Supporting Information

Detection and Occurrence of Chlorinated By-products of Bisphenol A, Nonylphenol and Estrogens in Drinking Water of China: Comparison to the Parent Compounds

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Detailed descriptions of target analytes, synthesis, dansylation procedure, nonylphenol standards and estimation of matrix effects and BPA equivalent estrogenic activity, Figures and tables addressing method validation, parameters of drinking water treatment plants (DWTPs), correlations between analytes and parameters of DWTPs, and between concentrations of BPA, NP, estrogens and their chlorinated by-products in source water and drinking water of all DWTPs.

Synthesis of Chlorinated By-products of BPA. The synthesis of chlorinated BPAs referred to the method used to synthesize chlorinated BPS.[1] An aqueous solution of sodium hypochlorite (1%, 10 ml) was added dropwise to a solution of BPA (300 mg) in 10 ml of 50% methanol with stirring. The solution was stirred for 2 h at room temperature. After addition of saturated aqueous sodium sulfite, the solution acidified with 2M hydrochloric acid was extracted with ethyl acetate. The organic layer was washed with brine, dried over magnesium sulfate, and concentrated to 2 mL under reduced pressure. The residue was subjected to a preparative HPLC (Waters 2690) with UV absorbance detector (Waters 2487) to isolate four chlorinated products, including monochloro-BPA, dichloro-BPA, trichloro-BPA and tetrachloro-BPA. The UV detector was at 228 nm. The chromatographic separation was conducted by a Waters HR C18 column (6 μm; 19 mm × 300 mm) with acetonitrile (A) and ultrapure water (B) were used as mobile phases. The column was maintained at 40°C, and the flow rate and the injection volume were 6 mL/min and 500 μL, respectively. 10% A was increased to 100% in 90 min and kept for 10 min, followed by a decrease to initial conditions of 10% A and held for 20 min to allow for equilibration. The synthesized products were characterized by ESI-UPLC-MS and NMR spectra. Although 2,6'-dichloro-BPA and 2,6-dichloro-BPA could not be separated chromatographically, the structures and abundance ratio of 2,6'-dichloro-BPA and 2,6-dichloro-BPA was determined (1/0.25) based on NMR spectra.

Monochloro-BPA. MS *m/z*: 261 $[M-H]^-$. ^{1}H NMR (MeOD): δ: 1.56 (6H, s, 2 × CH_3), 6.70 (2H, dt, *J* = 3.0, 8.7 Hz, 2 × ArH), 6.79 (1H, d, *J* = 8.2 Hz, ArH), 6.96 (1H, dd, *J* = 2.4, 8.5 Hz, ArH), 6.96 (2H, dt, *J* = 2.3, 8.9 Hz, 2 × ArH), 7.10 (1H, d, *J* = 2.3 Hz, ArH).

2,6'-Dichloro-BPA. MS *m*/*z*: 295 $[M-H]^-$. ^{1}H NMR (MeOD): δ: 1.57 (6H, s, 2 × CH_3), 6.81 (2H, d, *J* = 8.5 Hz, 2 × ArH), 6.95 (2H, dd, *J* = 2.4, 8.5 Hz, ArH), 7.16 (2H, d, *J* = 2.3 Hz, ArH).

2,6-Dichloro-BPA. MS *m*/*z*: 295 $[M-H]^-$. ^{1}H NMR (MeOD): δ: 1.57 (6H, s, 2 × CH_3), 6.71 (2H, m, *J* = 2.2, 8.9 Hz, 2 × ArH), 7.03 (2H, m, *J* = 2.2, 8.9 Hz, ArH), 7.06 (2H, s, ArH).

Trichloro-BPA. MS *m*/*z*: 331 $[M-H]^-$. ^{1}H NMR (MeOD): δ: 1.57 (6H, s, 2 × CH_3), 6.84 (1H, d, *J* = 8.5 Hz, ArH), 6.84 (1H, dd, *J* = 2.4, 8.5 Hz, ArH), 7.07 (2H, s, 2 × ArH), 7.13 (1H, d, *J* = 2.4 Hz, ArH).

Synthesis of Chlorinated By-products of 4-Nonylphenol (Mixture of Chain Isomers). Chlorinated NPs were synthesized according to the method reported in a previous study.[1] An aqueous solution of sodium hypochlorite (2.5%, 12 ml) was added dropwise to a solution of NP (1.1 g) in 50% methanol (50 ml). The solution was stirred for 3 h and an aqueous solution of sodium sulfite was added. The mixture acidified with 2M hydrochloric acid was extracted with diisopropyl ether. The organic solution was dried over magnesium sulfate and concentrated to 5 mL under reduced pressure. The residue was subjected to the same preparative HPLC and C18 column which were used for the isolation of chlorinated BPAs, and the UV detector was at 277 nm to afford two chlorinated NPs, monochloro-NP and dichloro-NP. 60% acetonitrile was increased to 100% in 30 min and then kept for 10 min, followed by a decrease to initial conditions of 60% acetonitrile and held for 20 min to allow for equilibration. The products were characterized by ESI-UPLC-MS (Figure S5) and their purities were identified by HPLC-UV (Figure S6).

Synthesis of Chlorinated By-products of E1. According to the report of Hideyuki

Nakamura et al.,[2] an aqueous solution of sodium hypochlorite (0.6 ml, 6% available chlorine) was added to a solution of E1 (1 mmol) in methanol (100 ml) and stirred. After 30 min of stirring at room temperature, an aqueous solution of sodium sulfite was added in an ice bath. The mixture was acidified with 2M hydrochloric acid, and methanol was removed under reduced pressure. The aqueous residue was extracted with dichloromethane after adding sodium chloride. The dichloromethane solution was washed with brine, dried over sodium sulfate and concentrated to 2 mL under reduced pressure. The residue was subjected to the same preparative HPLC and C18 column which were used for the isolation of chlorinated BPAs and NPs, and the UV detector was at 200 nm to afford three chlorinated products, 2-chloro-E1, 4-chloro-E1 and dichloro-E1. 40% acetonitrile was kept for 40 min and then increased to 100% in 10 min, followed by a decrease to initial conditions of 40% acetonitrile and held for 20 min to allow for equilibration. The synthesized products were characterized by ESI-UPLC-MS and NMR spectra.

