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Analytical and statistical approaches to preselect relevant organic compoundsin the non-target screening by coupling passive sampling and high resolution mass spectrometry: application to groundwater

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One of ongoing challenge is to protect and preserve water resources. This involves an increased monitoring and the characterization of micropollutants, emerging substances and their metabolites or transformation products. Emerging compounds are mostly released by wastewaters discharge into surface waters and then into other environmental compartment. All these compounds are present in complex mixture at low concentration, implying the need of specific analytical methodology to identify them.

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 low concentration levels and mix of pollutants from various sources. No therefore there is a strong interest to combine passive sampling and high resolution mass spectrometry (HRMS). On the one hand passive sampling tools allow accumulating compounds during exposure and improving the sensitivity by their integration abilities. The Polar Organic Chemical Integrative Sampler (POCIS) were used to sampling polar and semi-polar compounds. On the other hand HRMS allows detecting and identifying organic compounds. The high resolving power, mass accuracy and the sensitive full spectrum acquisition of this technique are the key points for organic compounds screening.

Different groundwater impacted by agricultural, urban or rural pressures 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 approach 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 wasappliedusingstatistical tools such as principal components analysis (PCA) with direct connections between original chromatograms and ion intensity.Trend plots are used to preselect relevant compounds for their identification.

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 compounds never revealed in these sampling sites.

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