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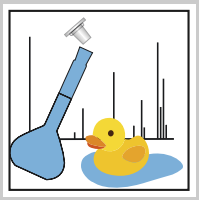

Highlights of Analytical Sciences in Switzerland

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Mass Spectrometric Analysis of Short-Chain Chlorinated Paraffins in Plastic Consumer Products

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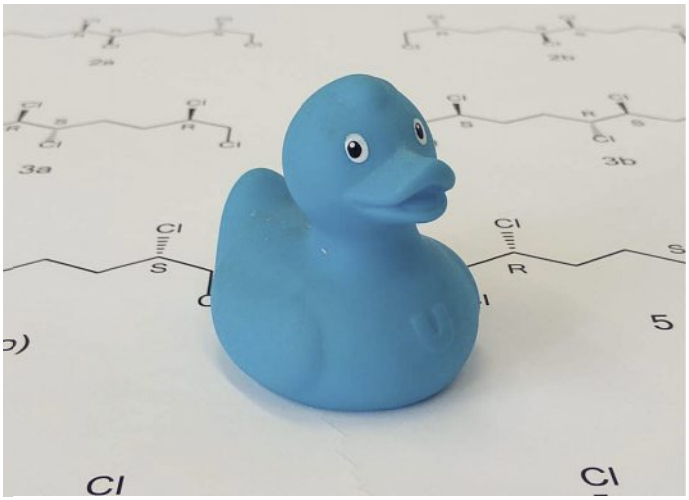
Chlorinated paraffins (CPs) are industrial chemicals with a production volume of more than 1 million tons per year. Technical CPs are complex mixtures of thousands of isomers, covering a range of carbon chain lengths (C_{10}–C_{30}) and degrees of chlorination (30–70% Cl by mass). They are applied in plastic consumer products as plasticizers or flame retardants. In 2017, short-chain chlorinated paraffins (SCCPs, C_{10}–C_{13}) were listed under the UN Stockholm Convention on Persistent Organic Pollutants (POPs) for global elimination. Accordingly, acceptable SCCP levels in consumer products have been recently lowered to 0.15% by mass (EU and Switzerland).

Mass spectrometry is the method of choice to analyze CPs. Due to high degrees of chlorination, CPs have many isotopologues (^{35}Cl, ^{37}Cl) resulting in broad isotope clusters that overlap for different CP homologues. If mass resolution is low (R < 7,000), these clusters interfere, which impedes a correct quantification of CPs. We could show that high-resolution mass spectrometry (HRMS, R > 100,000) is required to resolve mass interferences of (a) different CP homologues, (b) transformation products (*e.g.* chlorinated olefins), (c) other chlorinated organic compounds (*e.g.* polychlorinated biphenyls), and (d) fragment ions formed in the ion source. If mass resolution is insufficient, mathematical deconvolution procedures can be applied to derive non-interfered data.

In a pilot study, we tested whether SCCP levels in selected plastic consumer products are below the limit of 0.15%. Samples were cut and extracted with solvent (dichloromethane). Processed extracts were analyzed using HRMS. SCCP levels ranged between 1% and 4.4%. Hence, the tested plastic products exceeded the legal limit by 7 to 29 times. Many plastic products are imported from countries that do not have legal limits for SCCPs. Monitoring of SCCPs in imported goods is therefore an important but challenging task. **High-resolution mass spectrometry is the preferred tool for the accurate quantification of SCCP levels in consumer products and other samples.**



CPs are applied as plasticizers or flame retardants in various plastic consumer products.

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Reference

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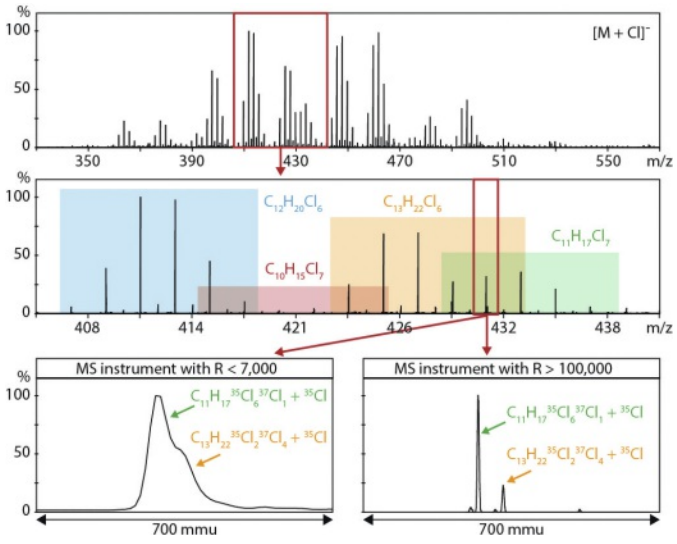

Mass spectrum of a SCCP mixture. Chloride-adducts $[M+Cl]^-$ are forced under the given ionization conditions. Isotope clusters of different CP homologues overlap and interfere in case of insufficient mass resolution (R), but can be resolved with HRMS.

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