Supporting information

Synthetic Phenolic Antioxidants and Their Metabolites in Sediments from the Coastal Area of Northern China: Spatial and Vertical Distributions

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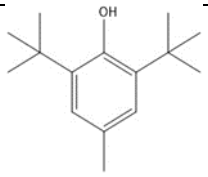
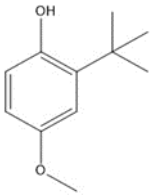
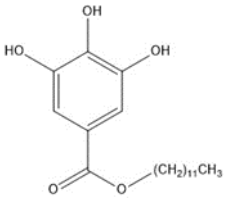
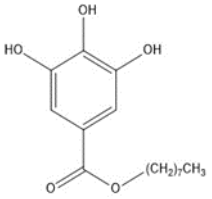
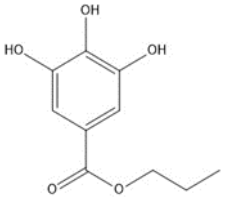
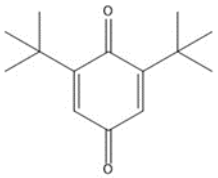
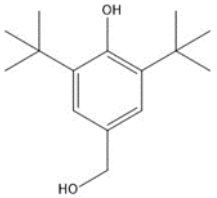
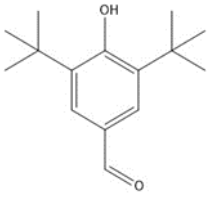
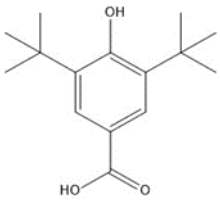
Table S1. The chemical name, CAS registry number, Log K_{ow}, Log K_{oa} and molecular structure of the target analytes.

Acronym	Chemical name	CAS	Structure	Log K_{ow}[a]	Log K_{oa}[a]
BHT	2,6-di-*tert*-butyl-4-methylphenol	128-37-0		5.10	8.87
BHA	3-*tert*-butyl-4-methoxyphenol	121-00-6		3.50	8.96
DG	Dodecyl 3,4,5-trihydroxybenzoate	1166-52-5		6.21	19.7
OG	Octyl 3,4,5-trihydroxybenzoate	1034-01-1		3.66	17.6
PG	Propyl 3,4,5-trihydroxybenzoate	121-79-9		1.80	16.4
BHT-Q	2,6-di-*tert*-butyl-1,4-benzoquinone	719-22-2		4.42	10.6
BHT-OH	2,6-di-*tert*-butyl-4-(hydroxymethyl)phenol	88-26-6		3.56	11.8
BHT-CHO	3,5-di-*tert*-butyl-4-hydroxybenzaldehyde	1620-98-0		4.20	10.6

BHT-COOH	3,5-di-*tert*-butyl-4-hydroxybenzoic acid	1421-49-4		4.36	12.9

[a] The data are predicted using the US Environmental Protection Agency's EPISuite™ and obtained from the website of ChemSpider (http://www.chemspider.com).

Table S2. Latitude, longitude and contents of TOC (%) of the sediment samples collected from the Chinese Bohai Sea, the Yellow Sea and East China Sea.

Station	Longitude(°E)	Latitude (°N)	TOC (%) [a]
HF1	121.67	35.50	0.25
HF2	122.00	35.50	0.43
HF3	122.33	35.50	0.58
BF1	122.93	37.39	0.61
BF2	123.16	37.39	0.77
BF3	123.37	37.39	0.70
E01	122.42	31.27	1.41
E02	123.10	31.27	0.97
E03	123.91	31.28	0.73
E04	124.55	31.27	0.94
E05	125.33	31.27	0.68
H01	121.01	35.96	0.63
H02	121.34	35.97	0.51
H03	121.67	35.97	0.43
H04	121.99	35.96	0.93
H05	122.33	35.97	1.01
H06	122.66	35.97	1.08
H07	123.00	35.96	1.27
H08	123.50	35.96	1.34
H09	123.50	35.50	1.07
H10	123.49	35.00	1.01
H11	123.00	35.00	0.91
H12	122.67	35.00	1.18
H13	122.34	35.01	0.93
H14	122.00	35.00	0.60
H15	121.66	35.00	0.25
H16	121.33	34.99	0.35
H17	121.00	35.00	0.45
H25	122.34	34.01	1.01
H26	122.66	34.00	0.77
H27	123.09	34.00	0.88
H28	123.59	33.99	0.75
H29	124.00	33.99	0.93
H30	124.00	33.52	0.67
H31	124.02	32.99	0.93
H32	123.49	33.00	0.71
H33	122.99	33.00	1.07
H34	122.67	33.00	0.73
H35	122.35	33.00	1.14
H36	122.13	33.00	1.04
H37	122.31	32.29	0.61

