Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supplementary data

Table S1

Results for blanks analyzed with every set of 9 samples (ng ml^{-1}, mean ± SD).

Compound	A	B
	Sediments	Mussels
Naph	79±31	87±35
Acy	2.1±1.0	5.4±3.1
Ace	2.2±0.8	5.1±1.0
Flu	8.6±2.0	12±5.9
Phe	21±9.3	91±16
Ant	0.4±0.2	0.6±0.4
Flt	7.6±3.0	22±4.3
Pyr	11±6.1	5.7±1.3
B(a)A	1.1±0.6	1.1±0.7
Chr	1.9±0.9	8.6±1.4
B(b)F	1.4±0.8	5.0±1.6
B(k)F	0.6±0.2	nd
B(a)P	0.8±0.3	nd
I(cd)P	0.8±0.3	1.2±0.3
DB(ah)A	0.4±0.1	nd
B(ghi)P	1.4±0.8	1.3±0.6

nd - the concentration was below the detection limit.

Table S2

Sediment F < 63 μm fractions: OM content and concentrations of native and alkylated PAHs (ng g^{-1} dw sediment; mean ± SD) in selected locations in the southern Baltic Sea (sample codes reflect the collection sites).

Site	Gulf of Gdańsk (GoG)			Bornholm Basin (BB)		Słupsk Furrow (SF)	
Sample code	**Z10**	**P104**	**P110**	**BB25**	**BB45**	**Z7**	**Z8**
Sampling year	2013	2014	2014	2014	2014	2013	2013
OM (%)[1]	7.7±0.04	8.4±0.4^{bc}	13±0.5^{c}	8.9±0.6^{b}	7.5±0.2^{a}	6.7±0.2	5.8±0.3
Compound							
Naph	9.2	4.8±0.9^{ab}	23±3^{c}	3.1±1.0^{a}	7.0±2.5^{b}	2.8	0.5
C1-Naph	19	7.0±0.9^{a}	27±3^{b}	5.0±2.9^{a}	8.7±3.2^{a}	4.2	1.1
C2-Naph	26	12±0.4^{a}	35±3^{b}	11±3^{a}	12±4^{a}	4.5	1.9
Acy	1.6	0.8±0.1^{a}	2.5±0.3^{c}	1.6±0.1^{b}	1.2±0.4^{ab}	0.4	0.1
Ace	3.6	3.4±0.1^{b}	11±1^{c}	2.1±0.1^{a}	2.8±0.7^{ab}	0.6	0.2
C3-Naph	31	13±1^{a}	36±3^{b}	13±3^{a}	13±4^{a}	6.5	4.4
Flu	7.1	6.3±0.1^{b}	19±3^{c}	4.7±0.6^{a}	4.9±1.4^{ab}	1.3	0.5
Phe	38	26±1^{a}	66±8^{b}	31±3^{a}	29±7^{a}	9.1	4.0
Ant	9.1	6.1±0.2^{b}	19±4^{c}	4.9±0.4^{a}	5.1±1.3^{ab}	1.4	0.6
C1-DBT	5.5	3.6±0.2^{a}	10±1^{c}	4.8±0.2^{b}	3.5±0.9^{a}	2.0	1.2
C1-Phe/Ant	63	42±2^{a}	100±10^{b}	45±2^{a}	41±10^{a}	13	8.8
C2- DBT	8.4	5.4±0.3^{a}	18±2^{c}	7.0±0.2^{b}	4.7±1.4^{a}	2.8	2.3
Flt	114	85±4^{a}	216±25^{c}	92±4^{b}	97±13^{b}	31	11
Pyr	91	62±3^{a}	159±18^{c}	84±6^{b}	78±19^{ab}	23	9.1
C2-Phe/Ant	78	51±2^{a}	131±15^{c}	55±2^{b}	47±11^{ab}	22	17
B(a)A	50	33±2^{a}	85±11^{c}	44±3^{b}	40±10^{b}	12	4.3
Chr	43	29±2^{a}	71±10^{c}	40±3^{b}	36±8^{ab}	14	5.6
B(b)F	80	53±3^{a}	170±28^{c}	153±18^{bc}	121±34^{b}	55	19
B(k)F	59	39±3^{a}	121±18^{c}	94±9^{b}	76±20^{b}	36	12
B(a)P	88	56±3^{a}	146±21^{c}	89±6^{b}	79±20^{b}	22	8.1
I(cd)P	99	64±3^{a}	221±37^{b}	281±32^{c}	205±60^{b}	96	31
DB(ah)A	16	9±0.3^{a}	32±6^{b}	35±4^{b}	27±9^{b}	10	3.3
B(ghi)P	63	39±2^{a}	129±19^{b}	145±17^{b}	111±31^{b}	55	18
Σ3-ring PAHs	59	43±2^{a}	118±16^{b}	45±3^{a}	43±11^{a}	13	5.4
Σ4-ring PAHs	300	208±10^{a}	531±64^{c}	260±14^{b}	251±60^{ab}	79	30
Σ5-ring PAHs	242	158±9^{a}	469±72^{c}	371±35^{bc}	302±82^{b}	123	42
Σ6-ring PAHs	162	103±5^{a}	350±56^{b}	426±49^{c}	316±91^{b}	151	48
Σ_{16}PAHs[2]	772	517±25^{a}	1490±205^{c}	1104±99^{b}	919±246^{b}	369	126
ΣaPAHs[3]	231	134±6^{a}	358±35^{b}	140±11^{a}	130±35^{a}	55	36
ΣPAHs[4]	1002	650±31^{a}	1847±239^{c}	1244±108^{b}	1049±281^{b}	424	162
ΣaPAHs (%) [5]	23	21±0.2^{b}	19±1^{b}	11±1^{a}	12±0.4^{a}	13	21
Ant/(Phe+Ant)	0.20	0.19	0.22	0.14	0.15	0.13	0.12
Flt/(Flt+Pyr)	0.56	0.58	0.58	0.52	0.56	0.58	0.54
(C1-Phe/Ant)/Phe	1.67	1.59	1.52	1.45	1.39	1.41	2.22

