Supporting information

Occurrence of organic contaminants and microbial community structure in river sediments and mollusks from an e-waste recycling area in Southeast China

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Text S1 Extraction and analysis for organic pollutant

The large particles and organic debris were removed from the sediment samples, and the soft parts of the benthic mollusks were picked out and shredded. Then, all samples were freeze-dried at -50℃ and ground through a 100-mesh sieve.Prior to extraction, 10 ng mixture of two surrogate standards (2-fluorobiphenyl and 4-terphenyl-d_{14}, Sigma-Aldrich, Inc., St. Louis, Missouri, USA) were added to each sample. All samples were Soxhlet-extracted separately for 24 h using dichloromethane (DCM, Honeywell Burdick & Jackson, Muskegon, Michigan, USA). The extracts were concentrated to 1 mL by a rotary evaporator (Heidolph Instruments GmbH & Co. KG, Schwabach, Bavaria, Germany) and DCM was replaced by hexane (Honeywell Burdick & Jackson, Muskegon, Michigan, USA). Each sample was cleaned up using 9 mm i.d. alumina/silica column in turn containing anhydrous sodium sulphate (1 cm), neutral silica gel (3 cm, 3% deactivated) and neutral alumina (3 cm, 3% deactivated) (Analytical grade, Guangzhou Chemical Reagent Factory, Guangzhou, China). The column was washed with 15 mL DCM/hexane (1:1, v/v) and the eluent was collected into a 20mL brown sample bottle. The eluted samples were concentrated to to a final volume of 100 μL in hexane under a gentle stream of nitrogen. Finally, 20 ng of hexamethylbenzene (Aldrich Chemical, Gillingham, Dorset, USA) was added as an internal standard.

PAHs and PAEs were analyzed with a gas chromatograph-mass spectrometer (Thermo Fisher, TRACE 1310, TSQ 9000, , Waltham, Massachusetts, USA) equipped with a DB-5MS capillary column (30 m, 0.25 mm, 0.25 μm). The mass spectrometer was operated in SIM mode with an EI source (-70 eV). High purity helium was used as the carrier gas at a flow rate of 1.0 mL min^{-1}.Then, 1 μL of sample was injected in splitless mode. For PAHs, the temperatures of the injector and the transfer line were set at 290 °C and 300 °C, respectively. The initial temperature is set at 60 °C and held for 1 minute, then ramped up to 100 °C at a rate of 4 °C min^{-1}, followed by an increase to 290 °C at a rate of 10 °C min^{-1}, and held for 20 minutes. The solvent delay time is 9 minutes. Quantitative analysis is performed using masses ranging from m/z 50 to 500. For PAEs, the temperatures of the injector and the transfer line were set at 260 °C and 300 °C, respectively. The initial temperature is set at 60 °C and held for 2 minute, then ramped up to 150 °C at a rate of 30 °C min^{-1}, and held for 1 minutes followed by an increase to 220 °C at a rate of 20 °C min^{-1}, and held for 6 minutes, then up to 300 °C at a rate of 10 °C min^{-1}, and held for 6 minutes.

Text S2 Ecological risk assessment

Long et al. proposed the Effects Range Low(ERL) index to evaluate the biohazard of individual PAHs in sediments(Long et al., 1995). If the concentration of PAHs in the environment is below the ERL, it is considered to have almost no toxic side effects or the toxic side effects are not obvious. The Toxic Equivalency method was proposed by Nisbet et al. (Nisbet, 1992). Since different types of PAH monomers have varying toxicities, each type of PAH monomer has a Toxic Equivalency Factor (TEF) relative to the toxicity of BaP. The ERL and TEF values for various PAHs are detailed in below:

PAHs	**ERL（ng/g）**	**TEF**
Nap	160	0.001
Acy	44	0.001
Ace	16	0.001
Flu	19	0.001
Phe	240	0.001
Ant	85.3	0.01
Fla	600	0.001
Pyr	665	0.001
BaA	261	0.1
Chr	384	0.01
BbF	/	0.1
BkF	/	0.1
BaP	430	1
IcdP	/	0.1
DahA	63.4	5
BghiP	/	0.01
Σ16PAHs	4022	/

The larger the TEF value, the stronger the carcinogenicity. The BaP Toxic Equivalency Quotients (TEQs) for PAHs are calculated as follows:

$$TEQ_{BaP}=\Sigma(C_i \times TEF_i)$$

where C_i is the concentration of the i-th PAH (ng/g), TEF_i is the TEF value of the i-th PAH, TEQ_{BaP} is the total toxic equivalent of PAHs (ng/g): <70 ng/g is considered to be at an almost risk-free level, while >70 ng/g poses a potential risk (Wang et al., 2017).

