Comprehensive two-dimensional gas chromatography coupled to high resolution time-of-flight mass spectrometry for screening of organohalogenated compounds in cat hair

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Supporting Information:
- Detailed description of GC×GC–HR-TOFMS instrumental parameters.
- Mass spectra comparison with commercial mass spectral database results

GC×GC–HR-TOFMS instrumental parameters:
The instrument control, data acquisition (100 Hz) and processing was carried out using Chroma-TOF software (LECO Corporation, St Joseph, MI, USA). The GC×GC separation was achieved using a 15 m Rxi-5HT (0.25 mm I.D. × 0.1 μm df; Restek, Bellefonte, USA) as the first dimension (1D) column and 1 m Rxi-PAH (0.25 mm I.D. × 0.1 μm df; Restek, Bellefonte, USA) as the second dimension column. The injector and transfer line temperatures were maintained at 280 °C and 320 °C, respectively. The ion source temperatures was set at 250 °C and operated at 70 eV. Helium (99.999%; Air Products, Kempton Park, South Africa) was used as the carrier gas at 1.0 mL/ min. Injections of 1 μL aliquots were made in the splitless mode with a 60 s purge delay and the primary GC oven temperature was
kept constant at 90 °C for 1 min, raised at 10 °C per minute to 320 °C, and held for 5 min. The secondary oven temperature was programmed as the primary oven with a +20 °C offset. The modulation period was set to 6 s with a 1.8 s hot pulse and the modulator temperature was programmed as the primary oven with a +15 °C offset relative to the secondary oven temperature. During modulation, cold pulses were generated using dry nitrogen gas cooled by liquid nitrogen (Air Products, Kempton Park, South Africa), and hot pulses through dry nitrogen heated by a modulator heating block. Modulation gases were supplied from a nitrogen generator (Genius 1052, Peak Scientific, Scotland). Full scan data was collected at an acquisition rate of 60 spectra/ s and extraction frequency of 1.4 kHz in the high resolution mode (>25,000 FWHM at m/z 218.98).

**Mass spectra comparison with commercial mass spectral database results**

![Mass spectra comparison](image)

**Fig. S1.** Trichloroaniline
Fig. S2. Trisbromoneopentyl alcohol (TBNPA)

Fig. S3. Alpha-hexachlorocyclohexane
Fig. S4. Hexachlorobenzene (HCB)

Fig. S5. Beta-hexachlorocyclohexane
Fig. S6. Gamma-hexachlorocyclohexane

Fig. S7. Dichlorobiphenyl (Di-CB)
Fig. S8. Tri(2-chloroethyl) phosphate (TCEP)

Fig. S9. Tris(2-chloroisopropyl)phosphate (TCIPP)
Fig. S10. Delta-hexachlorocyclohexane

Fig. S11. Tris(2-chloroisopropyl)phosphate (TCIPP)
Fig. S12. Diazinone

Fig. S13. Trichlorobiphenyls (Tri-CB)
Fig. S14. Dichloroanthracene

Fig. S15. Chlorpyrifos
Fig. S16. Tetrachlorobiphenyls (Tetra-CB)

Fig. S17. trans-Chlordane
Fig. S18. cis-Chlordane

Fig. S19. Endosulfan I
Fig. S20. trans-Nonachlor

Fig. S21. 2,3,3',4,4',5,5'-Heptachloro-1'-methyl-1,2'-bipyrrrole
Fig. S22. Dichlorophenylaniline

Fig. S23. 4,4'-DDE
Fig. S24. Dieldrin

Fig. S25. Endrin
Fig. S26. Endosulfan II

Fig. S27. Pentachlorobiphenyls (Penta-CB)
Fig. S28. cis-Nonachlor

Fig. S29a. 4,4'-DDD
Fig. S29b. 2,4'-DDT

Fig. S30. Pentabromoethylbenzene (PBEB)
Fig. S31. Endosulfan sulfate

Fig. S32. 4,4'-DDT
Fig. S33. Hexachlorobiphenyls (Hexa-CB)

Fig. S34. Endrin ketone
Fig. S35. Heptachlorobiphenyls (Hepta-CB)

Fig. S36. Tetrabromodiphenyl ether (Teta-BDE)
Fig. S37. Biphenthrin

Fig. S38. Pentabromodiphenyl ether (Penta-BDE)
Fig. S39. Permethrin

Fig. S40. Cypermethrin
Fig. S41. Hexabromodiphenyl ether (Hexa-BDE)

Fig. S42. Hexabromocyclododecane isomers (HBCD)
Fig. S43. Heptabromodiphenyl ether (Hepta-BDE)

Fig. S44. Octabromodiphenyl ether (Octa-BDE)
Fig. S45. Nonabromodiphenyl ether (Nona-BDE)

Fig. S46. Decabromodiphenyl ether (Deca-BDE)
Fig. S47. Decabromodiphenyl ethane (DBDPE)