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The challenge of perfluoroalkylated surfactant analysis using LC-MS: Comparison of three different mass spectrometers

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Perfluoroalkylated surfactants (PFAS) are employed in the large-volume production of fire-fighting foams, herbicides and insecticides, lubricants, paints, adhesives and acid etching solutions. Perfluorooctane sulfonate (PFOS), a representative of this group, has recently gained considerable attention because of its wide distribution in the environment. Though most of the PFOS production volume is voluntarily phased out by the manufacturers, similar compounds with long polyfluorinated chains continue to be employed for comparable applications. Such compounds include fluorotelomer alcohols (FTOHs). It was shown earlier that FTOHs are metabolised to PFAS by rats.

Two liquid chromatographic separation systems were developed for five different PFAS and three FTOHs, respectively. Ionisation of the target compounds by atmospheric pressure chemical ionisation (APCI) and electrospray ionisation (ESI) in the negative ion mode was compared. Three different types of mass spectrometers (time-of-flight, ion trap and triple quadrupole) were evaluated concerning fragmentation patterns and efficiency, selectivity, sensitivity and linearity for the target analytes.

Partial separation and detection of nine (three major and six minor) isomers of PFOS as well as of its amide was achieved. The three MS types gave different structure information about these isomers. Up to now, PFOS has been analysed as just one compound. Including all major isomers in comprehensive environmental analysis would add additional information on sources and possible degradation and transformation processes. Furthermore, it was found that the commercial standards contain many by-products from the technical synthesis, mainly molecules with the same functional groups but shorter fluorinated carbon chains. This is an additional challenge for accurate and reliable quantification.