

## Detect

Non-targeted screening (NTS) with high-resolution mass spectrometry (HRMS) enables monitoring complex chemical mixtures released to the environment.



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# Toxicity guided inverse design of materials for environmental remediation

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## Identification

Tandem mass spectra alongside other analytical information such as retention time allow the identification of detected chemicals.



## Toxicity

MS2Tox predicts ecotoxicity and endocrine disruption activity of chemicals detected with HRMS prior to their identification.



## Exposure

MS2Quant enables predicting the concentration and therefore exposure to the detected contaminants, thereby enabling risk assessment.



## Removal

Inverse design is one of the most promising methods for the design of novel materials that enable reducing the toxicity of environmental water samples by focusing on the removal of high-risk chemicals.

