

Redesign of passive samplers increase sensitivity of Compound Specific Isotope Analysis.

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Compound-specific isotope analysis (CSIA) offers an important approach to track the biodegradation history of micropollutants, such as atrazine, in aquatic environments through measurement of significant changes in isotopic ratios (e.g. $^{13}\text{C}/^{12}\text{C}$ and $^{15}\text{N}/^{14}\text{N}$) inside the molecule. The low occurrence, however, of these micropollutants (i.e. ng/L range) combined with the limited sensitivity of gas chromatography hyphenated to isotope ratio mass spectrometers (GC-IRMS) makes sampling of water a great challenge for CSIA. For example, active sampling of 60-210 L of water is necessary to provide the required amount of 1 nmol C and 3.5 nmol N to the GC-IRMS to accurately analyze $^{13}\text{C}/^{12}\text{C}$ and $^{15}\text{N}/^{14}\text{N}$, respectively, in atrazine at environmental concentration of 10 ng/L. In contrast, passive sampling offers a promising alternative approach to extract atrazine directly in the field, alleviating thereby the tediousness of transporting and handling gigantic volumes of samples. Recently, Polar Organic Chemical Integrative Samplers (POCIS), have been combined with CSIA, giving promising results, where no isotopic fractionation has been observed.^[1] However, it is of a vital importance to increase the uptake kinetics of POCIS and achieve the GC-IRMS critical mass in reasonable sampling frames. Therefore, we redesigned POCIS by examining different membrane types and sorbents. To this end, we monitored under controlled laboratory conditions concentrations of different pesticides in three compartments, namely water, membrane, and sorbent. During the entire deployment time, flow rate (3cm/s), neutral water pH, and temperature were maintained constant. Our results, as a comparison between the redesigned and traditional POCIS, showed that: a) pesticides sampling rate increased up to 4 times, b) the deployment time decreased by a factor of 3, and c) no isotopic fractionation was observed ($\Delta\delta^{13}\text{C} < 0.5 \text{ ‰}$). We conclude that redesign of POCIS has a great potential to increase sensitivity of CSIA of environmental micropollutants.

References

[1] Gilevska. T, Masbou. J, Baumlin. B, Chaumet. B, Chaumont. C, Payraudeau. S, Tourneize. J, Probst. A, Probst. J.L, Imfeld. G., Do pesticides degrade in surface water receiving runoff from agricultural catchments? Combining Passive samplers (POCIS) and compound-specific isotope analysis *Science of Total Environment*, 2022, 842, 156-735.