The Effects Range Low (ERL) value is one of the commonly used sediment risk assessment indicators. Based on the ERL value, using the exceedance factor (K) to evaluate the ecological risk of pollutants in aquatic sediments is a relatively common method. Wezel et al. determined the ERL values for DBP and DEHP to be 700 ng/g and 1000 ng/g, respectively (Wezel et al., 2000), while the ERL values for other PAEs are based on the 610 ng/g specified by the warning standards of Washington, USA. The K value is calculated as follows:

$$K=MEC/ERL$$

where MEC is the measured environmental concentration of PAEs in sediments. Different K values represent different ecological risk levels: $K<0.1$ suggests no potential risk, $0.1\leq K<3$ suggests relative low potential risk, $3\leq K<7$ suggests medium potential risk, $7\leq K<10$ suggests relative high potential risk, and $K>10$ indicates that ecological risks may exist.

Text S3 Ratios of characteristic PAHs in sediments

The ratios of characteristic PAH,such as Ant/ (Ant + Phe), BaA/ (BaA + Chr), Fla/ (Fla + Pyr) and IcdP/ (IcdP + BghiP) are often used to identify emission sources of PAHs. Due to the low detection rate of Ant, Ant/ (Ant + Phe) was not discussed in this study. In general, the ratio of BaA/ (BaA + Chr) < 0.2 indicates an oil source, between 0.2 and 0.35 is a mixed source (including fossil fuel combustion, crude oil and vehicle emissions), and > 0.35 is considered a combustion source(Zhu et al., 2014). For Fla/ (Fla + Pyr), a ratio between 0.4 and 0.5 indicates the source of fossil fuel combustion, and a ratio > 0.5 indicates the impact of biomass or coal combustion. And the ratio of IcdP/ (IcdP + BghiP) between 0.2 and 0.5 indicates liquid fossil fuel combustion. Ratios of characteristic PAHs in sediments were shown in the table below:

Sampling site	**Fla/（Fla + Pyr）**	**BaA/（BaA + Chr）**	**IcdP/（IcdP + BghiP）**
Site 1	0.58	0.44	0.44
Site 2	0.47	0.33	0.29
Site 3	0.54		0.26
Site 4	0.51		0.31
Site 5	0.47		0.26
Site 6	0.48	0.45	0.48
Site 7	0.43		
Site 8	0.43	0.30	0.26
Site 9	0.44	0.31	0.31
Site 10	0.45	0.30	0.32
Site 11	0.57		0.23
Site 12	0.51	0.37	0.39
Site 13	0.54	0.40	0.42
Site 14			

Table S1 The latitude and longitude of the fourteen sampling sites.

Sampling site	Latitude	Longitude
Site 1	121.42	28.53
Site 2	121.43	28.52
Site 3	121.44	28.49
Site 4	121.44	28.55
Site 5	121.46	28.55
Site 6	121.49	28.56
Site 7	121.50	28.55
Site 8	121.49	28.54
Site 9	121.50	28.52
Site 10	121.44	28.47
Site 11	121.46	28.47
Site 12	121.52	28.50
Site 13	121.60	28.50
Site 14	121.62	28.50

Table S2 Validation parameter of PAHs and PAEs according Eurachem Guidlines.

Validation Parameter	**PAHs**	**PAEs**
Linearity (R^2)	>0.997	>0.995
LOD (µg/kg)	1	1-16
LOQ (µg/kg)	3.3	3-48
Recovery (%)	82-109	90-115
Repeatability(%)	<19	1-8.9
Intermediate precision (%)	<20	<20
Measurement uncertainty	10-20%	5-15%

Table S3 Alpha diversity index of sediments and mollusks samples .

