Supplementary material:

Development of passive sampling devices for analysis of bioavailable contaminants of current and emerging concern: Waitemata Harbour case study

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Figure S1. Picture (on retrieval) of DGT deployed in plastic burley cage for protection

Figure S2. Picture (on retrieval) of POCIS. These were deployed in plastic burley cage (separate to DGT) for protection

Figure S3. Picture (on retrieval) of PED deployed in metal fish cage for protection

Table S1. LC Gradient.

Step	Total Time(min)	Flow Rate(μ l/min)	A (%)	B (%)
0	0.00	500	95.0	5.0
1	2.00	500	95.0	5.0
2	10.00	500	0.0	100.0
3	11.00	500	0.0	100.0
4	11.10	500	95.0	5.0
5	15.00	500	95.0	5.0

Table S2. MS/MS parameters.

Q1	Q3 (Quant)	Q3 (Qual)	Analyte	Internal Standard
Negative Mode				
205.0	161.1	159.0	Ibuprofen	Ketoprofen 13C-D3
286.8	35.0	35.0	Triclosan	Tolfenamic acid-13C6
286.9	145.0	142.8	Estriol	Estrone-D4
268.9	144.9	142.7	Estrone	Estrone-D4
271.0	144.8	142.6	b-Estradiol 1	Estrone-D4
295.2	144.8	142.8	Ethynyl estradiol	Estrone-D4
227.3	212.1	133.0	Bisphenol A	BPA-13C12
293.7	249.9	213.9	Diclofenac	Tolfenamic acid-13C6
244.9	135.1	108.7	2,2',4,4'-Tetrahydroxybenzophenone (BP-2)	4-fluoro-4'-hydroxybenzophenone
227.0	211.2	182.8	2-Hydroxy-4-methoxybenzophenone (BP-3)	4-fluoro-4'-hydroxybenzophenone
273.0	146.8		Estrone-D4	
266.0	222.1		Tolfenamic acid - 13C6	
238.7	224.2		BPA-13C12	
214.9	91.8		4-fluoro-4'-hydroxybenzophenone	
421.0	376.0		Perfluorooctanoic acid - 13C8	
Positive Mode				
152.0	109.8	65.0	Paracetamol	Tolfenamic acid-13C6
195.1	137.9	109.9	Caffeine	Cotinine-D3
237.1	163.1	189.9	Carbamazepine	Cotinine-D3
177.0	79.9	97.9	Cotinine	Cotinine-D3
748.2	590.2	83.0	Clarithromycin	Ketoprofen 13C-D3
259.1	213.0		Ketoprofen 13C-D3	
180.0	80.1		Cotinine-D3	

Table S3. Internal Standard Recovery Statistics

Internal Standard	Average Recovery (%)	RSD (n=13, %)
Estrone-D4	57	22
Tolfenamic acid-13C6	48	45
BPA-13C12	59	23
BP-IS	64	23
Ketoprofen 13C-D3	45	42
Cotinine-D3	47	33

Internal Standard	Average Recovery (%)	RSD (n=12, %)
13C12-BDE-15	56	21
13C12-BDE-28/33	73	27
13C12-BDE-47	87	4
13C12-BDE-77	100	4
13C12-BDE-100	102	8
13C12-BDE-99	93	28
13C12-BDE-126	109	15
13C12-BDE-154	88	11
13C12-BDE-153	112	10
13C12-BDE-138/166	117	14
13C12-BDE-156/169	109	19
13C12-BDE-183/175	89	14
13C12-BDE-197	99	9
13C12-BDE-205	98	14
13C12-BDE-207	96	4
13C12-BDE-209	66	20
13C6-Hexabromobenzene (HBB)	85	5
13C12-Hexabrominated biphenyl (BB-153 2)	93	12

Internal Standard	Average Recovery (%)	RSD (n=11, %)
13C6-naphthalene	64	24
13C6-acenaphthylene	70	13
13C6-acenaphthene	74	12
13C6-fluorene	69	24
13C6-phenanthrene	78	14
13C6-anthracene	78	14
13C6-fluoranthene	87	6
13C3-pyrene	85	6
13C6-benz[a]anthracene	88	9
13C6-chrysene	85	9
13C6-benz[b]fluoranthene	91	8
13C6-benz[k]fluoranthene	90	10
13C4-benz[a]pyrene	86	9
13C6-indeno[1,2,3-cd]pyrene	82	14
13C6-dibenz[a,h]anthracene	76	18
13C12-benz[ghi]perylene	80	13

Table S4. Analyte Recovery from Spiked Sampler

	Spiked Amount (ng)	Recovery of Spiked Sampler (%)
Ibuprofen	500	102
Triclosan	50	92
Estriol	500	110
Estrone	50	98
b-Estradiol	2000	92
Ethynyl estradiol	2000	85
Bisphenol A	500	97
Diclofenac	50	91
2,2',4,4'-Tetrahydroxybenzophenone	50	103
2-Hydroxy-4-methoxybenzophenone	500	61
Paracetamol	10	117
Caffeine	40	102
Carbamazepine	40	94
Cotinine	10	95
Clarithromycin	40	63

	Spiked Amount (pg)	Recovery of Spiked Sampler (%)
BDE7	100	104%
BDE15	100	96%
BDE30	100	93%
BDE17	100	99%
BDE28/33	100	104%
BDE49	250	97%
BDE71	250	94%
BDE47	250	99%
BDE66	250	83%
BDE77	250	87%
BDE100	250	87%
BDE119/120	250	95%
BDE99	250	103%
BDE85	250	91%
BDE126	250	102%
BDE154	250	97%
BDE153	250	94%
BDE139	250	101%
BDE140	250	103%
BDE138/166	250	98%
BDE156/169	250	88%
BDE184	500	87%
BDE183	500	87%
BDE191	500	82%
BDE180	500	86%
BDE171	500	79%
BDE201	500	94%
BDE204	500	80%
BDE197	500	79%
BDE203	500	85%
BDE196	500	93%
BDE205	500	87%
BDE208	1000	127%
BDE207	1000	117%
BDE206	1000	116%
BDE209	1000	117%
PBEB	100	94%
HBB	100	100%
BB153	200	109%

	Spiked Amount (ng)	Recovery of Spiked Sampler (%)
naphthalene	100	96
acenaphthylene	100	105
acenaphthene	100	102
fluorene	100	110
phenanthrene	100	101
anthracene	100	110
fluoranthene	100	98
pyrene	100	102
benz[a]anthracene	100	105
chrysene	100	96
benz[b]fluoranthene	100	101
benz[k]fluoranthene	100	108
benz[a]pyrene	100	111
indeno[1,2,3-cd]pyrene	100	117
dibenz[a,h]anthracene	100	108
benz[ghi]perylene	100	114

Table S5. Limit of Reporting (LOR) for POCIS Sampler

	LOR (ng)
Ibuprofen	2.5
Triclosan	0.5
Estriol	5
Estrone	2.5
b-Estradiol	20
Ethinyl estradiol	20
Bisphenol A	5
Diclofenac	1
2,2',4,4'-Tetrahydroxybenzophenone	0.2
2-Hydroxy-4-methoxybenzophenone	2.5
Paracetamol	0.05
Caffeine	0.2
Carbamazepine	0.1
Cotinine	0.1
Clarithromycin	0.1