2-Chloro-E1. MS m/z: 303 $[M-H]^-$. ^{1}H NMR (Acetone-d_6): δ: 7.19 (1H, s, 1-H), 6.73 (1H, s, 4-H).

4-Chloro-E1. MS m/z: 303 $[M-H]^-$. ^{1}H NMR (CDCl3): δ: 7.14 (1H, d, J = 8.6 Hz, 1-H), 6.87 (1H, d, J = 8.56 Hz, 2-H).

2,4-Dichloro-E1. MS m/z: 337 $[M-H]^-$. ^{1}H NMR (Acetone-d_6): δ: 7.24 (1H, s, 1-H).

Dansylation procedure. According to the method reported in previous paper,[3] the sample extract/ standard solution was dried under a gentle flow of nitrogen and redissolved in 100 μL of aqueous sodium bicarbonate (100 mmol/L, pH adjusted to 10.5 with HCl) and 100 μL of dansyl chloride (1 mg/mL in acetone), vortex-mixed for 1 min and incubated at 60°C for 10 min. Then 1 mL of 18 MΩ water and 2×2 mL of hexane were added. After cooling to room temperature, organic fraction containing dansylated analytes was dried and redissolved with acetonitrile prior to UPLC–MS/MS analysis.

Comparison of Nonylphenol (CAS 84852-15-3) from Different Producers. In order to evaluate the potential deviation of quantification by technical mixture standard obtained from Hayashi (Tokyo, Japan), we compared its signal intensities of dansylated standards with Sigma-Aldrich (USA) and AccuStandard (USA). Figure S7 shows the chromatograms of three standards at 2 μg/L. According to the peak areas of three standards, the signal differences between Hayashi-NP and NP from other producers were 3% (AccuStandard) and 8% (Sigma-Aldrich).

Matrix Effects of Dansylation UPLC-MS/MS Method. Two sets of standard lines were prepared to evaluate the presence of matrix effect. The first set of three standard lines (set 1) was prepared to evaluate the MS/MS response for neat standards of all analytes injected in the mobile phase. The second set (set 2) was prepared in water extracts originating from five different sources and spiked after extraction. By comparing the slopes of the standard lines between the two different sets of standard lines, the presence of matrix effect on the quantification of target analytes was assessed. Figure S8 shows the linearity plots of standard lines using UPLC.

Set 1. Three standard lines were constructed using neat solutions of target analytes in MeOH. By mixing and diluting stock solutions, standard mixture solutions of 0.01, 0.05, 0.1, 0.5, 2, 10, 50 and 100 μg/L target analytes were prepared and transferred into autosampler vials. 5 μL was injected directly into the UPLC-MS/MS system.

Set 2. Five standard lines were constructed in five different lots of water extracts by following treatments: 1) 1 mL elution of HLB cartridge in 2-mL glass bottle and were dried under gentle nitrogen flow; 2) 100 μL standard mixture solution of 0.01, 0.05, 0.1, 0.5, 2, 10, 50 and 100 μg/L target analytes was added to reconstitute 8 sample extracts, respectively.

Matrix Effects of Non-dansylation UPLC-MS/MS Method. The matrix effect of non-dansylation UPLC-MS/MS method was assessed in the same way as the evaluation of the matrix effect of dansylation method. Figure S9 shows the linearity plots of standard lines using UPLC.

Estimation of BPA Equivalent Estrogenic Activity (EQ_{BPA}). The estrogenic activities of chlorinated BPAs in the water samples were estimated by comparison with the activity of BPA and expressed as BPA equivalent (EQ_{BPA}). For the calculation of EQ_{BPA}, the estrogenic effect factors (EEFs), which equals the ratio of EC_{50} values of a chlorinated BPA and BPA, were estimated to be 7.46 for monochloro-BPA, 4.95 for 2,6'-dichloro-BPA, 1.2 for 2,6-dichloro-BPA, 0.588 for trichloro-BPA, and tetrachloro-BPA < 0.193), and the EC_{50} values of chlorinated BPAs were collected from a previous paper.[4] Thus, we made an attempt to calculate the average estrogenic activities of chlorinated BPAs and BPA in drinking water. Although two isomers of dichloro-BPA, 2,6'-dichloro-BPA and 2,6-dichloro-BPA could not be separated chromatographically to determine their respective concentration, our previous study has identified the concentration ratio between 2,6'-dichloro-BPA and 2,6-dichloro-BPA to be 1/0.25,[5] which provides us the chance to estimate their concentrations in the drinking water samples. The total average estrogenic activity of BPA and its chlorinated BPAs in drinking water is displayed in Figure S3. Although the concentrations of chlorinated BPAs as described above were much lower than that of BPA (19.1 ng/L) in drinking water, monochloro-BPA, dichloro-BPA, trichloro-BPA, tetrachloro-BPA and BPA on average accounted for 55±17%, 9.4±7.3%, 1.4±2.1%, <0.1% and 34±18% of the EQ_{BPA}, respectively, showing the significant contribution of monochloro-BPA.

References

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(3) Chang, H.; Wan, Y.; Naile, J.; Zhang, X.; Wiseman, S.; Hecker, M.; Lam, M. H. W.; Giesy, J. P.; Jones, P. D. Simultaneous quantification of multiple classes of phenolic compounds in blood plasma by liquid chromatography-electrospray tandem mass spectrometry. *J. Chromatogr. A* **2010**, *1217* (4), 506-513.

(4) Kuruto-Niwa, R.; Terao, Y.; Nozawa, R. Identification of estrogenic activity of chlorinated bisphenol A using a GFP expression system. *Environ. Toxicol. Phar.* **2002**, *12* (1), 27-35.

