



Compound specific isotope analysis to investigate pesticide degradation in lysimeter experiments at field conditions

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The frequent detection of organic micropollutants such as pesticides, consumer care products or pharmaceuticals in water is an increasing concern for human and ecosystem health. Degradation analysis of these compounds can be challenging in complex systems due to the fact that metabolites are not always found and mass balances frequently cannot be closed. Many abiotic and biotic degradation pathways cause, however, distinct isotope fractionation, where light isotopes are transferred preferentially from the reactant to the product pool (normal isotope fractionation). Compound-specific isotope analysis (CSIA) of multiple elements is a particularly powerful method to evaluate organic micropollutant transformation, because it can even give pathway-specific isotope fractionation (1,2). Available CSIA field studies, however, have focused almost exclusively on volatile petroleum and chlorinated hydrocarbons, which are present in high concentrations in the environment and can be extracted easily from water for GC-IRMS analysis. In the case of micropollutants, such as pesticides, CSIA is more challenging since it needs to be conducted at lower concentrations and requires pre-concentration, purification and high chromatographic performance (3).

In this study we used lysimeters experiments to analyze transformation of atrazine, acetochlor, metolachlor and chloridazone by studying associated isotope fractionation. The project combines a) analytical method development for CSIA, b) identification of pathways of micropollutant degradation and c) quantification of transformation processes under field condition. The pesticides were applied both, at the soil surface and below the top soil under field-relevant concentrations in May 2014. After typical irrigation of the lysimeters, seepage water was collected in 50L bottles and stored for further SPE and CSIA. Here we present the very first result of a) analytical method development, b) improvement of SPE methods for complex pesticide mixtures and c) transformation of pesticides in lysimeters during the year 2014.

1 Elsner, M. Stable isotope fractionation to investigate natural transformation mechanisms of organic contaminants: principles, prospects and limitations. *J. Environ. Monit.* 12, 2005-2031 (2010).

2 Hofstetter, T. B. & Berg, M. Assessing transformation processes of organic contaminants by compound-specific stable isotope analysis. *TrAC Trends in Analytical Chemistry* 30, 618-627 (2011).

3 Elsner, M. et al. Current challenges in compound-specific stable isotope analysis of environmental organic contaminants. *Anal. Bioanal. Chem.* 403, 2471-2491, doi:10.1007/s00216-011-5683-y (2012).