Supporting Information

Sequestration of Nonylphenol in Sediment from Bohai Bay, North China

Fen Jin[1,2], Jianying Hu[1]*, Jinlin Liu[1], Min Yang[2]*, Fu Wang[3] and Hong Wang[3]

[1] College of Urban and Environmental Sciences, Peking University, Beijing 100871, China

[2] State Key Lab of Environmental Aquatic Chemistry, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing 100085, China

[3] Tianjin Institute of Geology and Mineral Resources, Tianjin 300170, China

Instrumental Conditions for NP and 4-n-NP. NP was measured with gas chromatograph with mass spectrometer (GC-MS). GC-MS analysis was performed with a Hewlett-Packard 5890 gas chromatograph connected to a Hewlett-Packard 5971 mass spectrometer. The mass spectrometer was operated in the electron impact ionization mode with an ionizing energy of 70 eV. The injector temperature was maintained at 250˚C, and the transfer line temperature was kept at 280˚C. An HP-5MS capillary column (30 m × 0.25 mm i.d. with a film thickness of 0.25 μm) used for NP and 4-n-NP analysis, and was programmed from 50˚C (2 min) to 200˚C at 20˚C /min (2 min), and to 260˚C at 5˚C /min, and then to 280˚C at 20˚C /min (5 min). The injection volume was 1 μL, and the splitless mode was used. Quantitative analysis was performed using selected ion monitoring mode, and the fragment ions were selected according to the most abundant ions in each oligomer. The concentrations of NP were quantified by comparing the integrated peak area by the summed selected ion monitor (*m*/*z* 179, 193, 221, 207) with the peak area of the injection internal standard (4-n-NP, *m*/*z 179)* (*15*, *22*).

Quantitation and Quality Assurance Quality Control (QA/QC). NP is ubiquitous throughout the world. Procedural blanks for the sedimentary sample originated from the SPE column itself and also from the analytical procedure, despite all the precautions taken to avoid it. In this study, all SPE cartridges used in this study were rinsed 4 times with the eluted reagents before conditioning in order to minimize blanks from the SPE cartridges. The procedural blanks provided a means to accurately assess background contamination throughout the sample extraction and clean-up process. In this study, the composition of each sample batch consisted of 2 procedural blanks and 3 to 6 sedimentary samples, and procedural

blanks for the sedimentary samples consisted of approximately 20 g of pre-baked sodium sulfate that underwent all the sample extraction and cleanup steps. Mean NP concentration in the procedural blanks was 0.08 ng/g. All samples were blank-corrected by subtracting the mean NP concentration in the batch blanks from each sample.

Method detection limits (MDLs) were defined as the mean blank concentration of 3 standard deviations. Based on the procedural blanks, MDLs were determined as 3 standard deviations above the mean NP concentrations in the blanks. The MDLs of NP were determined to be 0.1 ng/g using all sediment batch procedural blanks since inter-batch variability was negligible.

TABLE S1. Concentrations (ng/g dw) of Extractable and Nonextractable NP in Sedimentary Core (Station A) from Bohai Bay, North China

Depth (cm)	NP(ng/g dw)	
	Extractable	Nonextractable
7-10	9.5	5.9
10-13	5.4	4.6
13-16	6.1	5.4
16-21	4.0	5.3
21-24	6.4	6.4
31-34	7.2	3.6
34-36	6.1	1.9
36-39	2.5	4.3
39-41	0.4	3.0
44-46	0.8	2.6
46-49	1.0	3.3
49-51	3.2	2.3
51-54	3.0	5.8
54-56	3.0	4.3
56-58	4.3	7.9
61-66	3.7	14.0
66-71	5.6	7.6
71-78	3.7	7.8
78-83	3.5	6.8
83-88	2.3	4.9
88-94	2.3	9.9
94-99	1.3	10.3
99-105	0.7	7.3
105-110	0.8	1.4
110-115	0.8	2.5
115-121	0.6	5.5
121-125	0.1	7.6
129-134	1.9	3.2
134-138	0.5	6.2
138-141	0.6	3.0
141-146	1.2	5.0
146-150	0.9	6.8

TABLE S2. Production of NP in China (t/year)

Year	Production of NP in China
1995	14,378
1996	15,300
1997	17,920
1998	18,070
1999	18,550
2000	20,678
2001	24,290

