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Developing Unique Nontarget High-Resolution Mass Spectrometry Signatures to Track Contaminant Sources in Urban Waters

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ABSTRACT

Diffuse pollution in urban receiving waters often adversely impacts both humans and ecosystems. Identifying such pollution sources is challenging and limits the effectiveness of management actions intended to reduce risk. Here, we evaluated the use of nontarget analysis via high-resolution mass spectrometry (HRMS) to develop chemical fingerprints/signatures for source tracking. Specifically, we applied nontarget HRMS to characterize and differentiate two urban chemical sources: roadway runoff and wastewater influent. We isolated 112 and 598 nontarget compounds (both known and unidentified chemicals) that co-occurred in all roadway runoff and wastewater influent samples, respectively, and were unique relative to other sampled sources. For example, methamphetamine, often considered wastewater derived, was detected in all samples, implying that individual wastewater indicators may lack sufficient specificity in urban receiving waters impacted by multiple sources. Hierarchical cluster analysis differentiated source types, and normalized abundance profiling prioritized nontarget compounds with consistent relative abundance patterns across field sites for a given source. Hexa (methoxymethyl) melamine, 1,3-diphenylguanidine, and polyethylene glycols co-occurred in roadway runoff across geographic areas and traffic intensities, supporting continued development of a universal roadway runofffingerprint based on ubiquitous compounds. This study provides a proof-of-concept for isolating nontarget source fingerprints to track diffuse contamination in urban receiving waters.