Supporting Table S1: Parent and alkyl PAH detection limits, toxic unit equivalents, and SPME-GC/MS relative response factors

	d-PAH internal standard	Target Detection Limit, ng/mL	Conc for one toxic unit, ng/mL	SPME-GC/MS RRF[b] vs. parent	Measured Detection Limit, ng/mL	Basis for detecion limit[c]
naphthalene	X	5.7	193.47	1.00	0.500	B
2-methylnaphthalene[a]		2.4	81.69	1.10	0.200	B
1-methylnaphthalene	X	2.4	81.69	0.88	0.200	B
C2 naphthalenes		0.89	30.24	1.44	0.600	B
C3 naphthalenes		0.33	11.10	0.88	0.300	B
C4 naphthalenes		0.12	4.05	0.71	0.050	C
acenaphthylene		9.0	306.85	1.00	0.100	B
acenaphthene	X	1.6	55.85	1.00	0.050	B
fluorene	X	1.2	39.30	1.00	0.050	B
C1 fluorenes		0.41	13.99	0.73	0.100	B
C2 fluorenes		0.16	5.30	0.59	0.100	B
C3 fluorenes		0.06	1.92	0.35	0.050	S
phenanthrene	X	0.56	19.13	1.00	0.200	B
anthracene	X	0.61	20.72	1.00	0.050	B
C1 phenanthrenes/anthracenes		0.22	7.44	0.57	0.200	B
C2 phenanthrenes/anthracenes		0.09	3.20	0.32	0.050	B
C3 phenanthrenes/anthracenes		0.04	1.26	0.29	0.020	B
C4 phenanthrenes/anthracenes		0.02	0.56	0.12	0.020	S
fluoranthene	X	0.21	7.11	1.00	0.040	B
pyrene	X	0.30	10.11	1.00	0.040	B
C1 fluoranthenes/pyrenes		0.14	4.89	0.51	0.050	C
benz[a]anthracene	X	0.066	2.23	1.00	0.010	B
chrysene	X	0.060	2.04	1.00	0.010	B
C1 chrysenes/benz[a]anthracenes		0.025	0.86	0.62	0.020	C
C2 chrysenes/benz[a]anthracenes		0.014	0.48	0.29	0.008	S
C3 chrysenes/benz[a]anthracenes		0.005	0.17	0.23	0.008	S
C4 chrysenes/benz[a]anthracenes		0.002	0.07	0.17	0.008	S
benzo[b+k]fluoranthene[d]	X	0.019	0.65	1.00	0.010	C
benzo[e]pyrene		0.026	0.90	1.00	0.005	C
benzo[a]pyrene	X	0.028	0.96	1.00	0.005	C
perylene	X	0.026	0.90	1.00	0.005	C
indeno[1,2,3-cd]pyrene		0.008	0.27	1.00	0.002	C
dibenz[ah]anthracene	X	0.008	0.28	1.00	0.002	C
benzo[ghi]perylene	X	0.013	0.44	1.00	0.002	C

[a]Alkyl PAHs used to determine the SPME-GC/MS relative response factors including alkyl naphthalenes (1-methyl-, 2-methyl-, 1,2-dimethyl-, 1,3-dimethyl- 1,8-dimethyl-, 2,7-dimethyl-, 1-ethyl, 2-ethyl, 1,4,5-trimethyl-, 2,3,5-trimethyl-, and 2-isopropyl-), 1-methylfluorene, 2-methyl- and 9-methylanthracene, 1-methyl-, 2-methyl-, and 3-methylphenanthrene, 9,10-dimethylanthracene, 2-ethylanthracene, 2-tertbutylanthracene, 1-methyl-7-isopropylphenanthrene, 1-methylpyrene, 7-methylbenz[a]anthracene, and 7,12-dimethylbenz[a]anthracene.

[b]All relative response factors are based on the SPME-GC/MS peak area per ng of the alkyl PAH in a water standard compared to that of its parent PAH as determined by SPME followed by GC/MS. When several isomers were available, (e.g., C2-naphthalenes), the mean relative response factor is reported. The relative response factors of alkyl PAHs for which no standards were available were estimated based on the closest analogous alkyl PAH.

[c]Detection limits were determined by background concentrations from the SPME fiber based on the analysis of water blanks ("B"), the lowest calibration standard which consistently yielded a signal to noise ratio of at least 3:1 ("C"), or (for when no calibration standard was available) for the lowest concentrations consistently found in pore water samples with a signal to noise ratio of at least 3:1 ("S"). Detection limits for alkyl PAHs are based on a single isomer.

[d]Benzo[b]fluoranthene and benzo[k]fluoranthene are reported as their sum because of insufficient chromatographic resolution. Benzo[b]fluoranthene-d12 was used as the internal standard.

