

Performance and limits of liquid chromatography isotope ratio mass spectrometry system for halogenated compounds

T. GILEVSKA *, M. GEHRE AND H. H. RICHNOW

Department of Isotope Biogeochemistry, Helmholtz Centre for Environmental Research – UFZ, 04318 Leipzig, Germany
(*correspondance: tetyana.gilevska@ufz.de)

Compound specific isotope analysis has become an important tool for assessing the fate and origin of contaminants in the environment [1]. Since 2004 liquid chromatography isotope ratio mass spectrometry (LC-IRMS) has become commercially available technique for carbon isotope analysis of non volatile, aqueous soluble compounds from complex mixtures [2]. This innovation created the possibility of new applications of compound-specific $\delta^{13}\text{C}$ analysis.

The aim of this study was to analyze the oxidation capacity of the interface of the LC-IRMS system and to determine which parameters could improve the oxidation of compounds resistant to persulfate oxidation. Oxidation capacity of the LC-IRMS system was tested with halogenated acetic acids and aromatic compounds. Acetic acid was taken as a reference compound for complete oxidation. Correct values (with reference to elementary analyzer connected to an isotope mass spectrometer; EA-IRMS) were obtained for di- and mono chlorinated and fluorinated and for tribrominated acetic acids as well as for all studied aromatic compounds. Incomplete oxidation of trichloroacetic acid and trifluoroacetic acid resulted in lower recovery compared to acetic acid and in depleted carbon isotope composition compared to values obtained on EA-IRMS. Several optimization steps, which lead to longer reaction time in the coil and increase in the concentration of radicals, were tried in order to improve the oxidation but complete combustion of highly chlorinated or fluorinated compounds was not achieved. Our study revealed for the first time the limits of a LC-IRMS system for highly halogenated compounds.

[1] Elsner *et al* (2012) *Analytical and Bioanalytical Chemistry* **403**, 2471-2491 [2] Krummen *et al* (2004) *Rapid Communications in Mass Spectrometry* **18**, 2260-2266