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Analytical strategies to highlight and identify organic compounds in groundwater

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One of ongoing challenge is to protect and preserve water resources. Nowadays it is increasingly important for public policy to know what compounds are present in groundwater, which of them must be monitored and their transfer / behavior. This implies the need of specific analytical methodology to identify these micropollutants, including emerging substances or transformation products potentially present at low concentrations. The high resolution mass spectrometry (HRMS), complementary method to routine quantitative analytical ones, has gained increasingly in importance for monitoring these organic compounds but application to groundwater samples remains rare. Its high resolving power, mass accuracy and the sensitive full spectrum acquisition are the key points to identify compounds.

Groundwater samples were analyzed by liquid chromatography coupled with hybrid quadrupole time-of-flight mass spectrometry (LC-QToF). All organic compounds present in samples are acquired and recorded to the extent that compounds are analyzable by the analytical methodology. No component is targeted before analysis. Results depend of raw data process, three types are identified: target, suspect and non-target screening. The first one is based on research from compounds listed on our homemade database (around 450 with experimental data) and suspect screening from bibliography and online databases. This suspect list will be supplemented by compounds of interest for studied area. The non-targeted screening compares samples to each other by statistical tools such as principal components analysis (PCA) and gives multidimensional visualization of chemical patterns such as

molecular fingerprints. Trend plots are also used to highlight relevant compounds for their identification.

This methodology was applied during several months on four groundwater sites impacted by agricultural, or urban pressures and has demonstrated its interest in environmental monitoring. Indeed several compounds were identified as targeted and suspected compounds including transformation products. The workflow used allows identifying sentinel molecules and molecular clusters as compounds never in these sampling sites.