H38	122.50	31.97	0.55
H42	124.50	32.00	0.48
H43	122.97	35.49	1.07
H44	122.66	35.50	1.34
B01	123.22	36.27	1.06
B02	122.97	36.46	0.62
B03	122.79	36.65	0.60
B04	122.59	36.83	0.42
B05	122.66	36.97	0.41
B06	122.88	37.00	0.61
B07	123.17	36.99	0.65
B08	123.42	36.99	0.56
B09	123.72	36.98	0.59
B12	123.06	37.88	0.39
B13	123.25	38.14	0.33
B14	123.48	38.43	0.15
B15	123.72	38.74	0.09
B21	123.00	38.75	0.23
B23	122.88	38.50	0.59
B24	122.74	38.22	0.65
B25	122.61	37.97	0.72
B26	122.49	37.70	0.52
B28	121.99	37.70	0.49
B29	121.99	37.95	0.85
B32	122.01	38.74	0.98
B33	121.62	38.67	0.28
B36	121.27	38.27	0.56
B37	121.22	38.11	0.44
B38	121.16	37.91	0.42
B40	120.45	38.34	0.48
B41	120.19	38.34	0.56
B42	119.79	38.33	0.73
B43	119.45	38.33	1.03
B44	119.18	38.33	0.91
B45	119.00	38.33	0.90
B46	119.00	38.50	0.79
B48	119.00	38.83	0.59
B49	119.00	39.00	0.10
B50	119.71	39.31	0.58
B51	120.06	39.18	0.49
B52	120.33	39.12	0.14
B53	120.60	39.06	0.47
B54	120.80	39.01	1.09
B55	120.90	39.29	0.94
B56	120.91	39.55	0.30
B59	120.44	39.48	0.64

B60	120.24	39.32	0.49
B61	119.89	39.05	0.60
B62	119.67	38.87	0.72
B63	119.38	38.63	0.89
B64	119.16	38.47	0.91
B65	119.26	37.94	0.75
B66	119.40	37.76	1.02
B67	119.58	37.75	0.76
B68	119.75	37.74	0.74
B69	119.94	37.73	0.70
B71	120.30	37.95	0.37

Core	**Longitude (°E)**	**Latitude (°N)**
1	123.18	36.07
2	126.12	31.73
3	122.47	28.50

[a] Zeng, L. X.; Chen, R.; Zhao, Z. S.; Wang, T.; Gao, Y.; Li, A.; Wang, Y. W.; Jiang, G. B.; Sun, L. G. Spatial distributions and deposition chronology of short chain chlorinated paraffins in marine sediments across the Chinese Bohai and Yellow seas. *Environ. Sci. Technol*. **2013**, 47 (20), 11449-11456.

Table S3. Optimized MRM parameters in GC-MS/MS quantification analysis.

Compound	BHT		BHT-d_{21}	
Precursor ion (m/z)	220.2		240.3	222.3
Product ion (m/z)	205	177.2	222.3	191.3
Collision energy (eV)	10	20	10	10

Table S4. Optimized MRM parameters in UPLC-MS/MS quantification analysis.

