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# Targeted and non-targeted liquid chromatography-mass spectrometric workflows for identification of transformation products of emerging pollutants in the aquatic environment

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## HIGHLIGHTS

- Biotic and abiotic formation of transformation products of emerging pollutants
- Comprehensive database on transformation products of emerging pollutants
- Workflows for suspect and non-target screening
- The use of high-resolution mass spectrometry to identify transformation products
- Gaps and future outlook for identification using high-resolution mass spectrometry

## ABSTRACT

Identification of transformation products (TPs) of emerging pollutants is challenging, due to the vast number of compounds, mostly unknown, the complexity of the matrices and their often low concentrations, requiring highly selective, highly sensitive techniques. We compile background information on biotic and abiotic formation of TPs and analytical developments over the past five years. We present a database of biotic or abiotic TPs compiled from those identified in recent years. We discuss mass spectrometric (MS) techniques and workflows for target, suspect and non-target screening of TPs with emphasis on liquid chromatography coupled to MS (LC-MS). Both low- and high-resolution mass analyzers have been applied, but HR-MS is the technique of choice, due to its high confirmatory capabilities, derived from the high resolving power and the mass accuracy in MS and MS/MS modes, and the sophisticated software developed.

*Keywords:*

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