Analytical and processing methodologies for non-target screening by coupling passive sampling and high resolution mass spectrometry

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Nowadays with technological advances, the use of environmental forensic approaches could help to characterize the various sources of groundwater contamination. This implies the need of specific analytical methodology to identify micropollutants, emerging substances or transformation products present at low concentrations. The high resolution mass spectrometry (HRMS) has gained increasingly in importance for monitoring organic compounds. Its high resolving power, mass accuracy and the sensitive full spectrum acquisition are the key points. Contamination profile and pattern of a specific site could be highlighted by this technique with the use of automatic data processing softwares.

The aim is to support public policy development by highlighting and identifying relevant compounds to be monitored in groundwater. The main difficulties for the implementation of monitoring are sometimes low and fluctuating concentration levels and complex mixture of pollutants. No therefore there is a strong interest to combine passive sampling to HRMS. Passive samplers allow accumulating compounds during exposure that improve trace detection and integrating pollution fluctuations. The Polar Organic Chemical Integrative Sampler (POCIS) was employed to sampling polar and semi-polar compounds (pesticides, pharmaceuticals, phenolic compounds, triazoles….).

Different sites impacted by agricultural, urban or industrial pollution sources were investigated and sampled during several months. Grab and passive sampling were deployed and analyzed by LC-QTof. To process data, different approaches were investigated according to identification confidence of NORMAN Network (Schymanski et al., 2014). The first one is based on research from target compounds listed on our homemade database (around 450 with experimental data on our system as retention time, exact masses for molecular and fragment ions) or in bibliography. The second one concerns non-targeted screening. The identification of unknown compounds was tried by using several databases such as Norman Mass Bank or Chemspider and different application manager for MassLynx software.

This approach allows highlighting the use of passive samplers as storage tool becausemore compounds are identified with POCIS. Transformation products of pesticides or pharmaceutical compounds were present in most of samples.

Keywords: non-target screening, passive sampling, POCIS, high resolution mass spectrometry

Bibliography:

Schymanski E., Jeon J., Gulde R., Fenner K., Ruff M., Singer H. and Hollender J.(2014), Identifying small molecules via high resolution mass spectrometry: communicating confidence. Environmental Science and Technology, 48, 2097-2098.