Supporting Table S2: Sediment concentrations, mg/kg dry wt. [a]

Sediment	Sediment A		Sediment B		Sediment C		Sediment D	
	mean	SD	mean	SD	mean	SD	mean	SD
naphthalene	0.40	0.06	8.1	0.6	135	12	690	75
2-methylnaphthalene	0.33	0.04	7.6	0.7	86	4	554	79
1-methylnaphthalene	0.27	0.04	4.4	0.5	50	2	291	40
C2 naphthalenes	1.67	0.06	10.0	1.0	134	6	835	118
C3 naphthalenes	3.72	0.98	4.6	0.7	61	3	399	55
C4 naphthalenes	1.31	0.43	2.2	0.3	23	3	135	20
acenaphthylene	0.55	0.13	2.4	0.6	16	3	35	4
acenaphthene	0.11	0.07	5.8	1.3	63	3	395	41
fluorene	0.17	0.06	4.1	1.1	37	1	251	36
C1 fluorenes	0.70	0.22	4.3	2.6	42	4	204	77
C2 fluorenes	0.79	0.22	3.2	1.1	40	6	135	19
C3 fluorenes	2.27	0.49	ND[c]		28	5	ND	
phenanthrene	0.94	0.10	12.6	1.7	119	8	563	125
anthracene	0.87	0.30	4.4	0.7	65	4	381	57
C1 phenanthrenes/anthracenes	2.2	0.2	14.8	3.2	155	21	752	114
C2 phenanthrenes/anthracenes	8.2	2.6	23.0	6.0	180	32	742	100
C3 phenanthrenes/anthracenes	4.8	2.0	10.6	2.6	72	12	219	33
C4 phenanthrenes/anthracenes	1.51	0.57	ND		13	1	84	20
fluoranthene	1.82	0.50	9.9	1.7	75	7	378	61
pyrene	1.65	0.38	10.1	1.9	77	9	392	53
C1 fluoranthenes/pyrenes	2.61	0.67	16.8	4.0	130	21	589	90
benz[a]anthracene	0.88	0.23	4.5	1.1	35	5	203	19
chrysene	1.2	0.3	4.8	1.0	33	5	185	20
C1 chrysenes/benz[a]anthracenes	3.0	0.6	13.4	3.4	65	11	290	70
C2 chrysenes/benz[a]anthracenes	5.6	1.6	21.4	6.0	107	18	261	35
C3 chrysenes/benz[a]anthracenes	2.5	0.5	ND		128	24	ND	
C4 chrysenes/benz[a]anthracenes	2.4	0.2	ND		121	29	ND	
benzo[b+k]fluoranthene	1.2	0.3	4.0	0.8	23	3	206	30
benzo[e]pyrene	0.59	0.13	2.4	0.5	11	1	53	8
benzo[a]pyrene	0.74	0.18	4.0	1.0	34	5	187	28
perylene	0.88	0.08	1.3	0.5	7	1	48	5
indeno[1,2,3-cd]pyrene	1.48	0.49	10.9	2.8	41	6	244	30
dibenz[ah]anthracene	0.27	0.08	2.0	0.5	9	2	82	12
benzo[ghi]perylene	0.63	0.17	4.1	0.9	17	2	90	11
Sum total "34" PAHs	58	13	232	46	2232	230	9873	1125
Sum total "16" PAHs [b]	13	2	92	14	779	49	4281	390

[a]Concentrations and standard deviations are based on 18-hour Soxhlet extractions of quadruplicate samples.
[b]Total PAHs based on the sum of the 16 parent PAHs as normally reported from EPA method 610.
[c] ND=Not detected.

Table S3: Effect of removing colloids from pore water on PAH concentrations (ng/mL)[a]

