SUPPLEMENTARY DATA FOR ABDALLAH ET AL, 2012

ONE-STEP EXTRACTION/CLEAN-UP METHOD FOR DETERMINATION OF PCBs, PBDEs AND HBCDs IN ENVIRONMENTAL SOLID SAMPLES

Mohamed Abou-Elwafa Abdallah, Daniel Drage and Stuart Harrad

8 pages, 4 figures and 3 tables

Figure SI-1: Locations and detailed information of sediment sampling sites.

Site Name	Latitude	longitude	Altitude (m)	Area (ha)	Mean Depth (m)	Population density (people/ km^2) of local/unitary authority of lake site	Population density (people per sq km) of local/unitary authorities within 25km of site
Fleet Pond	51.2890	-0.8257	68	26.4	0.5	250-499	>2500
Edgbaston Pond	52.4546	-1.9209	127	7.2	0.9	>2500	>2500
Marton Mere	53.8093	-3.0004	7	10.8	1.35	>2500	>2500
Crag Lough	55.0058	-2.3672	244	10.1	1	≤99	≤99
Chapman's Pond	53.9344	-1.1201	16	0.6	2.13	500-999	1000-2499

Altitudes and areas from www.UKLakes.net
Population Density of England by local or unitary authority, 2007
Data from:http://www.statistics.gov.uk/default.asp
Regional Snapshots of Population data: http://www.statistics.gov.uk/regionalsnapshot/

Figure SI-2: LC-MS/MS chromatogram showing peaks of target compounds in a dust sample.

