

## Multiple-element compound-specific isotope analysis (C, N, Cl) to assess photodegradation of herbicides atrazine and metolachlor

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Due to their extensive use in agriculture, herbicides are widely detected in surface water. Atrazine and metolachlor are among the most frequently detected compounds in agricultural areas with potential harmful effects on ecosystems and human health. These contaminants can be degraded by various processes in surface water, among which photodegradation is expected to play an important role. These processes are often difficult to disentangle based on conventional approaches relying on concentration measurements or metabolite to parent compound ratios. Furthermore, limited degradation is not always detected based on these approaches. Compound-Specific Isotope Analysis (CSIA) is a promising tool to address these issues. During their transformation, molecules with light isotopes (e.g., <sup>12</sup>C) are usually degraded at a different rate than those with heavy isotopes (e.g., <sup>13</sup>C), creating an isotope fractionation in the undegraded fraction, which has the potential to provide conclusive evidence of pesticide turnover and unique insight into the transformation mechanisms of pesticides. However, the interpretation of isotope field data in terms of degradation processes requires the knowledge of isotope fractionation associated to each process for each element monitored, information missing or incomplete for many compounds, including atrazine and metolachlor. The goal of this study was to determine carbon, nitrogen and chlorine isotope fractionation associated with direct and indirect photodegradation of metolachlor and atrazine.

Direct and indirect photodegradation experiments were run in a photoreactor simulating sunlight, hence simulating natural photodegradation. Concentrations of herbicides and selected degradation products were monitored by LC-MS/MS, while C and N isotopes of parent compounds were determined by GC-IRMS, and Cl isotopes were analyzed by GC-MS. For direct and indirect photodegradation of atrazine and metolachlor, the reactions resulted in normal isotope effects for carbon ( $\delta_{C\text{-atrazine-direct}} = -3.8 \pm 1.2\text{‰}$ ,  $\delta_{C\text{-metolachlor-direct}} = -0.9 \pm 0.4\text{‰}$ ,  $\delta_{C\text{-atrazine-indirect}} = -1.4 \pm 0.5\text{‰}$ , and  $\delta_{C\text{-metolachlor-indirect}} = -0.4 \pm 0.1\text{‰}$ ), while the first Cl results for direct photodegradation of atrazine and metolachlor point toward an inverse isotope effect. It is expected that once