	Sediment A				Sediment B				Sediment C			
	not flocculated		flocculated		not flocculated		flocculated		not flocculated		flocculated	
	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD
naphthalene	1.56	0.73	1.79	0.38	135	18	139	22	863	64	827	19
2-methylnaphthalene	0.35	0.17	0.35	0.08	47	6	44	6	162	9	144	2
1-methylnaphthalene	0.35	0.09	0.32	0.06	44	6	43	7	211	11	188	1
C2 naphthalenes	9.09	6.34	5.58	3.19	58	8	52	10	1660	228	922	40
C3 naphthalenes	3.36	0.80	1.82	0.14	50	8	44	13	1718	336	450	33
C4 naphthalenes	2.94	0.52	1.53	0.10	11.0	2.1	7.8	2.3	968	96	351	30
acenaphthylene	0.13	0.04	0.16	0.08	2.0	0.4	2.2	1.0	53	6	26	1
acenaphthene	0.20	0.03	0.26	0.09	37	4	37	7	191	10	165	2
fluorene	0.16	0.05	0.19	0.06	11.2	1.4	10.7	2.2	104	4	91	4
C1 fluorenes	0.31	0.05	0.34	0.17	5.7	0.5	3.8	0.9	230	32	63	3
C2 fluorenes	0.65	0.14	0.67	0.40	3.5	0.9	2.1	0.4	110	12	20	1
C3 fluorenes	ND[b]		ND		ND		ND		ND		ND	
phenanthrene	0.66	0.22	0.63	0.06	17.5	2.8	13.5	2.1	220	7	166	4
anthracene	0.08	0.03	0.07	0.01	3.5	0.8	2.3	0.5	34	0	23	0
C1 phenanthrenes/anthracenes	0.35	0.11	0.56	0.28	9.6	1.9	5.6	1.7	892	45	213	11
C2 phenanthrenes/anthracenes	0.54	0.15	0.50	0.08	6.8	1.7	1.8	0.6	494	136	81	4
C3 phenanthrenes/anthracenes	0.34	0.27	0.39	0.10	2.1	0.5	1.1	0.3	126	13	15	1
C4 phenanthrenes/anthracenes	0.52	0.10	0.30	0.03	1.1	0.2	1.0	0.5	53	7	7	1
fluoranthene	0.26	0.08	0.24	0.03	3.1	0.7	1.5	0.2	50	1	32	1
pyrene	0.21	0.05	0.24	0.05	3.2	0.7	1.4	0.2	36	1	25	2
C1 fluoranthenes/pyrenes	0.11	0.02	0.10	0.06	2.1	0.6	0.7	0.2	100	11	13	2
benz[a]anthracene	0.014	0.005	0.020	0.003	0.22	0.08	0.06	0.01	8.5	0.5	1.1	0.2
chrysene	0.018	0.005	0.022	0.003	0.24	0.09	0.06	0.01	6.9	0.7	0.9	0.1
C1 chrysenes/benz[a]anthracenes	0.029	0.006	ND		0.20	0.08	0.06	0.05	5.2	0.5	0.6	0.1
C2 chrysenes/benz[a]anthracenes	ND		ND		ND		ND		2.3	0.3	0.3	0.0
C3 chrysenes/benz[a]anthracenes	ND		ND		ND		ND		ND		ND	
C4 chrysenes/benz[a]anthracenes	ND		ND		ND		ND		ND		ND	
benzo[b+k]fluoranthene	0.011	0.003	0.014	0.003	0.09	0.04	0.02	0.00	2.6	0.3	0.3	0.0
benzo[e]pyrene	0.009	0.002	0.008	0.003	0.06	0.03	0.01	0.00	1.4	0.2	0.2	0.0
benzo[a]pyrene	0.007	0.002	0.014	0.006	0.11	0.05	0.03	0.01	2.4	0.3	0.3	0.0
perylene	0.013	0.002	0.006	0.005	0.03	0.01	0.01	0.01	0.48	0.06	0.06	0.01
indeno[1,2,3-cd]pyrene	0.0004	0.0001	0.0003	0.0002	0.02	0.02	0.003	0.001	0.28	0.04	0.03	0.00
dibenz[ah]anthracene	ND		0.005	0.000	0.02	0.02	ND		0.30	0.06	0.02	0.00
benzo[ghi]perylene	0.004	0.001	0.004	0.001	0.04	0.04	0.006	0.000	0.43	0.08	0.05	0.01
Sum total "34" PAHs	22.3		16.1		455		414		8305		3824	

[a]Concentrations are based on the analysis of quadruplicate pore water samples before flocculation, and a separate quadruplicate set after flocculation compared to external standard calibration.

[b] ND=Not detected.

Table S4. Pore water PAH concentrations (Sediment E) before and after 14 days of storage

	Fresh		Stored 14 days	
	mean ng/mL[a]	SD	mean ng/mL	SD
naphthalene	26.0	2.3	24.2	1.2
2-methylnaphthalene	18.1	0.5	20.7	1.2
1-methylnaphthalene	25.2	0.7	29.7	1.1
acenaphthylene	1.87	0.28	2.60	0.51
acenaphthene	23.8	0.3	27.5	2.7
fluorene	10.6	0.1	11.4	0.5
phenanthrene	16.9	0.3	16.7	0.7
anthracene	3.2	0.1	3.6	0.2
fluoranthene	2.4	0.1	2.5	0.1
pyrene	2.3	0.0	2.3	0.1
benz[a]anthracene	0.10	0.01	0.11	0.02
chrysene	0.10	0.01	0.10	0.00
benzo[b+k]fluoranthene	0.035	0.001	0.024	0.006
benzo[e]pyrene	0.021	0.002	0.021	0.004
benzo[a] pyrene	0.037	0.008	0.061	0.029
perylene	0.010	0.002	0.028	0.015
indeno[1,2,3-cd]pyrene	0.004	0.001	0.003	0.000
dibenz[ah]anthracene	0.008	0.001	0.007	0.004
benzo[ghi]perylene	0.008	0.001	0.008	0.001

[a]Concentrations and standard deviations are based on the analysis of quadruplicate pore water samples on each day.