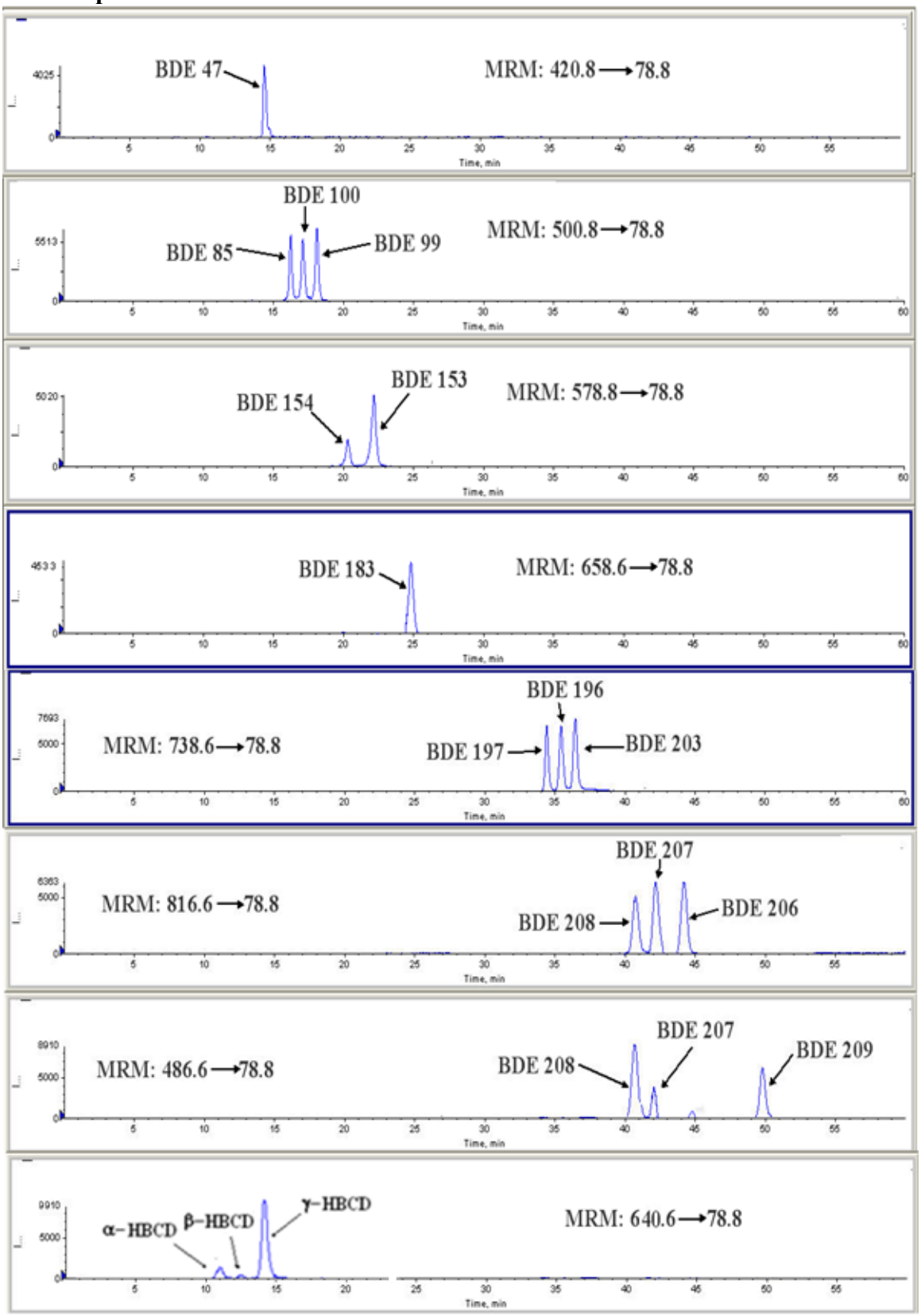
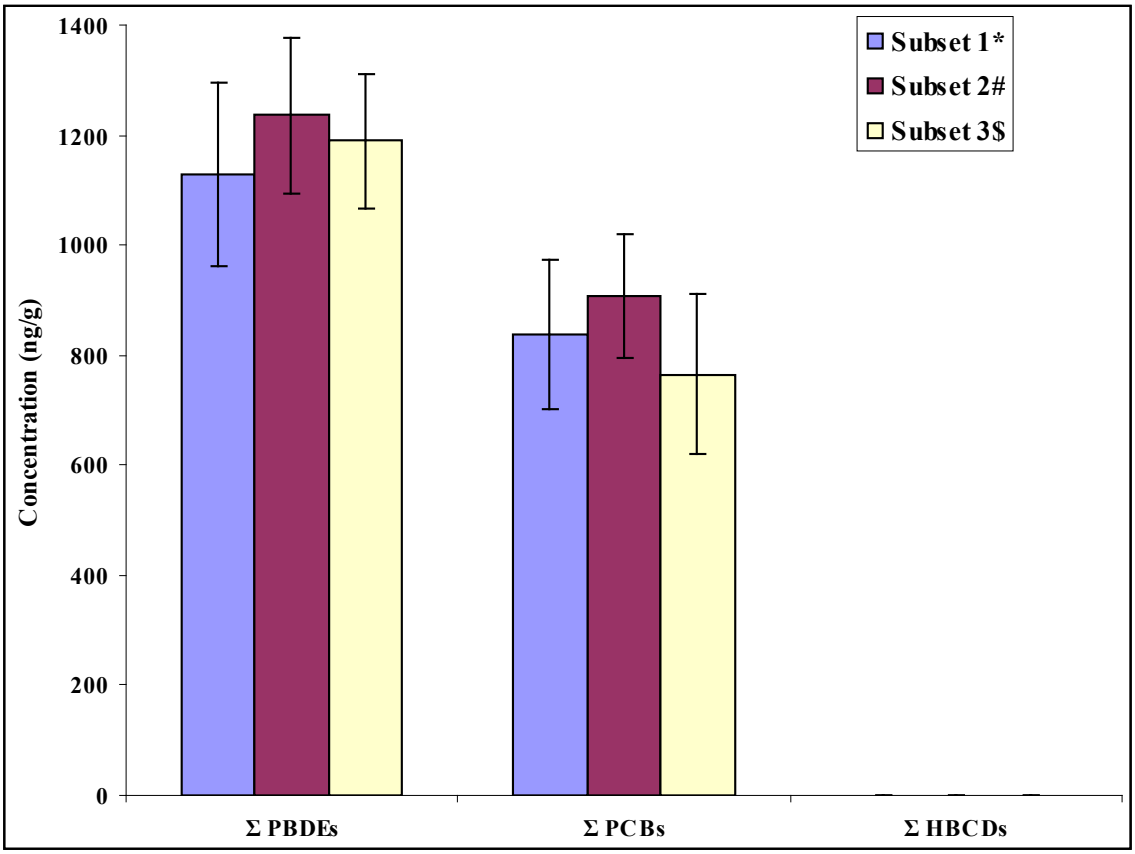