(5) Hu, J. Y.; Aizawa, T.; Ookubo, S. Products of aqueous chlorination of bisphenol A and their estrogenic activity. *Environ. Sci. Technol*. **2002**, *36* (9), 1980-1987.

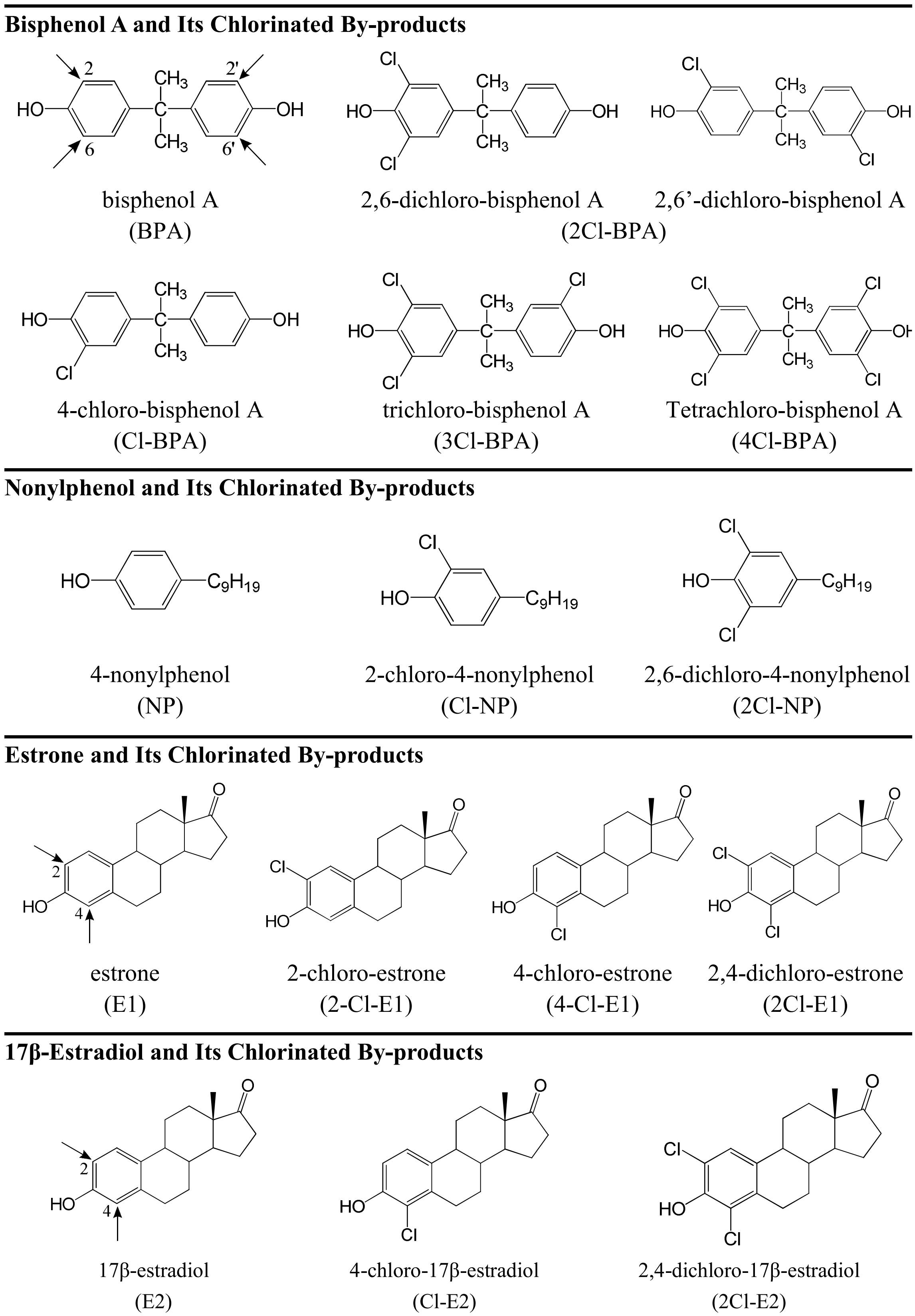

FIGURE S1. Structures of target four parent compounds and their chlorinated by-products.

