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Experts Workshop on the Ecotoxicological Risk Assessment of Ionizable Organic Chemicals: Towards a Science-Based Framework for Chemical Assessment

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There is a growing need to develop analytical methods and tools that can be applied to assess the environmental risks associated with charged, polar, and ionisable organic chemicals, such as those used as active pharmaceutical ingredients, biocides, and surface active chemicals. Ionisation of an organic chemical can lead to a change in the sorption behaviour of a chemical, with anionic compounds possibly having lower sorption and cationics experiencing higher binding affinity, relative to their neutral counterparts. Changes in sorption behaviour will have a direct influence on bioavailability. Modelling the freely dissolved concentration is further complicated by the role of salinity and pH on the sorption of ionised chemicals to organic matter, but also to clay minerals. Changes in pH can also result in substantial differences in ecotoxicological effects, implying the need to determine pH-specific toxicity data. As part of an experts workshop on the ecotoxicological risk aassessment of ionisable organic chemicals, factors influencing the sorption behaviour, and hence the bioavailability of these chemicals was investigated. This understanding is further complemented by an assessment of the factors important for understanding the internal distribution, metabolism, and excretion of the chemicals, as well as an investigation of tools aimed at better understanding ecotoxicological effects. Three workgroups were commissioned with investigating the various issues, with an objective of providing insight towards the development of a science-based framework for assessing the environmental risks of ionisable organics. Here we summarise the key findings from each of the workgroups, with an emphasis on addressing limitations of current testing methods for applicability of ionisable organics and recommendations for key approaches or models than can be developed.