Sample ID*	ace	chao	coverage	shannon	simpson	sobs
S1	3876.89	3802.24	0.977	6.423	0.005	3027
S2	4864.80	4772.22	0.970	5.918	0.049	3694
S3	4787.39	4719.20	0.974	6.814	0.006	3947
S4	4797.29	4675.90	0.972	6.751	0.005	3789
S5	5998.50	5515.07	0.966	6.760	0.009	4821
S6	6132.29	5677.36	0.966	7.114	0.004	5076
S7	5707.60	5305.24	0.967	6.697	0.009	4625
S8	5620.30	5189.85	0.966	6.802	0.006	4323
S9	5856.30	5481.00	0.967	7.053	0.003	4827
S10	5925.52	5529.38	0.968	6.454	0.038	4945
S11	4828.05	4498.00	0.974	6.634	0.006	3970
S12	5581.10	5402.12	0.967	6.894	0.008	4387
S13	4569.34	4441.35	0.973	6.708	0.005	3567
S14	3755.71	3601.62	0.976	5.768	0.011	2568
LS1	663.93	673.57	0.997	3.443	0.076	576
LS2	769.22	746.55	0.996	1.984	0.345	624
LS4	650.22	484.76	0.996	1.488	0.447	321
LS7	313.69	246.50	0.998	1.222	0.566	175
LS9	429.32	421.60	0.997	2.392	0.173	318
LS10	332.27	353.08	0.998	1.902	0.269	274
LS11	684.47	652.00	0.996	2.434	0.230	477
LS12	124.58	130.75	0.999	1.152	0.455	92

Note: *S is the sediment samples, LS is the mollusks samples.

Table S4 Proportion of dominant microorganisms abundance at phyla level in sediment samples (%).

Sample ID	Proteobacteria	Bacteroidota	Firmicutes	Chloroflexi	Desulfobacterota	Campilobacterota	Acidobacteriota	Actinobacteriota	Verrucomicrobiota	Cyanobacteria
S1	47.96	15.10	4.77	2.57	6.84	0.15	5.99	2.84	0.67	2.42
S2	27.60	13.03	4.63	4.71	7.85	21.88	2.90	1.26	1.13	3.38
S3	38.91	10.97	9.30	5.33	9.04	3.00	4.55	2.94	1.51	3.09
S4	40.79	13.29	8.66	4.38	6.83	1.06	4.20	3.48	1.13	3.13
S5	28.03	8.81	7.06	14.81	6.99	7.19	3.13	2.09	4.60	1.75
S6	37.44	10.80	6.11	14.03	6.66	0.41	3.77	3.24	4.28	1.19
S7	28.31	8.04	15.43	13.79	7.24	1.77	2.94	3.46	6.96	1.82
S8	33.00	9.31	11.05	12.05	8.80	0.89	4.29	3.79	3.58	1.35
S9	32.12	11.69	8.71	11.42	7.64	1.75	3.70	3.02	3.84	1.94
S10	19.94	8.17	7.11	11.07	6.06	20.43	2.69	3.41	3.72	3.37
S11	41.20	13.29	9.76	7.44	7.16	0.18	2.46	3.50	3.93	3.14
S12	20.42	5.87	8.13	17.87	9.55	8.85	4.73	2.99	3.93	1.37
S13	30.99	7.94	13.44	10.64	8.00	1.93	4.88	6.45	1.56	2.78
S14	32.62	12.54	28.95	0.66	7.45	0.97	0.72	6.07	0.80	5.36

Table S5 Proportion of dominant microorganisms abundance at phyla level in mollusk samples (%).

Sample ID	Proteobacteria	Bacteroidota	Firmicutes	Actinobacteriota	Cyanobacteria	Campilobacterota	Spirochaetota	Chloroflexi	Verrucomicrobiota
LS1	75.22	4.80	7.89	6.19	3.19	0.9	0.09	0.22	0.36
LS2	60.59	31.11	1.27	2.19	1.28	0.19	0.67	0.42	0.07
LS4	69.01	20.15	1.87	3.74	3.01	0.04	0.02	0.02	0.01
LS7	96.61	1.01	1.10	0.38	0.52	0	0	0.01	0.01
LS9	75.58	1.67	15.88	0.80	1.60	0.01	0.13	0.03	0.10
LS10	91.20	3.48	1.34	1.34	0.71	0.02	0	0.06	0.08
LS11	77.04	1.52	7.23	10.83	2.35	0.01	0	0.08	0.17
LS12	67.64	13.11	0.39	0.07	0.08	0.08	0.10	0.01	0.01