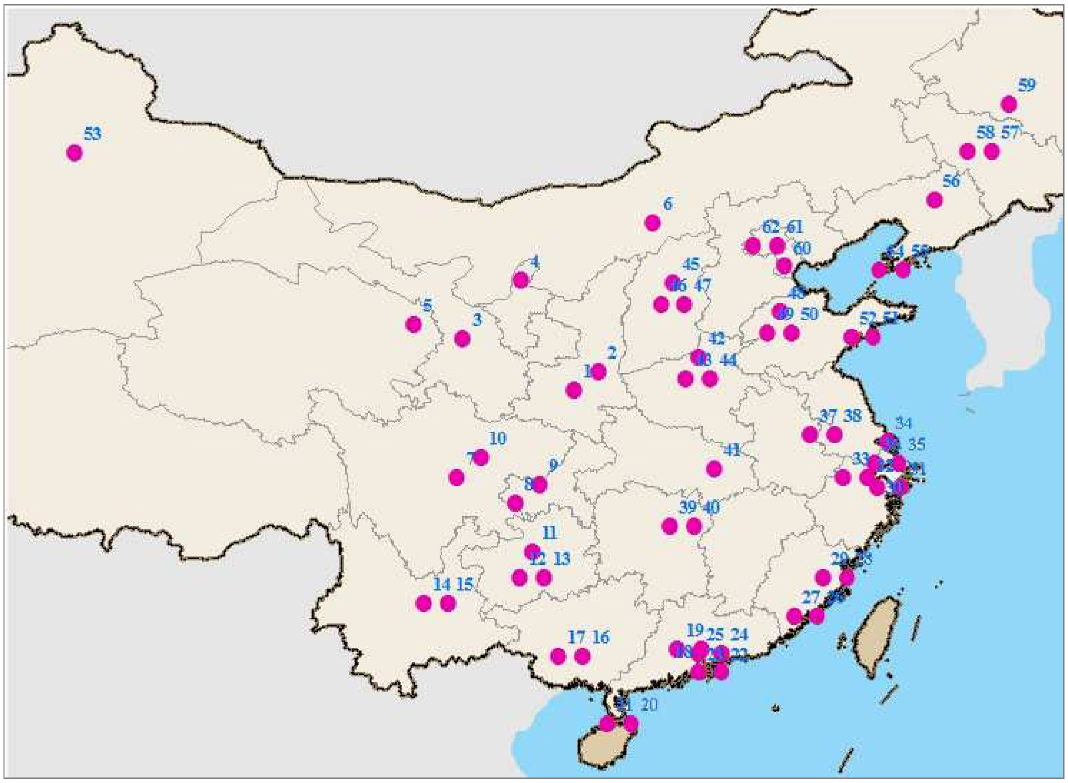

FIGURE S2. Drinking water treatment plants (DWTPs) locations across China.

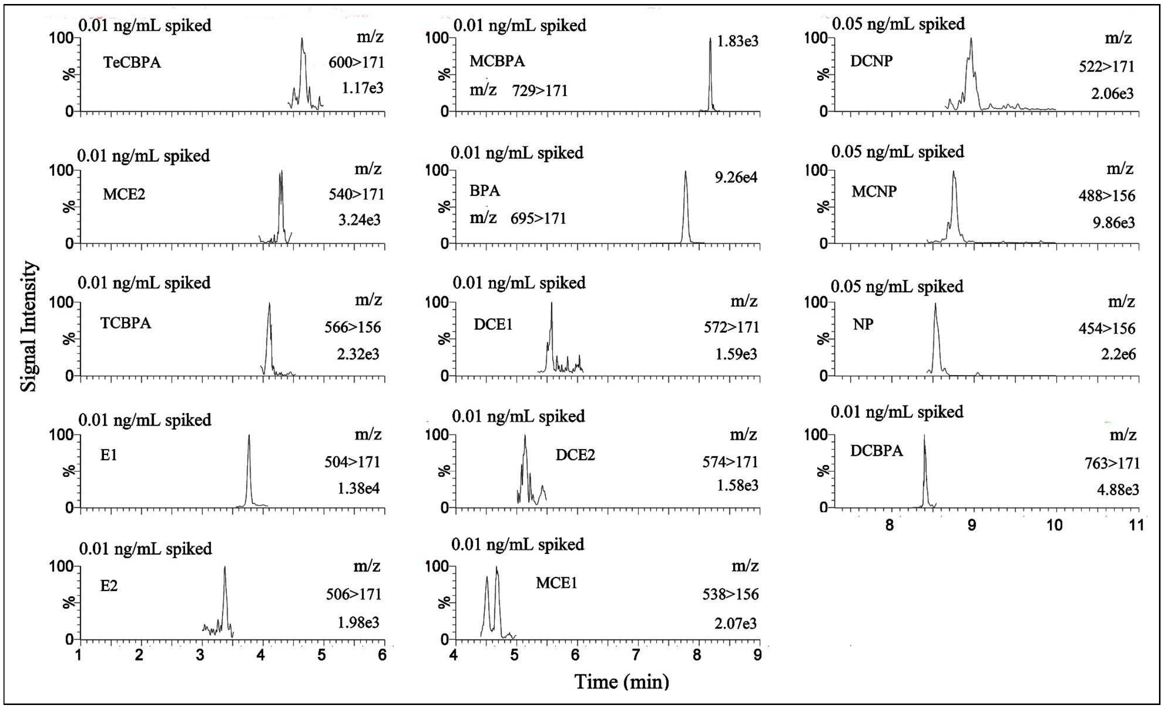

FIGURE S3. UPLC-MS/MS MRM chromatograms of a water sample spiked with low levels of target analytes.

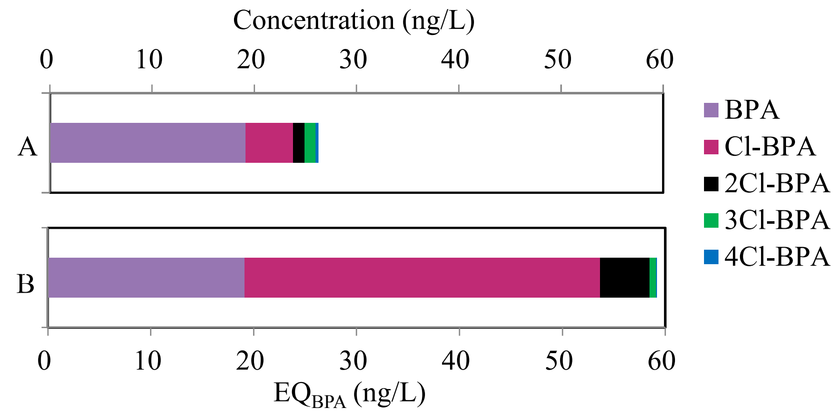

FIGURE S4. Comparison of average concentrations in drinking water (A) with their average equivalent (EQ_{BPA}) of bisphenol A (BPA) and its chlorinated products (B).

