

#### **Track 4. Chemistry and Exposure Assessment**

### **Quantitative Non-Targeted Analysis (qNTA): Bridging the Gap Between Characterization and Quantitation**

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Traditional targeted chemical measurements have failed to meet the demands of an increasingly complex chemical landscape. Non-targeted analysis (NTA) methods are increasingly used to satisfy an overwhelming need for environmental monitoring, exposure assessment, and novel compound characterization for a vast, and growing, list of environmentally relevant chemicals. NTA has promised the ability to analyze hundreds to thousands of compounds in a single analysis of a sample, and has frequently been paired with follow-up targeted analysis in order to satisfy a need for defensible, reproducible quantitative estimates of chemical concentration. Targeted analysis has therefore remained complementary to NTA as the provider of quantitative information and NTA has been viewed as largely qualitative thereby limiting the scope of quantitative information available about the environmental contaminants. Recent advancements in computational methods and beyond have progressed quantitative non-targeted analysis strategies (qNTA) to provide concentration estimates for chemicals detected in NTA experiments. Methods using qNTA approaches can better support risk-based decision making, toxicology, and other downstream analyses that require concentration estimates while still providing the breadth of analytes observed in NTA methods. This session will present various advances and applications in making quantitative usage of NTA data. Presentations may focus on development of new modeling techniques for qNTA (considering parameters such as chemical response, extraction/recovery, and method amenability), advances in study design that enable more accurate and/or reproducible quantitative estimates (considering QA/QC and method validation), and practical applications of qNTA to solve research questions (including combining qNTA results with hazard data to inform chemicals risks). A primary goal of this session is to highlight recent scientific advancements and initiate a much-needed dialogue on innovative approaches for conducting qNTA studies and recommended best practices for reporting qNTA results.