Compound	BHA		BHT-Q		BHT-OH		BHT-CHO		BHT-COOH		OG		PG		DG		PrP-d_4		MeP-d_4	
Precursor ion (m/z)	179		220		235		233		249		281		211		337		183		155	
Product ion (m/z)	164	149	205	148	217	160	217	203	205	189	169	124	169	124	169	124	140	96	140	96
Declustering potential (V)	-60		-120		-120		-120		-100		-120		-80		-120		-100		-100	
Collision energy (eV)	-20	-34.2	-32.7	-41.9	-27	-36	-44.1	-46	-28.2	-44.3	-30.6	-40	-23.8	-37.5	-36.2	-42.3	-23.1	-31.3	-19.3	-39
Collision cell exit potential (V)	-11	-8.64	-8.06	-5.69	-10.1	-10.9	-8.02	-10	-8.27	-11.2	-10	-8	-8	-8	-13.6	-9	-9.82	-6.82	-8.93	-14

Table S5. The method quantification limits (MQLs) and recoveries from matrices for SPAs in sediment.

Compound	MQL (ng/g)	Matrix spike recovery (%)
BHT	1.0	110 ± 12
BHA	0.3	77 ± 24
BHT-CHO	0.8	86 ± 8
BHT-COOH	0.5	87 ± 11
BHT-OH	0.6	92 ± 27
BHT-Q	1.1	101 ± 12
DG	0.03	83 ± 10
OG	0.03	81 ± 15
PG	0.8	76 ± 23

Table S6. Correlation analysis of target compounds in surface sediment samples.

	BHT	BHA	BHT-CHO	BHT-COOH	BHT-OH	BHT-Q	DG	OG	PG	$\sum_5$SPAs	MTs	$\sum_9$SPAs
BHT	1											
BHA	0.009	1										
BHT-CHO	0.277**	0.215*	1									
BHT-COOH	-0.033	0.672**	0.105	1								
BHT-OH	0.545**	0.179*	0.418**	0.249**	1							
BHT-Q	0.247**	-0.001	0.480**	-0.038	0.252**	1						
DG	0.225**	0.272**	0.263**	0.084	0.370**	0.092	1					
OG	0.143	0.502**	0.287**	0.337**	0.360**	0.071	0.947**	1				
PG	0.194*	0.816**	0.289**	0.534**	0.391**	0.150	0.692**	0.834**	1			
$\sum_5$SPAs	0.998**	0.038	0.291**	-0.017	0.561**	0.249**	0.282**	0.202*	0.243**	1		
MTs	0.270**	0.068	0.592**	0.037	0.316**	0.989**	0.130	0.128	0.212*	0.276**	1	
$\sum_9$SPAs	0.635**	0.070	0.595**	0.022	0.487**	0.895**	0.222**	0.186*	0.270**	0.640**	0.915**	1

**, Correlation is significant at the 0.01 level.

*, Correlation is significant at the 0.05 level.

Table S7. Correlation analysis of target compounds in sediment core samples.

	BHT	BHA	BHT-CHO	BHT-COOH	BHT-OH	BHT-Q	DG	OG	PG	$\sum_5$SPAs	MTs	$\sum_9$SPAs
BHT	1											
BHA	0.035	1										
BHT-CHO	0.540**	-0.126	1									
BHT-COOH	-0.043	0.046	-0.066	1								
BHT-OH	0.036	0.297**	0.154	-0.001	1							
BHT-Q	0.247**	-0.167	0.306**	-0.077	-0.018	1						
DG	0.117	0.384**	-0.051	-0.027	0.100	0.073	1					
OG	0.148	0.625**	-0.109	0.092	0.260**	-0.086	0.759**	1				
PG	0.100	0.728**	-0.130	0.125	0.277**	-0.151	0.615**	0.909**	1			
$\sum_5$SPAs	0.951**	0.230*	0.459**	-0.021	0.103	0.208*	0.381**	0.435**	0.372**	1		
MTs	0.432**	-0.156	0.706**	0.275**	0.084	0.797**	0.014	-0.077	-0.119	0.373**	1	
$\sum_9$SPAs	0.533**	-0.119	0.727**	0.256**	0.093	0.779**	0.062	-0.017	-0.066	0.484**	0.992**	1

**, Correlation is significant at the 0.01 level.

*, Correlation is significant at the 0.05 level.