

Alleviating the need of standards and Leveraging advances in High Resolution Mass Spectrometry for integrated, holistic environmental monitoring of emerging contaminants

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Thousands of chemicals are released daily into the environment, posing potential risks to ecosystems and human health. Recent advancements in high-resolution mass spectrometry (HRMS) and software development have facilitated comprehensive contaminant monitoring in complex matrices. To investigate environmental samples, methodologies such as LC-ESI (RPLC and HILIC) and GC-APCI-HRMS, along with advanced workflows (target, suspect, and non-target screening) and chemometric tools, have been developed to detect known contaminants and identify unknowns. For target screening, extensive datasets of over 2,400 organic pollutants—including various compound classes and transformation products—have been developed, while the integration of ion mobility-derived CCS values and TIMS technology into LC-QTOFMS has improved sensitivity and detection accuracy. New algorithms for suspect screening enable the chemical curation of regulatory databases, yielding a comprehensive suspect list with in-silico predictions of properties (e.g., RT, RTI, fragments, toxicity). Machine learning models now optimize the selection of LC-HRMS or GC-HRMS methods, increasing identification confidence, and novel semi-quantification techniques improve concentration estimations for newly identified chemicals. These methodologies have been applied in environmental studies globally, including research on the Danube River, Black Sea, and biomonitoring in apex predators, making significant strides in the field of chemical management.