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Identification of pesticides and their transformation products in groundwater

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Nowadays it is increasingly important for public policy to know what compounds are present in groundwater and which of them must be monitored. This implies the need of specific analytical methodology to identify these micropollutants, emerging substances or transformation products present at low concentrations. The high resolution mass spectrometry (HRMS) has gained increasingly in importance for monitoring these organic compounds. Its high resolving power, mass accuracy and the sensitive full spectrum acquisition are the key points.

On the other hand, the main difficulties for the implementation of monitoring are sometimes low and fluctuating concentration levels and complex mixture of pollutants. 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....).

Two drinking water supplies were investigated and sampled during several months. Passive sampling was deployed monthly and analyzed by LC-QToF. To process data, different approaches were investigated. The first one is based on research from compounds listed on our homemade database (around 450 with experimental data on our system as retention time, exact masses for molecular and fragment ions) and suspect database (from bibliography and online databases). This suspect list was supplemented by crop protection agents and their degradation products of interest for these sites. The second approach concerns the non-target screening that could give information on the presence of other degradation products or unknown compounds present in all samples.

These approaches allow highlighting the use of passive samplers as storage tool because more compounds are identified with POCIS. The use of these two techniques (passive sampler and HRMS) identified some target and suspect compounds present in groundwater on several month.

Keywords: Drinking water supply, Polar Organic Chemical Integrative Sampler (POCIS), high resolution mass spectrometry, screening