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Compound-Specific Chlorine Isotope Analysis: A Method Comparison Study

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Chlorine isotope analysis in chlorinated hydrocarbons like trichloroethylene (TCE) is of emerging demand, since they are important environmental pollutants. Continuous flow analysis of non-combusted TCE molecules, either by gas chromatography – isotope ratio mass spectrometry (GC-IRMS) or by GC - mass spectrometry (GC-MS), was recently brought forward as an innovative analytical solution. Despite early implementations a benchmark for standard routine applications has been missing. This work systematically compared the performance of GC-MS versus GC-IRMS in five laboratories involving four different instruments (GC-IRMS: Isoprime and Thermo MAT-253, GC-MS: Agilent 6890N and Thermo Trace GC – DSQII MS). Calibrations of “raw” delta37Cl data against the international SMOC scale (Standard Mean Ocean Chloride) deviated between instruments and even between measurement days. Therefore, at least two calibration standards must always be included to obtain true differences in delta37Cl values between samples. Amount-dependency of delta37Cl was pronounced for some instruments, but could be eliminated by corrections, or by adjusting the amplitudes of standard and sample. Precision decreased in the order GC-IRMS (1delta≈0.1‰, Agilent GC-MS (1delta≈0.2‰0.5‰, Thermo GC-MS (1delta≈0.4‰0.9‰. Nonetheless, delta37Cl values between laboratories showed good agreement when the same external standards were used. These results lend confidence to the methods and may serve as a benchmark for future applications.