Environmental forensic in groundwater by coupling passive sampling and high resolution mass spectrometry for non-target screening

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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 and their metabolites or transformation products presents 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 of highlighting and identifying compounds of interest present 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 and integrating pollution fluctuations. The Polar Organic Chemical Integrative Sampler (POCIS) were 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. The first one is based on research from compounds listed on homemade database (around 450 with experimental data on our system as retention time, exact masses for molecular and fragment ions). The non-targeted screening was applied using statistical tools such as principal components analysis (PCA) with direct connections between original chromatograms and ion intensity. Trend plots are used to highlight relevant compounds for their identification. In tandem with this work laboratory calibration was made with POCIS in order to obtain uptake rate constants for target compounds.

This approach allows making comparison of samples and giving multidimensional visualization of chemical patterns as molecular fingerprint and highlighting recurrent or specific peaks of each site. The identification of relevant signal was partially succeeded by using different database such as Norman Mass Bank or Chemspider. The workflow used allows identifying sentinel molecules and molecular clusters as compounds never revealed in these sampling sites. From data acquired by the results post-processing it has been possible to quantify targeted compounds by using acquired data on POCIS laboratory calibration.

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