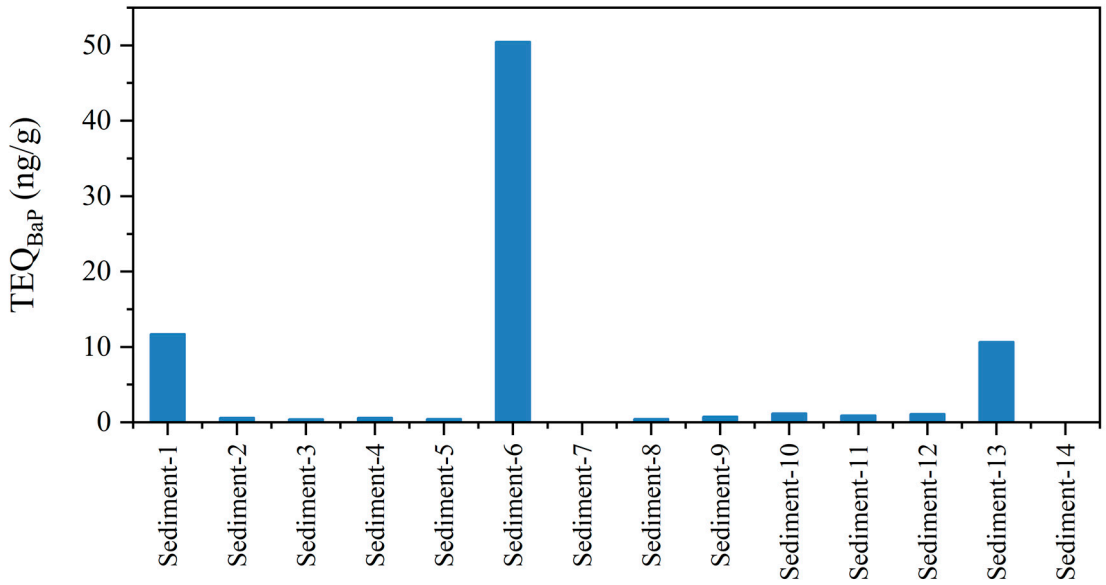


Fig. S1. TEQ_{BaP} of PAHs in sediments at each sampling sites.

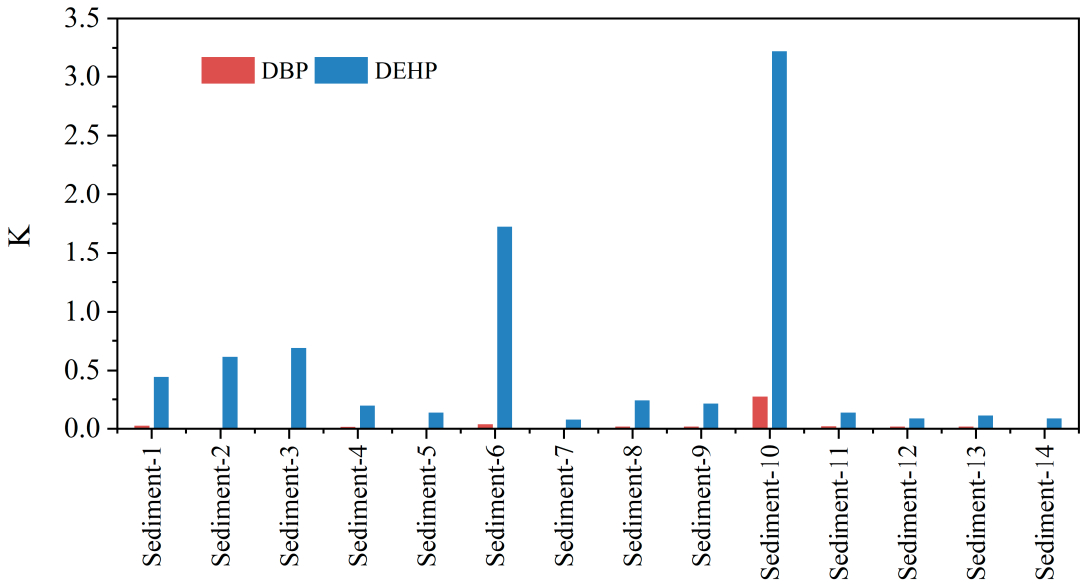


Fig. S2. K values of DBP and DEHP in sediments at each sampling sites.

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