

Evaluation of Enhanced Comprehensive 2-D Gas Chromatography-Time-Of-Flight Mass Spectrometry for the Separation of Recalcitrant Polychlorinated Biphenyl Isomers

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Abstract

The separation of some recalcitrant polychlorinated biphenyl (PCB) isomers in extracts from environmental compartments has been a daunting task for environmental chemists. Summed quantitation values for coeluting PCB isomers are often reported. This composite data obscures the actual concentration and toxicity of the more toxic isomer. Using the individual 209 PCB congeners as analytes of interest, this research evaluated the current state of development of a comprehensive 2-D GC coupled with a time-of-flight mass spectrometer (GCxGC/TOFMS). A sequence of 1-D and 2-D modes of separation was adopted after a series of experimental GC/TOFMS and GCxGC/TOFMS runs. In two chromatographic runs, 196 PCB congeners were distinguished, including 43 of the 46 pentachlorobiphenyl isomers. Some individual chlorinated biphenyls that could not be resolved chromatographically from others were distinguished using the “ortho effect,” when only they were present. The “ortho effect” can distinguish PCBs having 2,2’-; 2,2’6’-; and 2,2’,6,6’- chlorine substituted positions from other congeners without these substitutions. Although not all 209 PCB congeners were separated, a cost effective tool for a better front-end separation of PCB-specific congeners and isomers has been demonstrated. It has the potential to acquire more accurate data for human and environmental exposure risk assessments.

Keywords: GCxGC/TOFMS, Comprehensive gas chromatography; time-of-flight mass spectrometry; polychlorinated biphenyls; congeners, ortho-effect, PCB