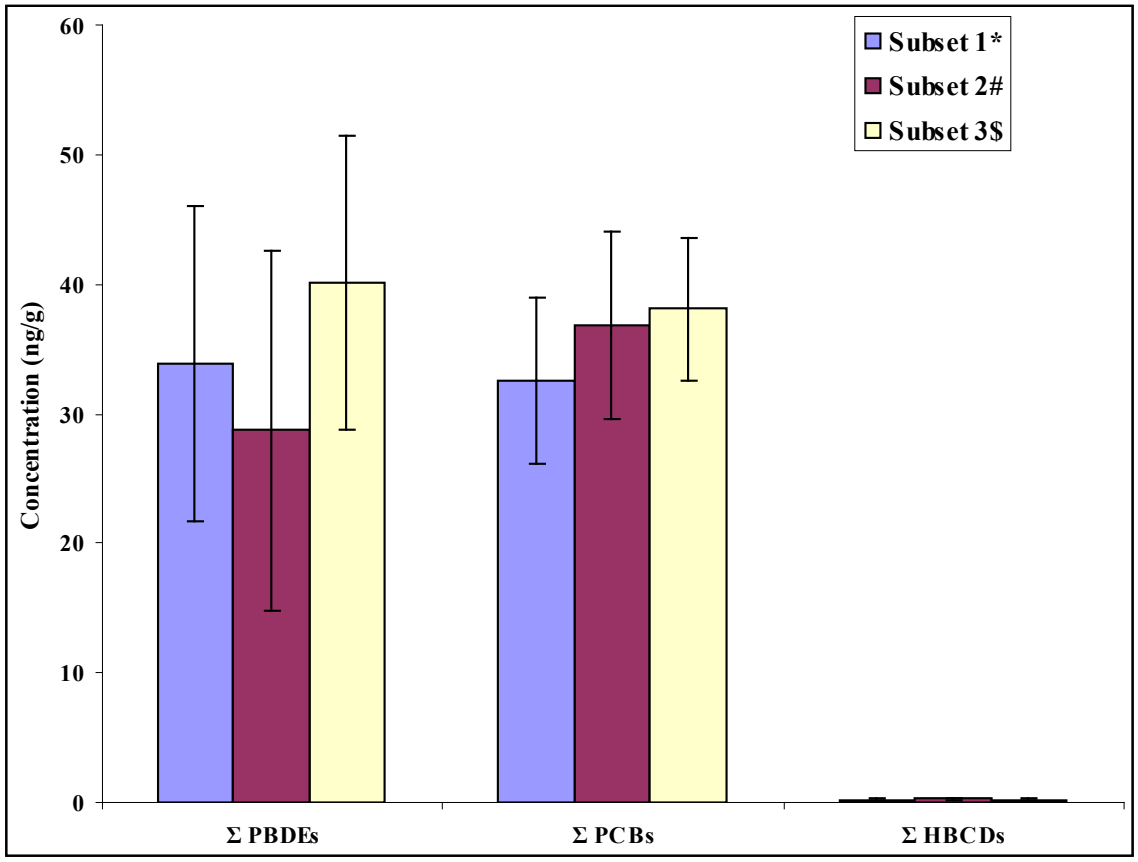


