

Electronic Supplementary Material (ESI) for Analytical Methods.

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Supplementary data to:

Optimizing a simple procedure to determine organochlorine compounds in sediment samples: practical considerations

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Table S11. Mass fractions (ng g⁻¹) obtained from the analyses of a real sample of sediment applying different drying treatments.

ng g ⁻¹	Freeze drying (-110 °C) & milled			Air drying (~25 °C) & milled			Light oven drying (50 °C) & milled			Wet, as received (untreated)		
PeC1bzn	115	110	128	96	100	107	87	91	90	95	93	118
α-HCH	82	111	127	83	66	75	37	34	38	44	40	80
β-HCH	368	474	390	419	379	379	234	261	331	164	180	323
γ-HCH	12.8	22	24	29	38	35	8	13	6	26	29	40
HxC1bzn	794	664	788	556	548	596	874	906	930	426	432	629
o,p'-DDE	205	195	217	60	48	51	109	107	111	31	29	31
p,p'-DDE	1142	864	895	432	400	451	651	659	700	302	317	343
o,p'-DDD	1932	1686	1506	1748	1719	1827	1539	1595	1630	1235	1364	1469
p,p'-DDD	2881	2629	2134	2417	2077	2240	1876	1966	1940	1502	1755	1871
o,p'-DDT	762	790	284	738	741	885	219	266	221	156	198	221
p,p'-DDT	6152	5234	3596	3800	4703	4250	3032	5344	4149	1194	1625	2920
PCB 28	264	193	183	229	225	246	176	181	186	161	164	184
PCB 52	142	152	158	139	137	144	92	93	96	76	81	89
PCB 101	104	115	76	89	84	76	65	67	68	46	50	58
PCB 118	50	38	39	42	40	47	35	35	36	12	25	27
PCB 153	116	94	111	118	114	122	82	83	84	48	55	77
PCB 138	137	93	108	124	123	132	81	82	83	48	53	72
PCB 180	135	99	109	135	135	137	84	84	85	37	43	67

Table SI2. Parameters deduced for evaluation of possible constant bias of GC/MS analysis. The measured mass, expressed as ng and “t” statistical corresponded to 0.1, 0.25 and 0.6 g (x_1 , x_2 and x_3 , respectively). The constant bias is noted as b_{cte} (in ng) and its relative uncertainty contribution is noted as $u(b_{cte})$ %. A value of “t” noted bold implies significant constant bias

(ng)	Sub-sample ₁	Sub-sample ₂	Sub-sample ₃	b_{cte}		$u(b_{cte})$ %		$t(b_{cte})$	
	$x_1=0.1$	$x_2=0.25$	$x_3=0.6$	x_1-x_2	x_2-x_3	x_1-x_2	x_2-x_3	x_1-x_2	x_2-x_3
Pentachlorobenzene	13±1.0	23±0.41	57±3.1	4.0	3.0	0.15	0.051	2.07	2.57
α-HCH	4.0±1.9	8.0±1.2	22±14	0.34	2.09	0.90	0.54	0.094	0.48
β-HCH	29±3.3	67±13	199±51	4.1	30	0.27	0.38	0.51	1.17
γ-HCH	2.1±0.29	2.9±0.72	7.6±2.3	1.3	0.51	0.34	0.48	1.79	0.36
Hexachlorobenzene	124±12	239±15	557±79	23	5.0	0.19	0.15	0.97	0.14
o,p'-DDE	14±3.4	24±5.5	86±50	4.0	21	0.52	0.58	0.57	1.51
p,p'-DDE	122±38	201±20	548±116	52	55	0.59	0.23	0.72	1.17
o,p'-DDD	342±68	712±19	1191±19	12	361	0.38	0.047	0.59	11
p,p'-DDD	338±98	635±20	1789±148	73	214	0.52	0.081	0.70	4.1
o,p'-DDT	29±6.0	50±12	141±499	10	18	0.44	0.57	0.81	0.63
p,p'-DDT	482±188	703±159	1751±12	285	68	0.76	0.45	0.78	0.22
PCB-28	24±2.6	51±2.9	121±5.2	0.53	0.23	0.21	0.10	0.10	0.043
PCB-52	13±2.1	26±1.2	64±3.1	1.0	2.1	0.31	0.090	0.26	0.89
PCB-101	8.9±1.2	18±1.5	45±1.8	0.50	1.2	0.26	0.14	0.21	0.45
PCB-118	3.7±0.69	8.8±1.2	22±1.4	0.72	0.84	0.37	0.25	0.52	0.39
PCB-138	10±1.0	22±2.5	55±4.5	0.25	2.8	0.21	0.21	0.12	0.62
PCB-153	10±1.0	22±2.7	57±5.2	0.23	3.4	0.21	0.22	0.10	0.69
PCB-180	8.3±0.48	19±2.5	53±13	0.87	6.6	0.16	0.29	0.66	1.2

Table S13. Intermediate precision estimated from analysis of sediment samples with different mass fraction levels of target compounds. Empty cells correspond to measured levels below detection limits.

(ng g ⁻¹)	sediment	sediment	sediment	sediment	sediment	sediment	sediment	sediment	Intermediate precision %	
	1	2	3	4	5	6	7	8	This work	Previous [17]
PeClBzn	15.0±0.93	156±1.9	172±20	201±16	97±5.2	80±2.5	123±18	12.4±0.63	8.5	43
α-HCH	5.5±0.34	6.6±1.8	20±5.2	412±101	34±16	27±5.5	145±21	11±5.4	29	31
β-HCH			140±38	896±64	328±85	559±76	346±26	379±56	15	36
γ-HCH	1.85±0.057	1.5±0.31	4±1.4	146±42	15±6.6	11±1.8	47±7.7		30	25
HxclBzn	614±188	2656±33	711±112	896±83	964±128	388±15	1032±143	140±14	15	39
o,p'-DDE	24±1.9	21.8±0.31	646±89	68±10	145±81	250±8.1	193±50	54±10	24	23
p,p'-DDE	218±5.6	155±8.1	1221±91	973±65	938±204	1461±76	1150±110	204±32	11	24
o,p'-DDD	237±11	273±5.3	1064±174	1465±113	1864±219	1915±219	1875±146	455±71	10	23
p,p'-DDD	382±16	482±11	1715±124	1969±199	2634±535	2394±100	2731±278	531±89	11	36
o,p'-DDT	78±23	63.5±0.50	217±36	182±33	315±137	223±14	417±152	227±53	27	54
p,p'-DDT	487±52	467±102	2267±159	2851±379	3429±1216	3054±272	6822±3113	2440±576	26	63
PCB-28	15.2±0.39	35±2.6	153±11	192±7.1	205±11	189±3.1	241±22	172±9.3	6.0	27
PCB-52	10.7±0.25	16.4±0.21	60±1.9	73±6.4	104±7.4	98±6.2	106±11	128±8.6	6.9	24
PCB-101	12.5±0.51	18.1±0.57	58±2.7	85±21	74±4.9	66±4.6	78±3.9	107±9.1	10	30
PCB-118	5.87±0.052	8.05±0.035	27±2.1	85±21	74±4.9	30±2.7	43±2.2	49±14	14	24
PCB-138	20.2±0.48	29.5±0.67	87±10	91±8.4	92±11	85±13	107±5.9	121±13	9.6	37
PCB-153	20.9±0.34	28±1.2	88±6.5	92±8.5	97±13	81±12	114±2.7	121±13	8.8	32
PCB-180	18.8±0.23	38±3.4	108±11	86±12	85±22	79±18	115±3.7	129±13	14	33