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Effect Directed Analysis to assess transformation products formed during water treatment

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Motivation

Advanced oxidation processes (AOPs) play an important role in degrading micropollutants like pharmaceuticals and pesticides present in water. However, during treatment, so-called transformation products (TPs) might be formed as micropollutants are not completely mineralized. These TPs can have significantly different characteristics compared to their parent compound and, in some cases, might still be biologically active.

Depending on the micropollutant(s), matrix composition and treatment conditions, a broad range of TPs can be formed. However, many of these chemicals are unknown and are hence not included in conventional analytical techniques. There is a need to develop and implement a (bio)analytical platform capable of detecting and characterizing TPs, assessing their potential toxicity, and linking their formation to AOP conditions and water characteristics.

Technological challenge

We combine advanced (bio)analytical techniques (fig 1), such as high-resolution mass spectrometry (HRMS) and effect-directed analysis (EDA), with computational methods such as in-silico prediction and machine learning models to create a comprehensive platform [1]. Computational approaches will help us prioritize and identify relevant (i.e., potentially toxic) TPs.

The platform will be implemented to assess TPs formation during AOP treatment and to establish operational risk zones based on treatment conditions, matrix, and micropollutant characteristics.

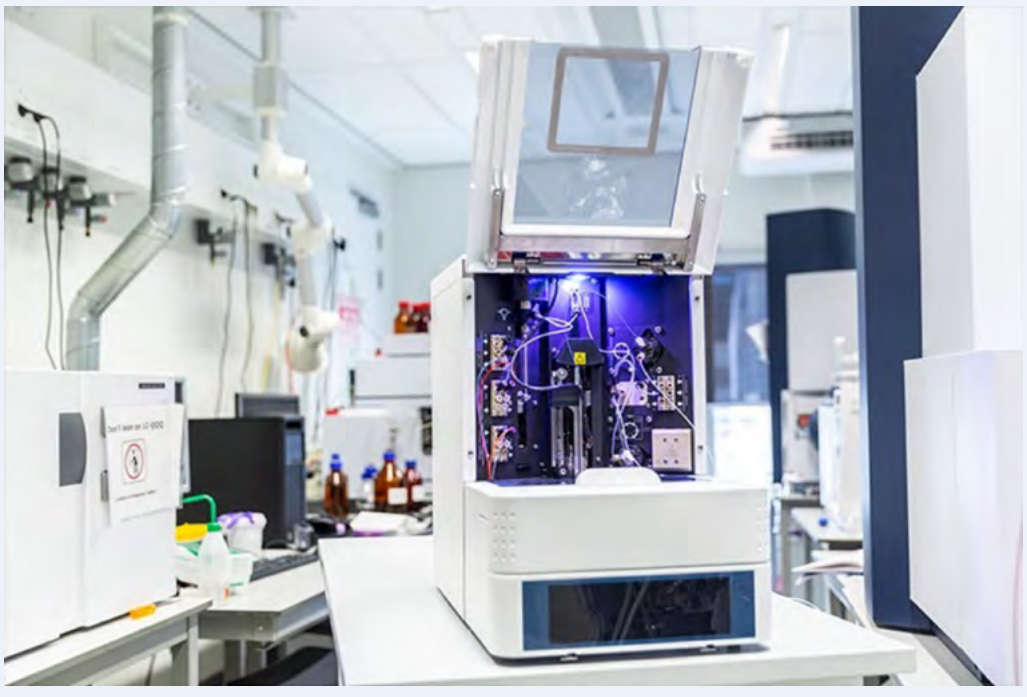

Fig 1. After a liquid chromatography (LC) separation step, the flow is split towards a) the FractioMate™, transporting eluent fractions to a high-resolution bioassay; and b) a high-resolution accurate mass spectrometer (MS) capable of identifying unknown compounds.