[1]Organic matter content; [2]The sum of 16 native PAHs; [3]The sum of alkylated PAH derivatives; [4]The sum of the native and alkylated PAHs; [5]ΣaPAH expressed as the percentage (%) of ΣPAHs; ^{a,b,c} ANOVA statistics (and Tukey test) or Kruskal-Wallis test.

Table S3

Correlations between the concentrations of PAHs and the content of fines (F < 63 μm) and organic matter (OM) in whole sediments (A and B, respectively), and between PAH concentrations and LOI in the sediment fraction < 63 μm (C).

Compound	A		B		C	
	Whole sediment F < 63 μm		Whole sediment OM		Fraction < 63 μm OM	
	R^2[a] or R_S[b]	*p*	R^2 or R_S	*p*	R^2 or R_S	*p*
Naph	R_s, 0.25	0.59	R_s, 0.46	0.29	R_s, 0.68	0.09
C1-Naph	R_s, 0.19	0.70	R_s, 0.14	0.76	**R^2, 0.64**	**0.03**
C2-Naph	R_s, 0.50	0.25	R_s, 0.75	0.05	**R^2, 0.69**	**0.02**
Acy	R^2, 0.001	0.94	**R^2, 0.68**	**0.02**	**R^2, 0.76**	**0.01**
Ace	R^2, 0.02	0.78	R^2, 0.54	0.06	**R_s, 0.75**	**0.05**
C3-Naph	R_s, 0.61	o.15	R_s, 0.50	0.25	**R^2, 0.61**	**0.04**
Flu	R^2, 0.01	0.80	**R^2, 0.57**	**0.05**	**R_s, 0.75**	**0.05**
Phe	R^2, 0.05	0.63	R^2, 0.44	0.10	**R^2, 0.87**	**0.002**
Ant	R^2, 0.02	0.78	R^2, 0.52	0.07	**R^2, 0.88**	**0.002**
C1-DBT	R_s, 0.50	0.25	**R_s, 0.75**	**0.05**	**R^2, 0.91**	**0.0008**
C1-Phe/Ant	R^2, 0.0007	0.86	**R^2, 0.58**	**0.04**	**R^2, 0.83**	**0.0004**
C2- DBT	R_s, 0.46	0.29	R_s, 0.68	0.09	**R^2, 0.92**	**0.0007**
Flt	R^2, 0.006	0.87	**R^2, 0.58**	**0.04**	**R^2, 0.88**	**0.002**
Pyr	R^2, 0.01	0.83	**R^2, 0.57**	**0.04**	**R^2, 0.85**	**0.003**
C2-Phe/Ant	R_s, 0.64	0.12	R_s, 0.71	0.07	**R^2, 0.86**	**0.003**
B(a)A	R^2, 0.003	0.91	**R^2, 0.63**	**0.03**	**R^2, 0.84**	**0.004**
Chr	R^2, 0.0006	0.96	**R^2, 0.65**	**0.03**	**R^2, 0.84**	**0.004**
B(b)F	R^2, 0.04	0.65	**R^2, 0.70**	**0.02**	**R^2, 0.61**	**0.04**
B(k)F	R^2, 0.03	0.72	**R^2, 0.70**	**0.02**	**R^2, 0.73**	**0.02**
B(a)P	R^2, 0.001	0.96	**R^2, 0.67**	**0.03**	**R^2, 0.80**	**0.007**
I(cd)P	R^2, 0.1	0.47	**R^2, 0.63**	**0.03**	R^2, 0.33	0.18
DB(ah)A	R^2, 0.07	0.56	**R^2, 0.68**	**0.02**	R^2, 0.44	0.11
B(ghi)P	R^2, 0.08	0.54	**R^2, 0.65**	**0.03**	R^2, 0.41	0.12
Σ_{16}PAHs	R^2, 0.008	0.85	**R^2, 0.68**	**0.02**	**R^2, 0.75**	**0.01**
ΣaPAHs	R_s, 0.50	0.25	**R_s, 0.75**	**0.05**	**R^2, 0.81**	**0.006**
ΣPAHs	R^2, 0.005	0.88	**R^2, 0.68**	**0.02**	**R^2, 0.80**	**0.006**
Σ3-ring PAHs	R^2, 0.03	0.71	R^2, 0.50	0.08	**R^2, 0.90**	**0.001**
Σ4-ring PAHs	R^2, 0.005	0.88	**R^2, 0.60**	**0.04**	**R^2, 0.86**	**0.003**
Σ5-ring PAHs	R^2, 0.02	0.75	**R^2, 0.70**	**0.02**	**R^2, 0.71**	**0.02**
Σ6-ring PAHs	R^2, 0.10	0.50	**R^2, 0.64**	**0.03**	R^2, 0.36	0.16