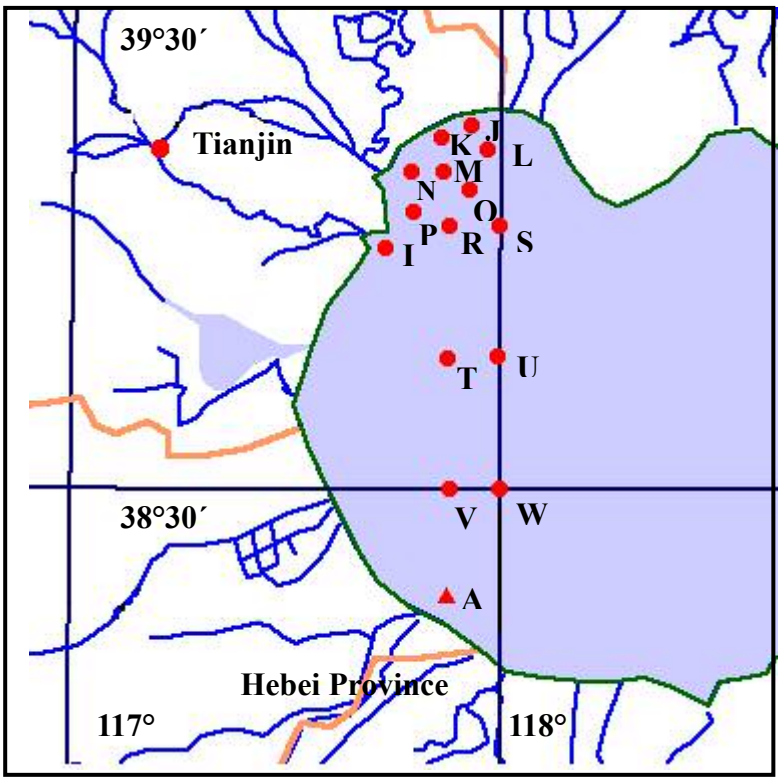

FIGURE S1. Map of sampling sites in Bohai Bay, north China. I-W: surface sediments; A: sedimentary core.