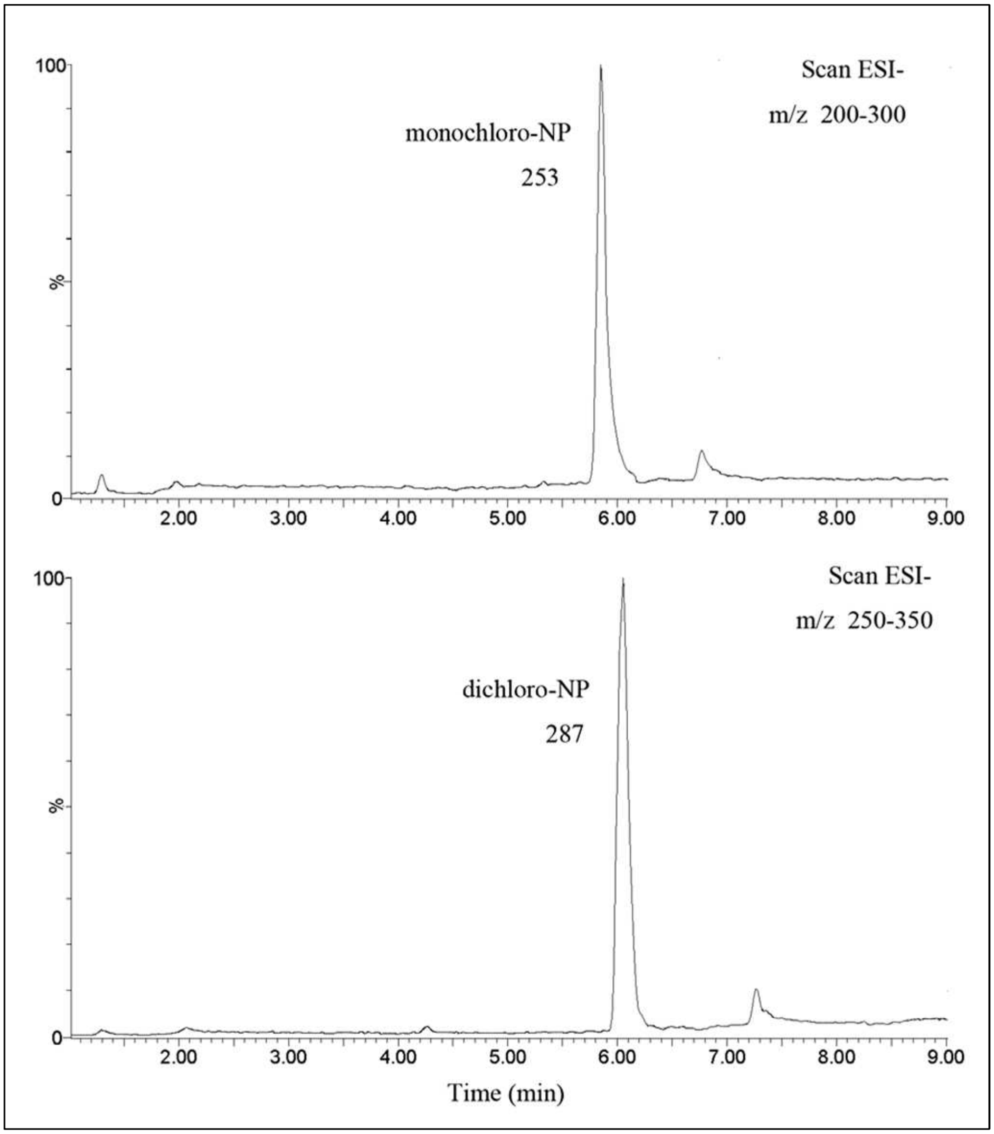

FIGURE S5. UPLC-MS chromatogram of synthesized monochloro-NP and dichloro-NP in methanol solution (500 ng/mL) in scan mode.

