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METHOD FOR THE MEASUREMENT OF DECHLORANE 602 IN HUMAN SERUM

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Quite recently, the presence of significant amounts of several Dechlorane flame retardants was reported in environmental samples from Canada[1]. Several molecules were identified, e.g. Dec 602, 603, 604, Dechlorane Plus (DP), and Chlordene Plus (CP)[2]. So far, no data are available on the possible presence of such analytes in human specimen, particularly in Europe where very few data on any matrices are available. Therefore, the aim of this study is to develop a GC-MS method for the measurement of 602, 603, 604 and CP in human serum. The particularity of the 600 family molecules is to exhibit a bicycle [2,2,1]-heptene halogenated structure. During mass spectrometric analysis, they can undergo retro Diels-Alder reactions and typically form hexchlorocyclopentadiene (HCCPD) fragments (m/z = 272). The quantification of those analytes is most of the time carried out on the most abundant ions of this fragment cluster (e.g m/z 271.8102/273.8072 for 602).

We decided to investigate the use of comprehensive two-dimensional gas chromatography (GCxGC) coupled to negative chemical ionisation (NCI) high resolution mass spectrometry (HRMS) to ensure sensitive, specific, and accurate quantification.

GCxGC with cryogenic modulation was used to reduce the risk of chromatographic co-elution and to enhance the instrumental detection limits (iDLs) of the MS instrument. We decided to use HR time-of-flight (TOF) MS because the instrument was equipped with a specific ion source filament that allowed performing in NCI mode at temperatures as low as 140°C with a low thermal emission filament expressing good stability. The use of such reduced temperature was ideal to minimize dissociative electron capture (DEC) and enhance resonance electron capture (REC) to favor high MS signal for the parent ion cluster. This is important for isotope dilution (ID) (once ^{13}C labels will be available) accurate quantification, but also for enhanced specificity in the identification of the target molecule. Also, the cluster of the Cl_{12}-containing molecule is very specific and ion ratios can be calculated.

After optimization of isotope dilution quantification, the method will be used to measure Dec 602 at background level in European population. An extended human biomonitoring study will be considered in the near future to confirm the presence of Dec 602 at measurable levels in human.

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[1] Sverko et al., Environ. Sci. Technol. (2010) 44, 574
[2] Shen et al., Environ. Sci. Technol. (2011) 45, 693