[a]R^2 – Pearson correlation; [b]R_S – Spearman correlation. Statistically significant correlations ($p \leq 0.05$) are bold.

Table S4

PCA results. A – whole sediment samples, B – sediment F < 63 μm fractions, C – mussels.

	A			**B**			**C**		
	Whole sediment			**Sediment fraction < 63 μm**			**Mussels**		
	PC1	**PC2**	**PC3**	**PC1**	**PC2**	**PC3**	**PC1**	**PC2**	**PC3**
% of variance	51	34	8.8	69	19	5.5	50	25	11
Eigenvalues	13	8.5	2.2	16.45	4.60	1.32	11.61	5.69	2.50
F<63μm	**-0.66**	-0.22	0.17	-	-	-	-	-	-
OM (%)	-0.11	-0.28	**0.94**	**0.52**	-0.45	**0.65**	-	-	-
Naph	0.29	**0.80**	0.44	**0.73**	-0.24	0.43	0.34	0.08	**-0.88**
C1-Naph	0.13	**0.97**	-0.01	**0.78**	0.03	-0.01	**0.69**	-0.28	**-0.59**
C2-Naph	0.14	**0.98**	0.08	**0.92**	0.12	-0.13	**0.92**	-0.33	-0.16
Acy	0.31	-0.28	**0.86**	**0.69**	-0.47	-0.25	-0.01	**0.64**	**-0.67**
Ace	**0.94**	-0.17	0.18	**0.90**	-0.22	0.33	0.36	0.30	**0.65**
C3-Naph	0.02	**0.99**	-0.06	**0.54**	**0.76**	-0.19	**0.87**	-0.41	0.23
Flu	**0.97**	-0.08	0.22	**0.92**	-0.15	0.33	**0.55**	0.24	0.30
Phe	**0.90**	-0.12	-0.31	**0.98**	-0.07	-0.07	-0.15	**0.97**	0.003
Ant	**0.95**	-0.27	0.05	**0.97**	-0.13	0.18	**-0.50**	**0.79**	0.07
C1-DBT	0.13	**0.96**	0.13	0.26	**0.94**	0.18	**0.73**	**-0.51**	0.38
C1-Phe/Ant	**0.91**	0.39	-0.08	**0.86**	0.45	-0.13	-0.16	**0.95**	0.12
C2- DBT	0.05	**0.94**	0.25	0.18	**0.92**	0.28	-0.10	**0.75**	0.36
Flt	**0.92**	-0.37	-0.07	**0.95**	-0.23	0.03	**-0.72**	**-0.61**	0.07
Pyr	**0.92**	-0.31	-0.19	**0.94**	-0.27	-0.13	**-0.87**	-0.46	0.12
C2-Phe/Ant	0.32	**0.90**	0.07	0.41	**0.90**	0.04	**-0.68**	-0.22	0.03
B(a)A	**0.83**	**-0.53**	0.06	**0.93**	-0.33	-0.15	**-0.90**	-0.41	-0.06
Chr	**0.81**	-0.47	0.04	**0.94**	0.11	-0.21	**-0.92**	-0.26	-0.07
B(b)F	**-0.93**	-0.35	0.13	**-0.99**	-0.07	0.12	**-0.94**	-0.02	-0.06
B(k)F	**-0.74**	**-0.63**	0.10	**-0.95**	-0.04	0.21	**-0.95**	-0.05	-0.03
B(a)P	**0.56**	**-0.79**	0.13	**0.83**	-0.48	-0.25	**-0.88**	-0.36	-0.05
I(cd)P	**-0.99**	-0.11	-0.01	**-0.99**	-0.12	0.03	**-0.94**	-0.01	0.01
DB(ah)A	**-0.97**	0.01	0.02	**-0.88**	-0.43	-0.05	**-0.67**	**0.66**	-0.10
B(ghi)P	**-0.98**	-0.17	0.02	**-0.99**	-0.02	0.03	**-0.92**	-0.20	0.08