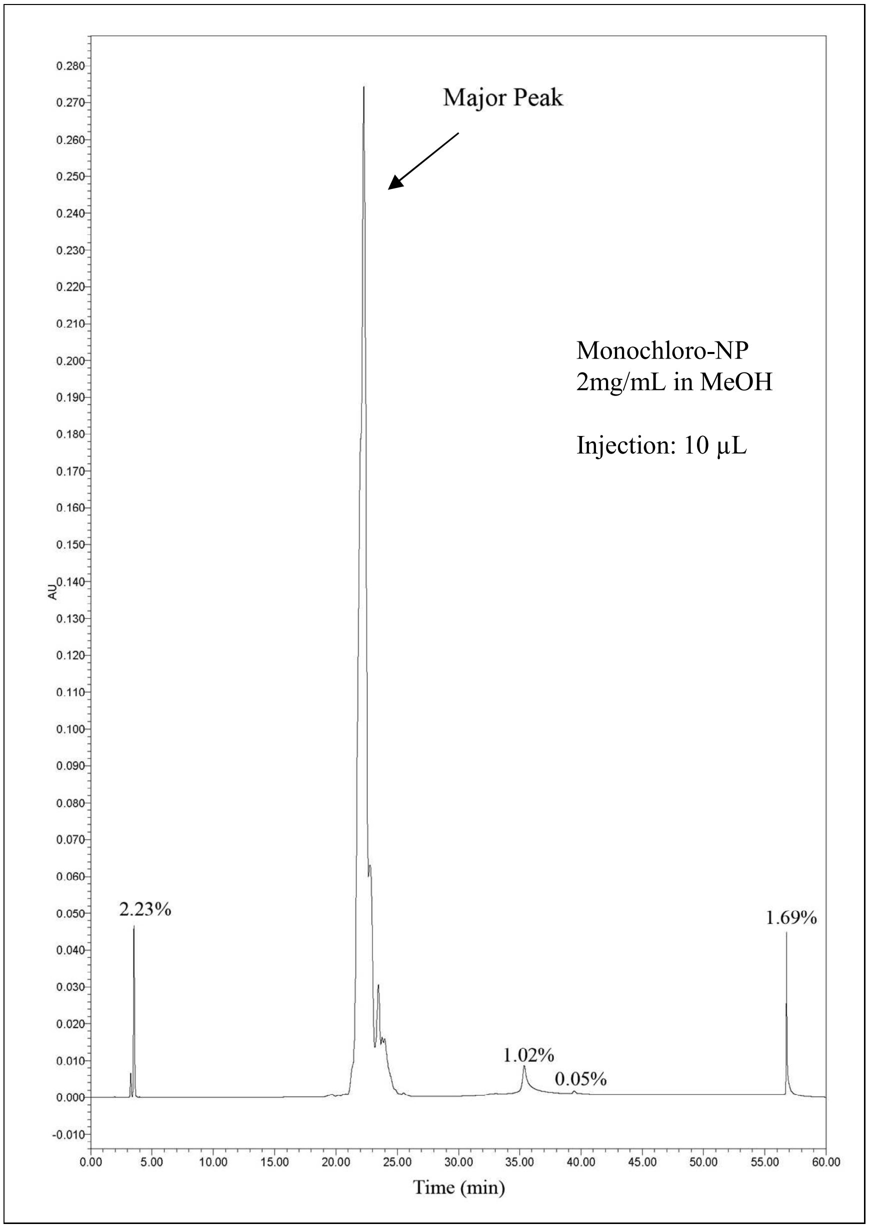

FIGURE S6(a). HPLC-UV chromatogram and impurities (%) of synthesized monochloro-NP detected at 277nm.

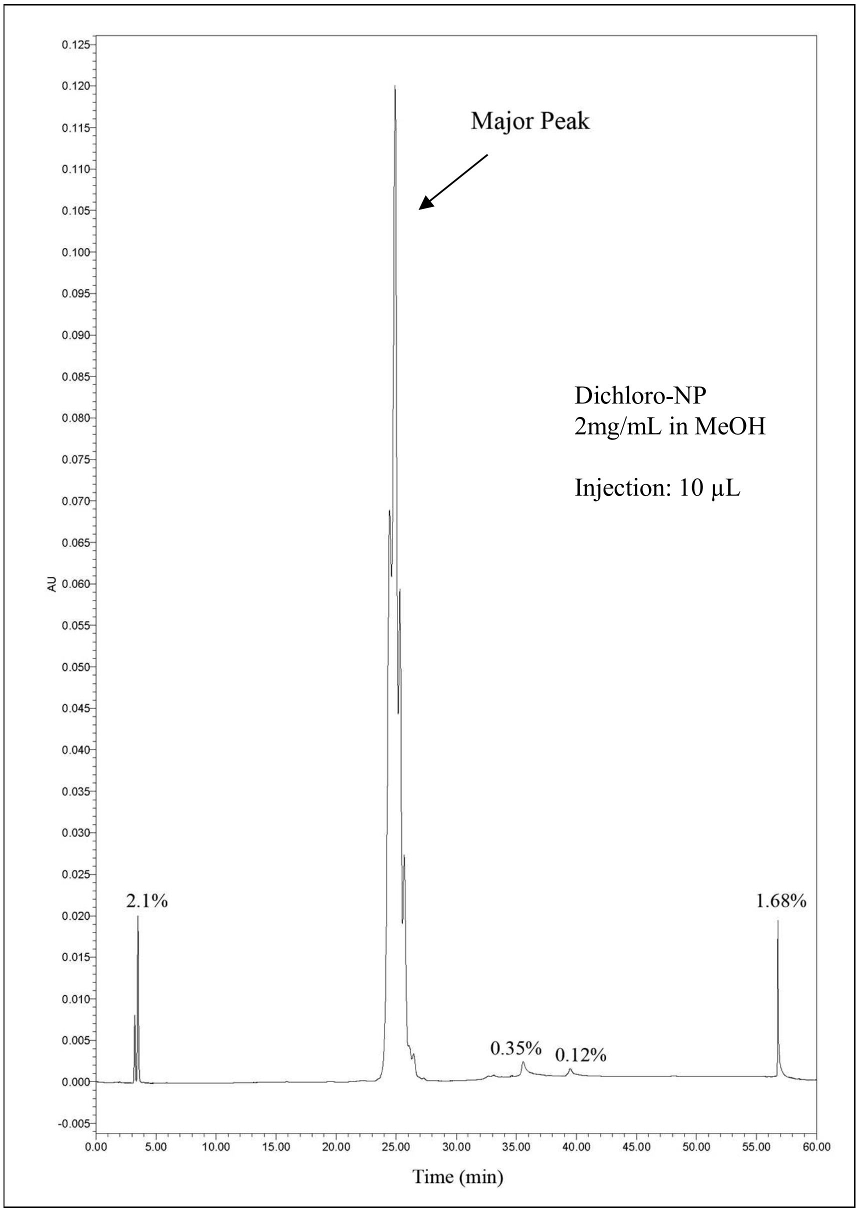

FIGURE S6(b). HPLC-UV chromatogram and impurities (%) of synthesized dichloro-NP detected at 277nm.

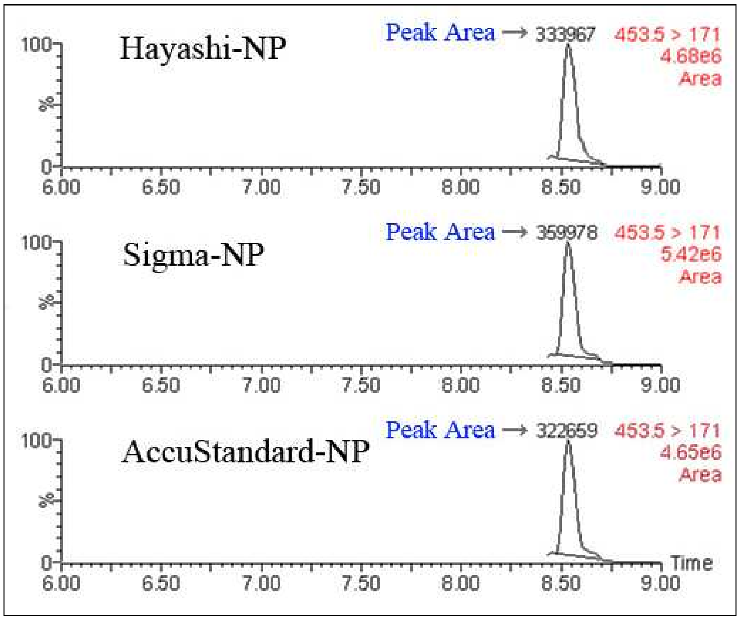

FIGURE S7. UPLC-MS/MS chromatograms of three NP standards at 2 μg/L.

