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USING QSPR TECHNIQUES FOR ASSESSING THE REMOVAL OF EMERGING ORGANIC CONTAMINANTS DURING WASTEWATER AND WATER REUSE TREATMENT PROCESSES

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ABSTRACT: Many utilities are currently using drinking water sources impacted by wastewater discharge, and others are attracted to reuse treated municipal wastewater effluents to augment drinking water supplies. However, there is an increasing concern of the presence of chemical contaminants of which some might have a potential adverse effect on human health. The continuous creation of new synthetic organic chemicals precludes comprehensive testing for all potentially toxic compounds and presents an ever-present uncertainty of human health and/or environmental risks. Thus, the absence or minimization of emerging organic contaminants in potable waters is pertinent for protecting human health and the environment. The near impossibility of experimentally studying the fate and transport of current and future emerging contaminants on an individual basis indicates a need to develop a framework which provides guidance on how effectively certain compounds can be removed during drinking water and indirect potable water reuse treatment processes. Quantitative structure property relationship (QSPR) models can aid the water industry by assessing the removal performance of their treatment processes for emerging organic contaminants. The objective of this research was to identify the critical compound descriptors for assessing the tendency of removal of known emerging organic chemical compounds during wastewater and water reuse treatment processes. A comprehensive literature review was conducted on the relevant QSPR descriptive parameters of organic compounds for the following fate and treatment routes: reactivity (chemical oxidation and biodegradation mechanisms), phase partitioning (soil-aqueous and activated carbon-aqueous interfaces) and membrane transport (membrane rejection). Molecular descriptors for relevant wastewater-derived organic compounds were generated using powerful molecular modeling software, Schrödinger. Significant descriptors were derived by correlating descriptors with removal of organic compounds in the following treatment processes: biodegradation (activated sludge treatment), adsorption (activated carbon), and physical separation (nanofiltration and reverse osmosis). The treatability of organic compounds was obtained from a comprehensive literature review and from past and ongoing full-, pilot-, and bench-scale studies.

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