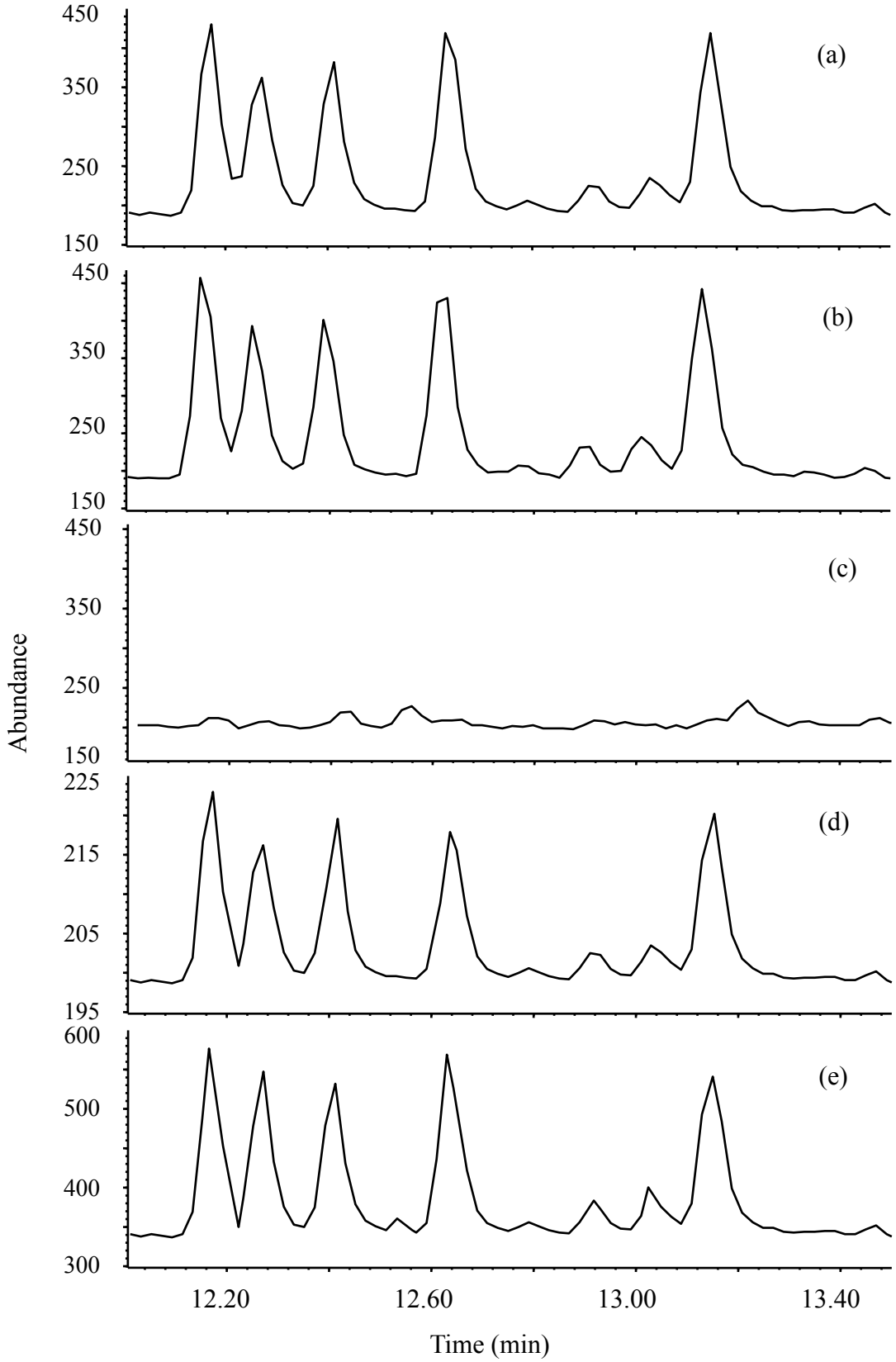

FIGURE S2. GC-MS chromatograms of NP. (a) standard (500 μg/L); (b) sample after application of the hydrolysis procedure; (c) sample after application of BBr_3-treatment procedure. (d) extractable fraction at site J (2.2 ng/g dw); (e) nonextractable fraction at site J (9.7 ng/g dw).

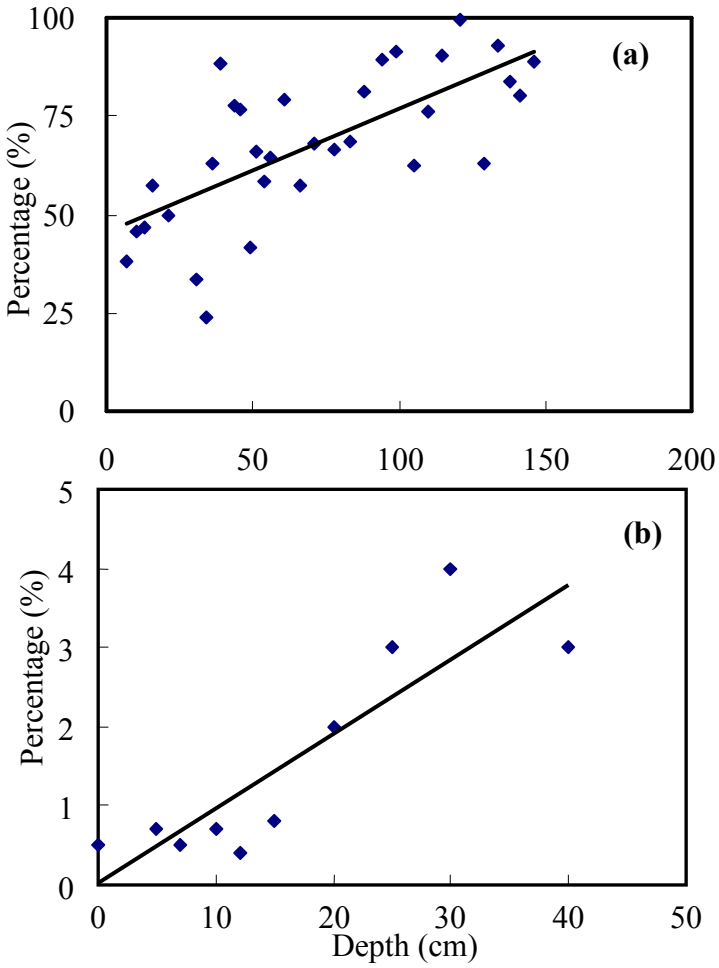

FIGURE S3. Relationship between the percentage of nonextractable fraction (%) and the depth in the sedimentary core. (a) Bohai Bay, north China (present study: $p<0.001$, $r^2=0.4915$); (b) Pawtuxet River, U.S.A *(9)* ($p<0.001$, $r^2=0.7685$).