



Reading signs from the past

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Topics: Pollutants

When water samples are analysed with a mass spectrometer, peaks of compounds appear that are completely unknown, or that weren't being looked for. If these compounds prove subsequently to be of interest to environmental researchers, evidence of their presence can be retrieved from the archived measurements.

Stored measurement results from mass spectrometers are a treasure trove. Eight reference laboratories in Europe and Australia, among them Eawag, now want to make use of this via "Retrospective Suspect Screening" in order to establish a world-wide early warning network. Data can thus be made available within a short time that show how widespread the newly-appeared problematic materials are in the environment.

Identifying compounds in existing mass spectra from a variety of sources presents a number of challenges, however. It is crucial, for example, that the data were produced by high-resolution mass spectrometers combined with chromatography, and that all the parameters of quality control were observed. In a pilot project, researchers have now searched archived mass spectra from 14 countries and 3 continents for new compounds, and have developed a set of recommendations on obtaining and analysing the data, as well as on quality control. The screening has enabled them to confirm the presence of various tensides, medications and chemicals used in industry and to show that the concept functions with disparate datasets from various countries.

Mass spectrometry

Environmental analysis without mass spectrometers is no longer imaginable. The technology

makes it possible to determine which compounds are contained in a sample, and in what quantities. The molecules are ionised, fragmented and separated by mass and charge. A specific pattern for each chemical compound is produced – the mass spectrum. For a compound, this is almost as unique as a person's fingerprint. Because innumerable substances are present in environmental samples, these are first separated chromatographically. This then results in much more specific analysis.

Publication

Alygizakis, N. A.; Samanipour, S.; Hollender, J.; Ibáñez, M.; Kaserzon, S.; Kokkali, V.; van Leerdam, J. A.; Mueller, J. F.; Pijnappels, M.; Reid, M. J.; Schymanski, E. L.; Slobodnik, J.; Thomaidis, N. S.; Thomas, K. V. (2018) Exploring the potential of a global emerging contaminant early warning network through the use of retrospective suspect screening with high-resolution mass spectrometry, *Environmental Science and Technology*, 52(9), 5135-5144, [doi:10.1021/acs.est.8b00365](https://doi.org/10.1021/acs.est.8b00365), [Institutional Repository](#)

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