

ASMS 2023: Environmental Applications Workshop Report

Tuesday, June 6, 2023, 5:45 PM

“Non-target analysis (NTA): Modern tools for unknown analysis”

Organized by the Environmental Applications Interest
Group, Co-chairs Ahmed Hamid and Kevin Tucker

Presided by Ahmed Hamid and Kevin Tucker

Summary: Environmental pollutants cause adverse health effects in humans and ecosystems. Due to rapid industrialization and urbanization, many pollutants have entered the environment, including pharmaceutical compounds, illicit drugs, pesticides, and personal care products. In addition, various per/polyfluoroalkyl substances (PFAS) have been found in many sources such as water, air, fish, soil, food, and food packaging, etc. Interestingly, PFAS degrade very slowly in the environment, which makes them one of the most important research topics for non-target environmental analysis. Liquid chromatography-mass spectrometry (LC-MS) and gas chromatography-mass spectrometry (GC-MS) have been used to analyze many pollutants in the environment. Many investigators reported that structural determination of ions can be achieved by high-resolution-MS, ion mobility spectrometry (IMS), and artificial intelligence. For example, one of the artificial intelligence tools is FluoroMatch, which is helpful for automated non-target analysis of PFAS. This workshop will discuss advances and challenges in the analysis of contaminants in the environment by non-target analysis, presented by several scientists in short overviews. This will be followed by a panel discussion led by researchers with relevant experience, along with active engagement of the audience. The goal is to share current experiences and knowledge about different instrumentation platforms for non-target analysis of pollutants in the environment to stimulate further thinking and perspectives among researchers, as well as new artificial intelligence software packages, development of libraries of contaminants, sample preparation, and the benefits of 4D workflows, such as LC-IM-MS/MS.

The Environmental Workshop attendance was more than 60 scientists at the beginning with others who were not counted trickling in during the workshop. We were pleased with the participation given the extensive workshop opportunities that were available this year. We kept with the new format enacted in 2019 with the first portion consisting of presentations and the remainder of the time used for a panel discussion.

Presentations and Panel Discussion on NTA in Environmental Applications

Anna Boatman, PhD Candidate, Erin Baker Lab, North Carolina State University

Ruth Marfil-Vega, Shimadzu Scientific Instruments

Enrico Davoli, Istituto di Ricerche Farmacologiche Mario Negri, IRCCS

Jeremy Koelmel, Post-Doc, Yale, School of Public Health

The panel was formulated to bring in application-specific knowledge for the new environmental focus on NTA from a variety of perspectives, student, post-doc, academic, and industry as well as including a variety of targets ranging from PFCs to GC-MS targets. Overall, audience participation was excellent consisting of several questions following each talk and a robust panel discussion that could have lasted beyond the allotted time. The session ended on time at 7pm, with the traditional dinner brought back for the first time post-COVID..

The room was perfectly size for the workshop, seemingly having capacity for 2 times the number of expected attendees.

Ahmed Hamid

Kevin Tucker

Co-Presiders