

## Levels of Short-Chain Chlorinated Paraffins in Consumer Products of the Swiss Market: From a Semi-Quantitative Approach to Specific C- and Cl-Homologue Quantification

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Chlorinated paraffins (CPs) are polychlorinated *n*-alkanes with the general molecular formula  $C_nH_{2n+2-x}Cl_x$ . CPs are commonly used as plasticizers, flame retardants or coolant fluids and are currently produced at a rate of 1.5 Mt/y.<sup>[1]</sup> Depending on their carbon-chain length, CPs are classified as very short-chain (vSC-,  $C_{<10}$ ) short-chain (SC-,  $C_{10}$ – $C_{13}$ ), medium-chain (MC-,  $C_{14}$ – $C_{17}$ ), long-chain (LC-,  $C_{18}$ – $C_{21}$ ) and very long-chain (vLC-,  $C_{>21}$ ) CPs. Since 2017, SCCPs are labeled as persistent organic pollutants by the Stockholm Convention and MCCPs are under evaluation since 2022. According to a regulation introduced in 2017, SCCP levels in consumer products in Switzerland should not exceed 0.15 % in mass. Due to evolving legislations, the levels of SC- and MCCPs are of concern in various markets.<sup>[2]</sup>

Technical CP mixtures can contain a broad range of carbon- ( $C$ -,  $n_C=9$ – $30$ ) and chlorine- ( $Cl$ -,  $n_{Cl}=2$ – $20$ ) homologues with millions of constitutional isomers and stereoisomers. CPs are commonly analyzed by liquid chromatography coupled with mass spectrometry (LC-MS). Due to the lack of representative standard materials, the levels of CPs are often determined only semi-quantitatively, assuming similar MS-response factors for different homologues. This means that the amount of CPs in a standard material are compared with the amount of CPs in a sample, regardless whether their C- and Cl-homologue composition match. This approach fails when homologue distributions of standards and samples are different due to different MS-response. We developed a method where the MS-responses of each C- and Cl-homologue are quantified individually in a standard material and can now be compared with the ones found in the samples.

Herein, 30 plastic items collected from the Swiss market in 2021 were analyzed by an LC system coupled with an atmospheric pressure chemical ionization source and an Orbitrap mass analyzer (LC-APCI-Orbitrap-MS). Adduct ions of  $[M+Cl]^-$  were monitored and the corresponding high-resolution MS data were evaluated by the newly developed data evaluation tool CP Hunter. Carbon- and chlorine-homologue distributions were obtained as qualitative analysis. Quantification of the SCCP content was achieved by the C- and Cl-homologue approach.<sup>[3]</sup>

[1] Chen, C. *et al.*, *Environ. Sci. & Technol.* (2022), 7895–7904.

[2] Guida, Y. *et al.*, *Environ. Sci. & Technol.* (2023), 13136–13147.

[3] Mendo Diaz, O., *et al.*, (in preparation).