ELECTRONIC SUPPORTING INFORMATION

COMPARISON OF DIFFERENT MASS SPECTROMETRIC TECHNIQUES FOR THE DETERMINATION OF POLYCHLORINATED BIPHENYLS BY ISOTOPE DILUTION USING ^{37}CL-LABELLED ANALOGUES

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Table S1. Experimental conditions employed in the GC-ICP-MS and GC-ICP-MSMS instruments.

GAS CHROMATOGRAPHY PARAMETERS		
Model	Agilent 6890	
Column	DB-5MS (15 m, 0.25 mm, 0.1 µm)	
Injection mode	Cool On-column	
Injection volume	1 µL	
Carrier gas flow	2.6 mL min-1 (He)	
Injection temperature	280ºC	
Oven program	100°C(2min); 30°C/min to 195°C(0 min); 5°C/min to 210°C(0 min); 30°C/min to 300°C(8.83 min)	
Interface temperature	300 ºC	
ION SOURCE AND MS PARAMETERS		
	GC-ICP-MS	**GC-ICP-MS/MS**
Model	Agilent 7700	Agilent 8800
Rf power	900	800
Carrier gas flow rate	0.95 L min-1	0.95 L min-1
Auxiliary gas pressure	30 Psi (N_2)	30 Psi (N_2)
Collision gas flow	2 mL min^{-1} (He)	
Reaction Gas flow		2 mL min^{-1} (H_2)
m/z measured	35, 37	35→37, 37→39
Ion lens setting	Daily optimization	

Table S2. Experimental conditions employed in the GC-NCI-MS instrument.

GC AND INTERFACE PARAMETERS	
Model	Shimadzu QP2010 Plus
Column	DB-5MS (30m, 0.25mm, 0.25 µm)
Injection mode	Splitless
Sampling time	0.50 min
Injection volume	2 µL
Carrier gas/Flow	He/ 2 mL/min
Injection temperature	280°C
Oven programme	80°C(1min); 20°C/min to 220°C(0min); 5°C/min to 232°C(0min); 30°C/min to 300°C(3 min)
Interface temperature	280°C
ION SOURCE AND MS PARAMETERS	
Source temperature	230°C
Source voltage	70 eV
Emission current	150 µA
Reagent gas	CH_4
Solvent delay	4 min
Acquisition mode	SIM
Selected m/z	35 and 37

Table S3. Experimental conditions employed in the GC-EI-MSMS instrument.

CHROMATOGRAPHIC PARAMETERS	
Chromatograph	7890A Agilent Technologies
Column	DB-5MS (30 m x 0.25 mm i.d. x 0.25 µm coating)
Carrier gas	He (2 mL/min)
Injection mode	Splitless (2 min of purge time)
Injector temperature	280ºC
Temperature program	80ºC (1min), 220°C (0 min) at 20°C/min; 232°C (0 min) at 5°C/min; 300°C (3 min) at 30°C/min
DETECTOR PARAMETERS	
Detector	Agilent 7000
Ionization current	35 µA
Ionization energy	70 eV
Source temperature	230ºC
Interface temperature	280ºC