

Highlights of Analytical Sciences in Switzerland

Division of Analytical Sciences

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

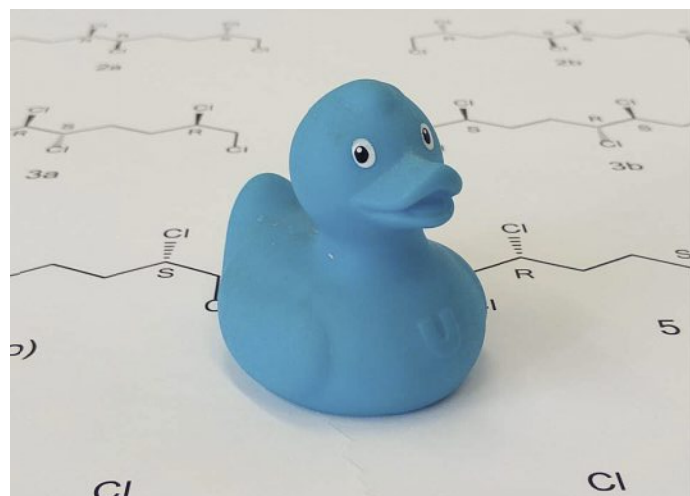
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Keywords: Chlorinated paraffins · High-resolution mass spectrometry · Persistent organic pollutants

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



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

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.**

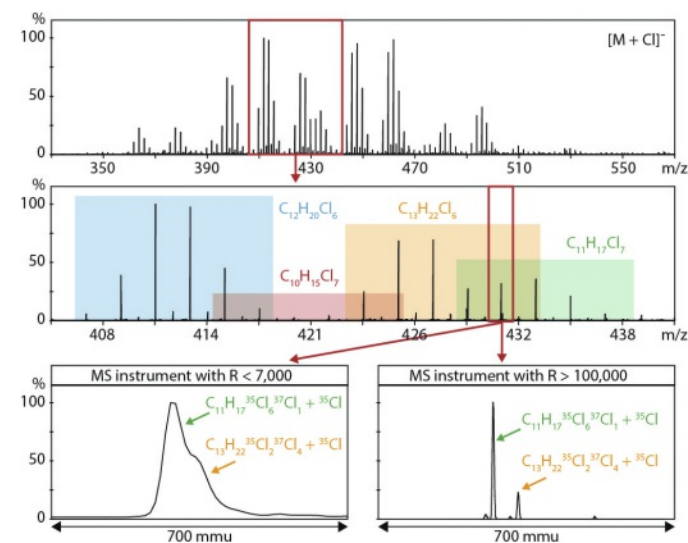
Acknowledgement

The Swiss Federal Office for the Environment (BAFU) is acknowledged for financing Empa's research on chlorinated paraffins.

Received: April 4, 2019

Reference

L. Schinkel, S. Lehner, N. Heeb, P. Marchand, R. Cariou, K. McNeill, C. Bogdal, *Trends Anal. Chem.* **2018**, *106*, 116, doi: 10.1016/j.trac.2018.07.002.



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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