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Application of biomimetic chromatography for the prediction of acute aquatic toxicity of organic pollutants

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The presence of organic pollutants in aquatic environments can have adverse effects on ecosystems and long-term consequences on human health [1]. Therefore, hazard assessment of compounds seems inevitable in order to evaluate their ecological risk [2]. In order to assess the impact of such pollutants on aquatic organisms, international authorities require completion of many ecotoxicological studies, such as the acute toxicity of compounds on organisms [3]. In this work, the potential of biomimetic chromatography to predict acute aquatic ecotoxicological endpoints of organic pollutants of emerging concern was investigated. For this purpose, the retention of a total of 88 structural diverse organic compounds was measured on immobilized artificial membrane (IAM), immobilized human serum albumin (HSA) and immobilized alpha-1-acid-glycoprotein (AGP) stationary phases [4]. The retention of the aforementioned compounds was also measured via reversed phase micellar chromatography using micellar mobile phases which consisted of polyoxyethylene(23) lauryl ether (Brij35), sodium dodecyl sulfate (SDS) and cetrimonium bromide (CTAB) surfactants above critical micelle concentrations [4]. The pollutants under study included 39 pesticides, 36 drugs and 13 UV-filter compounds which are commonly used in cosmetic formulations. As ecotoxicological endpoints, half-maximal lethal concentration (LC_{50}) values of fish and half-maximal effective concentration (EC_{50} - immobilization) values of water flea (daphnia magna) were considered [5]. Data was compiled from the US Environmental Protection Agency (EPA) [6], as well as the European Chemicals Agency (ECHA) [7]. For reasons of comparison, corresponding models were developed using the traditionally used octanol-water partition coefficient (logP). Models derived with biomimetic properties resulted in better statistics and superior predictive performance compared to those based on logP. Furthermore, models constructed upon biomimetic properties were compared with each other in order to highlight the best biomimetic property that can be used for the prediction of the acute toxicity of each organism. Overall, biomimetic chromatography can be suggested as a promising technique for high-throughput screening and ranking of chemicals according to their ecotoxicological risk, especially when the reduction of animal testing and the need of rapid and economical solutions are in question.

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