Comprehensive Screening of Pollutants in Household Dust Using High-Resolution Mass Spectrometry with Enhanced Chromatographic Resolution

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Introduction

• Dust is complex: Numerous, chemically diverse constituents in a wide concentration range
• Dust can be used to estimate human exposure to contaminants (e.g., Pesticides, PAHs, flame retardants)
• Analysis of dust has primarily been conducted using targeted methods and a variety of instrumental techniques

Objectives

1) Untargeted characterization of dust extracts using GC×GC and a novel multimode source with high resolution time-of-flight mass spectrometry
2) To perform quantitative analysis of Polychlorinated Paraffins (PCPs) in dust

Dust Sample Preparation

• Dust: 1) NIST SRM 2585, 2) Office Sample, and 3) Household Sample
• Extraction:

Advantages of GC×GC-HRT+ 4D Data

NIST SRM 2585: Halogenated Organic Compounds

• Soft ionization (less fragmentation)
• Higher sensitivity
• Better selectivity
• Identifiable in mixtures

Figure 3. ECNI and PCI contour plot displaying NIST SRM 2585 data collected using the Multi-Mode Source and GC×GC-TOFMS.

Table 1. HRT+ 4D instrument acquisition parameters.

Table 2. Representative compounds in SRM 2585.

Figure 4. EI plot displaying some of the major compounds in SRM 2585.

Figure 5. EI plot displaying halogenated compounds in SRM 2585.

Table 3. SRM 2585 selected halogenated compounds.

Figure 6. Peak True and library EI mass spectra for TDCPP and BDE-99 in SRM 2585.

Figure 8. ECNI plot displaying POPs in SRM 2585.

Figure 9. ECNI plot for PCPs in a calibration standard mix. Each group (cloud) region represents PCPs for which the number of carbon + chlorine atoms is constant.

Figure 10. ECNI Plot for Group 4 PCPs with formulas C_{11}H_{17}Cl_{7} and C_{12}H_{20}Cl_{6}. Mass accuracy values for the most abundant isotope in each cluster was -1.14 and 0.08 ppm respectively.

Figure 11. ECNI Plot for SCCPs and MCCPs in the NIST SRM and a household dust sample.

Polychlorinated Paraffins: Cloud Quant

• Hydrocarbons
• Aromatics
• Alcohols
• Ketones
• Fatty Acids
• Steroids
• Phosphates
• More

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