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Perspectives for sulfur isotope analysis of perfluorooctane sulfonic acid (PFOS)

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The emerging organic pollutant perfluorooctane sulfonic acid (PFOS) is a persistent and bioaccumulative chemical that has been detected in various environmental matrices. Compound-specific stable isotope analysis (CSIA) of PFOS can provide valuable information on its sources and potentially on precursors and transformation reactions of PFOS in the environment. While the applicability of CSIA to study the chemical transformation of perfluorooctanic acid (PFOA) has already been demonstrated, knowledge on the isotope fractionation during the transformation of PFOS is still limited due to the lack of a suitable derivatization method. In this study, different derivatization methods for PFOS have been investigated. The most promising method involves the use of bis-(4-tert-butyl phenyl)-iodonium (BtBpi) in an in-port dativization approach. The results showed an injector temperature dependent derivatization efficiency of PFOS. Thus, off-line derivatization methods at higher temperatures (> 300°C) and longer reaction times (> 5 mins) were conducted. The sulfur isotope ratios of PFOS were investigated by gas chromatography connected to multiple-collector inductively coupled plasma mass spectrometry (GC-MC-ICPMS). The newly developed derivatization method might be applied to future studies investigating the sources, transport, and fate of PFOS in the environment.