Figure SI-3: Concentrations of target analytes in EROS soil obtained at variable extraction conditions (method robustness).



* Extracted using optimized conditions (section 3.1); # extracted using 1:1 n-hexane:DCM and 70% flush volume at 85ºC; $ extracted using 1:1 n-hexane:DCM and 70% flush volume at 95ºC. All experiments were carried out in triplicates, error bars represent 1 standard deviation.

Figure SI-4: Concentrations of target analytes in SRM 1941b sediment obtained at variable extraction conditions (method robustness).



* Extracted using optimized conditions (section 3.1); # extracted using 1:1 n-hexane:DCM and 70% flush volume at 85ºC; $ extracted using 1:1 n-hexane:DCM and 70% flush volume at 95ºC. All experiments were carried out in triplicates, error bars represent 1 standard deviation.

Table SI-1: Concentrations of PCBs, PBDEs and HBCDs in in-house reference materials [26-29]**.**

	In-house reference dust	In-house reference sediment	In-house reference soil
BDE 47	56±6	1.6±0.7	114±33
BDE 85	7±3	0.05±0.03	*NR*
BDE 99	97±18	1.1±0.5	227±78
BDE 100	34±4	0.32±0.2	61±11
BDE 153	31±6	0.13±0.04	64±10
BDE 154	26±5	0.22±0.05	65±44
BDE 183	19±2	0.13±0.03	33±5
BDE 196	15±3	*ND*	*NR*
BDE 197	8±2	*ND*	*NR*
BDE 203	17±3	*ND*	*NR*
BDE 209	1184±67	27±6	588±55
PCB 28	5±2	4.9±1.5	29±14
PCB 52	16±2	4.1±0.9	23±11
PCB 101	18±3	3.6±1.2	78±22
PCB 118	11±2	2.9±0.5	124±26
PCB 138	17±2	1.9±0.7	229±38
PCB 153	24±3	3.1±0.8	238±33
PCB 180	12±2	1.7±0.5	107±19
α-HBCD	32±4	0.11±0.03	0.26±0.03
β-HBCD	7±2	0.08±0.02	0.05±0.02
γ-HBCD	41±5	0.61±0.05	0.17±0.03

Table SI-2: Limits of detection (LOD) and quantification (LOQ) of target analytes (pg/g dry weight) in indoor dust, lacustrine sediment, and soil

	Dust		Sediment		Soil	
	LOQ	LOD	LOQ	LOD	LOQ	LOD
BDE 47	7.1	2.1	6.4	1.9	7.3	2.2
BDE 85	5.4	1.6	5.3	1.6	6.2	1.9
BDE 99	6.1	1.8	5.9	1.8	6.5	2.0
BDE 100	5.7	1.7	6.2	1.9	6.1	1.8
BDE 153	5.3	1.6	5.8	1.7	5.4	1.6
BDE 154	5.9	1.8	5.2	1.6	6.0	1.8
BDE 183	6.8	2.0	6.2	1.9	5.7	1.7
BDE 196	5.9	1.8	6.4	1.9	6.3	1.9
BDE 197	6.6	2.0	5.7	1.7	5.9	1.8
BDE 203	6.1	1.8	6.3	1.9	5.6	1.7
BDE 209	10.7	3.2	11.2	3.4	10.2	3.1
PCB 28	4.7	1.4	4.2	1.3	5.2	1.6
PCB 52	5.3	1.6	4.8	1.4	4.6	1.4
PCB 101	4.8	1.4	4.4	1.3	4.9	1.5
PCB 118	5.1	1.5	5.4	1.6	5.4	1.6
PCB 138	4.4	1.3	4.7	1.4	5.2	1.6
PCB 153	4.5	1.4	4.1	1.2	4.7	1.4
PCB 180	5.7	1.7	5.2	1.6	5.0	1.5
α-HBCD	3.6	1.1	3.8	1.1	2.9	1.1
β-HBCD	2.9	1.0	3.4	1.0	3.2	1.0
γ-HBCD	3.9	1.2	3.3	1.0	2.6	1.0

Table SI-3: Percent recovery of internal standards in the analyzed samples.

	SRM 2585	SRM 1941b	EROS soil	Chapmans pond	Crag Lough	Edgbaston Pool	Marton Mere	Fleet Pond	H1	H2	H3	H4	H5	S1	S2	S3	S4	S5
^{13}C-BDE 47	93	102	102	101	88	94	98	103	99	87	87	97	89					
^{13}C-BDE 99	91	104	97	88	89	89	89	105	103	105	95	93	86	89	86	78	76	90
^{13}C-BDE153	101	94	87	103	91	97	88	100	102	102	103	96	104	117	110	86	94	106
^{13}C-BDE 183	98	99	102	97	94	105	86	87	90	86	92	87	88	118	107	81	84	101
^{13}C-BDE 209	90	95	86	90	96	90	89	95	91	91	93	93	92	126	118	101	116	114
PCB 34	96	101	102	104	90	92	95	93	97	100	95	105	93	116	127	109	91	111
PCB 62	90	97	86	101	91	88	103	104	93	96	95	87	89	99	119	82	102	99
PCB 119	85	102	88	105	105	100	104	99	90	106	102	98	95	96	114	78	96	111
PCB 131	101	99	97	93	92	102	104	103	98	105	97	104	96	100	119	86	92	109
PCB 173	103	96	91	95	87	98	100	93	92	94	85	102	103					
^{13}C-α-HBCD	86	99	89	85	100	99	104	99	89	96	104	85	91	90	75	77	79	87
^{13}C-β-HBCD	101	99	94	102	96	91	99	91	88	105	95	87	88	97	99	104	85	93
^{13}C-γ-HBCD	97	101	97	101	98	100	99	86	105	90	101	87	104					