Unmasking the Unknown: Non-target Analysis in the aquatic environment

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The detection and identification of organic pollutants in aquatic environments, particularly from sources such as agriculture, households, and industry, are crucial for understanding environmental contamination and potential risks for aquatic organisms. Liquid chromatography coupled with high-resolution mass spectrometry (LC-HRMS) has become the most important analytical tool for comprehensively evaluating the input, behavior, and fate of organic contaminants in the water cycle. Enhanced processing pipelines for LC-HRMS data, including preprocessing, prioritization, and identification steps, have been developed in recent years to enable the fast screening of target, suspect, and non-target contaminants in wastewater, surface water, and groundwater samples. [1]

Although the throughput of LC-HRMS measurements in the lab has been constantly enhanced over the past few years, the time delay between sampling and analysis remains significant. These limitations can be overcome by using transportable mass spectrometers that enable on-site measurements. The transportable platform MS2field integrates sample preparation, liquid chromatography–high-resolution mass spectrometry measurement, automated data processing, and remote control and surveillance. This system can detect pollutants at 20-minute intervals with sensitivity and operational stability comparable to lab-based analysis. [2]

In this presentation, the capabilities of laboratory-based LC-HRMS methods as well as the unique features of the MS2field platform will be illustrated with selected application examples. These examples include the analysis of high-frequency concentration time-series of plant protection products and their transformation products in small rivers [3], the monitoring of unknown organic chemicals in industrial wastewater [4], and illicit drug screening in raw wastewater to estimate drug consumption for entire communities [2], all demonstrated with both lab and on-site LC-HRMS measurements.

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[4] S. Anliker, S. Santiago, K. Fenner, H. Singer, *Water Research,* **2022**, 215, 118221.