Track 4. Chemistry and Exposure Assessment

Bridging the Gap Between the Unknown and the Known for PFAS Analysis

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Non-targeted and targeted workflows are foundational for understanding the impact of emerging compounds of concern, including PFAS, in the environment. Recent advancements in analytical instrumentation and data processing approaches have paved the way for the discovery of a growing number of PFAS structures in a variety of matrices using nontargeted analysis (NTA) techniques. However, the process of transitioning from an unknown feature to a known compound with a quantifiable concentration is often challenging. The lack of analytical standards, detailed structural information, comprehensive open access mass spectral libraries, and comprehensive analytical methods limit the ability to fully utilize NTA data for toxicological and environmental research. Furthermore, the inability to ensure data quality, lack of comparability between laboratories, data management challenges, and lack of understanding of the utility of NTA data inhibit widespread adoption. The scientific community has developed strategies to address some of these issues, using tools such as suspect list screening approaches, computational chemistry methods involving quantum mechanics, adjustments to chromatography conditions, confidence reporting, and semi-quantitative analysis. This session will provide a forum for discussing the current state of PFAS NTA, as well as the experimental and data processing approaches needed to fully utilize this data to address current challenges across the scientific community. Additionally, the session will allow researchers to share experiences regarding the steps and effort required to go from an unknown feature to a reportable or semi-quantifiable result, while highlighting methodologies that they found the most helpful.