

**A COMBINED MODELLING AND MONITORING SCREENING APPROACH TO
ASSESS EXPOSURE TO PESTICIDE TRANSFORMATION PRODUCTS IN SURFACE WATERS**

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ABSTRACT: One of the great challenges in chemical risk assessment and water quality management is assessing the extent of exposure to transformation products (TPs) of xenobiotic contaminants. From an analytical chemistry point of view the challenge is that they are mostly rather polar compounds whose individual concentrations usually lie in the ng/L range, thus requiring sophisticated enrichment, separation and detection techniques. Most importantly, however, for TPs there is often a lack of reference standards that would enable their unequivocal identification through the standard's characteristic chromatographic behavior and fragmentation pattern. The newly developed hybrid linear iontrap-orbitrap mass spectrometer that simultaneously exhibits high mass accuracy, mass resolution (100'000) and sensitivity (10 ng/L with sample enrichment) might close this gap by allowing one to identify compounds based on their exact mass and the fragmentation patterns alone, without the need for reference standards. The use of this technique, however, is still critically dependent on an initial list of target compounds. Here we present the first results of an ongoing combined modelling and monitoring study for 16 frequently used pesticides and 53 of their likely TPs. A multispecies, multimedia model representing agricultural soil connected to an average European river was developed to calculate estimates of relative aquatic concentrations (RAC) of the pesticides and their transformation products in the river. An intensive literature survey was performed to collect chemical fate data for parent pesticide and TPs as input into the model. Where such properties were not readily available, they were estimated using the EPISuite chemical property prediction software, whose predictive performance was simultaneously assessed using the available experimental fate data. The 20 compounds with the highest RAC indices composed the target list for screening surface water samples from different agricultural areas in Switzerland. The samples were enriched by SPE and screened for the target compounds using a single orbitrap run. Accurate mass full scan MS and MS/MS in a data-dependent fashion were used for identification of the target compounds. In this way, we managed to detect several TPs in the ng/L concentration range but also identified several points in the procedure that need further refinement.

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