identified, there is an increased need for tools to identify potential sources and delineate areas affected by individual sources. Differences in PFAS manufacturing processes over time produced different molecular structures that provide a means to distinguish sources. The two major manufacturing processes are electrochemical fluorination (ECF) and telomerization. Before 2002, the majority of PFAS was produced by the ECF process, with telomerization becoming the primary process post-2002. ECF produces a mixture of 70% to 80% linear and 20% to 30% branched isomers. Telomerization primarily produces PFAS with almost entirely linear isomers. Based on these characteristics, the relative proportion of linear and branched isomers, in conjunction with the carbon chain length distribution, can aid in source identification and delineation of PFAS in the environment. However, not all commercial laboratories are currently able to differentiate branched and linear isomers, and those that do report only the total of linear and branched isomers as few standards for branched isomers are available. Despite these limitations, qualitative information on presence and semiquantitative information on the relative quantities of branched and linear isomers can be obtained using data generated by standard PFAS analysis by examining ion current profiles. Such analysis can provide insight into identifying potential sources and delineating impacted areas at PFAS sites.

Approach/Activities. Ion current profiles from standard PFAS analysis of groundwater samples collected near an industrial site associated with linear isomers were examined to determine the presence of branched isomers and estimate the relative proportion of branched and linear isomers. The proportions of branched isomers were then mapped as part of the site investigation to determine if additional sources of PFAS were present.

Results/Lessons Learned. The analysis identified the presence of branched isomers in groundwater in certain areas indicating additional source(s) are present.