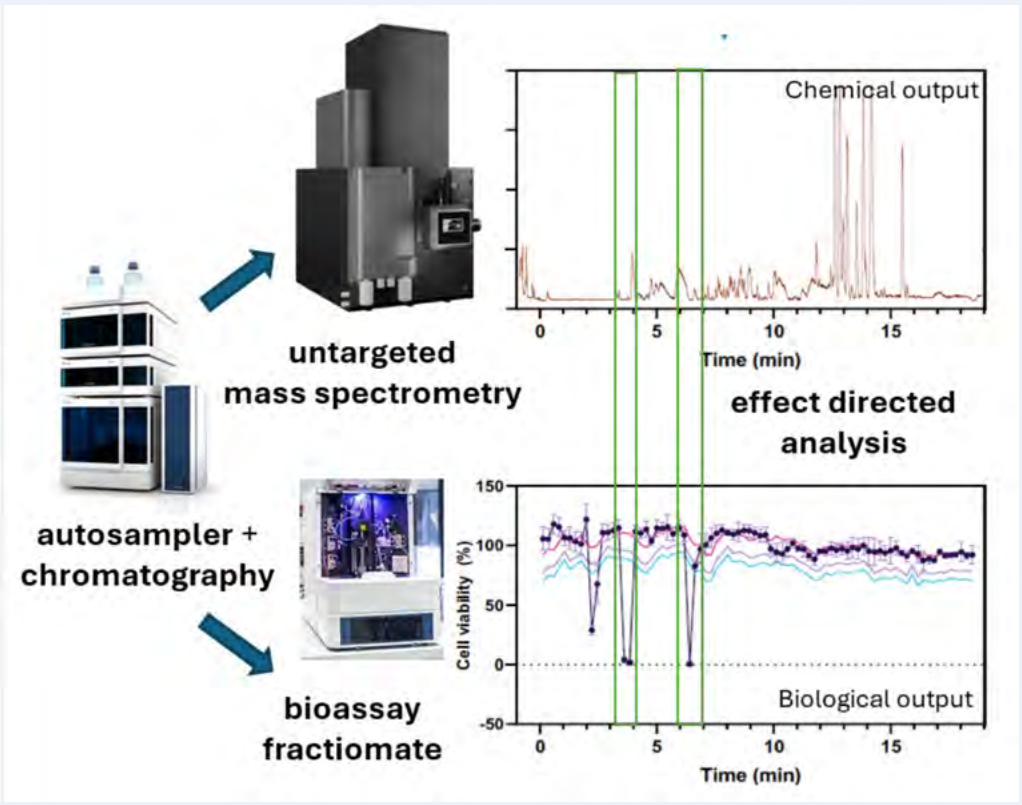

Fig 2 In Effect-Directed Analysis bioassay responses are correlated to mass compound data to identify potentially toxic compounds

Research goals

The goal is to develop an assessment framework to evaluate and identify operational risk zones for selected (waste)water treatment technologies, by:

- Linking the chemical and hazard space of TPs by understanding under which conditions they are formed and what their potential (in-vitro) toxicity is (fig 2);
- Selecting a relevant set of bioassays to be used in Effect-Directed Analysis (EDA) mode;
- Developing an EDA-platform, coupling high-throughput fractionation, effect and LC-HRMS analysis for the detection, identification, and toxicity assessment of TPs formed during AOPs;
- Performing controlled experiments and implementing the EDA-platform to investigate TPs formation during AOP treatment under various conditions;
- Complementing the EDA-platform through the implementation of in-silico approaches (e.g., machine learning algorithms) to (i) detect and prioritise TPs based on molecular structures and (ii) enhance the discovery and identification rate of TPs.

[1] Jonkers, Tim J. H., Jeroen Meijer, Jelle J. Vlaanderen, Roel C. H. Vermeulen, Corine J. Houtman, Timo Hamers, and Marja H. Lamoree. “High-Performance Data Processing Workflow Incorporating Effect-Directed Analysis for Feature Prioritization in Suspect and Nontarget Screening.” Environmental Science & Technology 56, no. 3 (February 1, 2022): 1639–51. https://doi.org/10.1021/acs.est.1c04168.]

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