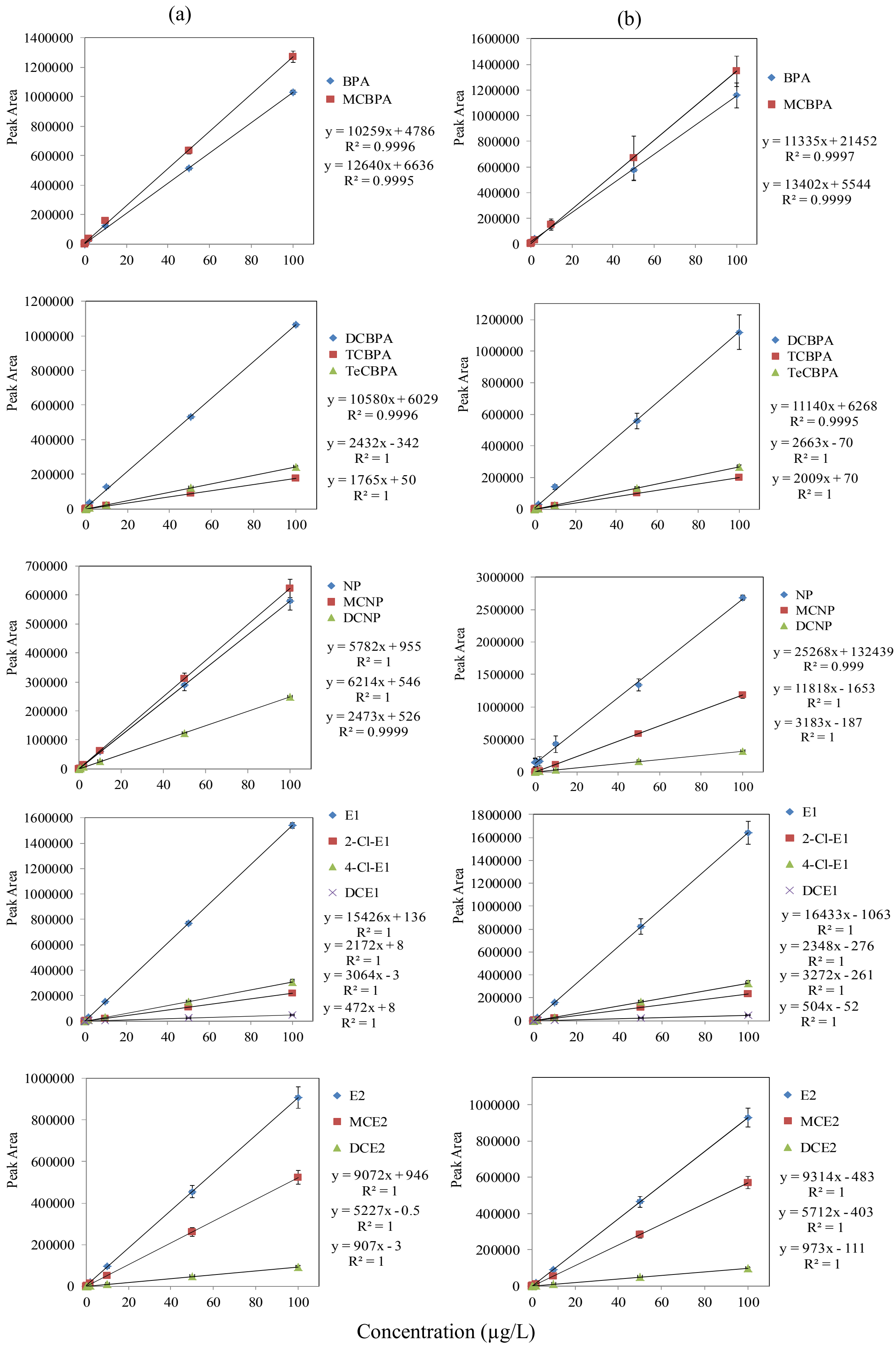

FIGURE S8. Linearity plots of standard lines of (a) neat standards and (b) spiked extracts using dansylation UPLC-MS/MS method.

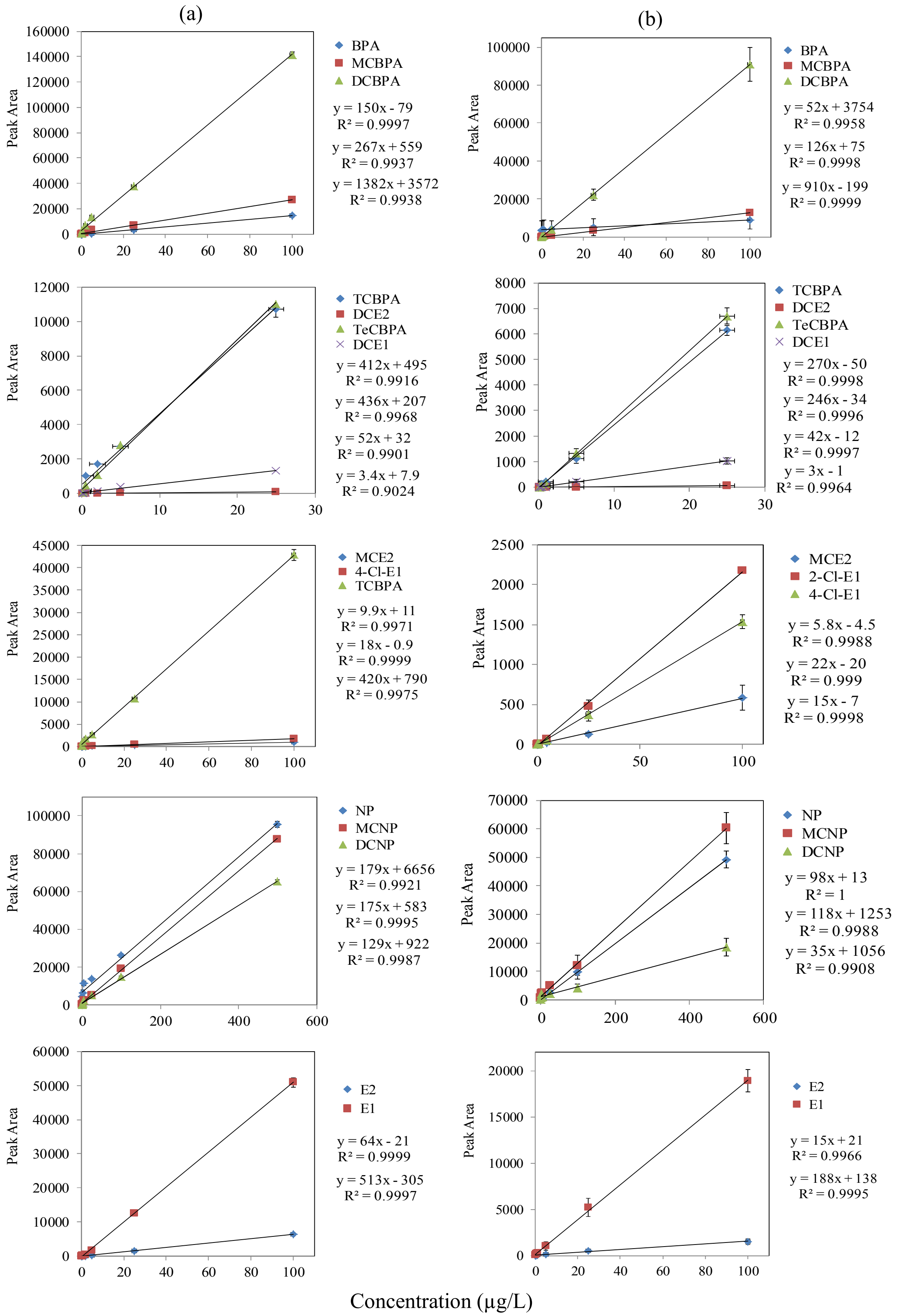

FIGURE S9. Linearity plots of standard lines of (a) neat standards and (b) spiked extracts using non-dansylated UPLC-MS/MS method.

TABLE S1. Located Cities, Sampling Time, Residual Chlorine, Temperature (Source - Finished) and Source Water Type of Drinking Water Treatment Plants.

DWTP	Source Water	TOC (mg/L)	Residual Chlorine (mg/L)	Sampling Time	Temperature (°C)
DWTP-1	R	5.45	0.1	08/17/2011	17 - 22
DWTP-2	R	4.07	NA	08/17/2011	22 - 23
DWTP-3	RW	3.82	0.66	08/19/2011	16 - 18
DWTP-4	GW	NA	0.07	08/23/2011	15 - 15
DWTP-5	RW	NA	0.3	08/25/2011	5.5 - 7
DWTP-6	R	NA	NA	08/28/2011	NA
DWTP-7	RW	1.45	0.06	09/14/2011	16 - 16.5
DWTP-8	RW	2.20	0.75	09/16/2011	NA
DWTP-9	RW	1.64	0.38	09/16/2011	24.5 - 25
DWTP-10	R	2.97	NA	09/20/2011	NA
DWTP-11	GW	1.06	0.49	09/20/2011	NA
DWTP-12	R	2.49	0.93	09/20/2011	NA
DWTP-13	R	1.63	0.41	09/20/2011	NA
DWTP-14	R	2.47	0.4	10/10/2011	17.5 - 18
DWTP-15	R	2.28	0.32	10/10/2011	12.5 - 17
DWTP-16	RW	NA	0.29	10/14/2011	24 - 25
DWTP-17	RW	1.61	0.31	10/14/2011	23 - 27
DWTP-18	RW	1.94	NA	10/25/2011	NA
DWTP-19	RW	2.41	0.95	10/25/2011	22 - 23
DWTP-20	RW	1.70	0.6	10/28/2011	NA
DWTP-21	R	2.19	NA	10/28/2011	26.6 - 27
DWTP-22	R	2.16	0.39	11/02/2011	27.5 - 28
DWTP-23	R	2.28	0.61	11/02/2011	NA
DWTP-24	R	2.17	0.67	11/02/2011	NA
DWTP-25	R	2.23	NA	11/02/2011	NA
DWTP-26	RW	1.11	0.26	11/22/2011	21.4 - 21.5
DWTP-27	RW	2.67	0.04	11/23/2011	22 - 22.2
DWTP-28	R	2.11	0.5	11/24/2011	20 - 20.5
DWTP-29	RW	1.98	0.4	11/24/2011	NA
DWTP-30	R	NA	0.1	11/28/2011	19 - 19.6
DWTP-31	R	NA	0.5	11/28/2011	17.5 - 18
DWTP-32	RW	NA	0.33	12/05/2011	15.9 - 18.5
DWTP-33	RW	3.10	0.47	12/05/2011	12.5 - 13.5
DWTP-34	RW	5.30	NA	12/08/2011	NA
DWTP-35	RW	2.53	NA	12/08/2011	NA
DWTP-36	R	2.38	1.09	12/08/2011	12 - 14
DWTP-37	RW	2.28	0.67	12/13/2011	11 - 12
DWTP-38	RW	2.28	0.43	12/13/2011	12.4 - 12.6

(continued)

DWTP	Source Water	TOC (mg/L)	Residual Chlorine (mg/L)	Sampling Time	Temperature (°C)
DWTP-39	R	1.74	NA	12/30/2011	12 - 15
DWTP-40	RW	2.37	0.08	12/30/2011	10 - 11
DWTP-41	RW	NA	0.44	01/05/2012	NA
DWTP-42	GW	1.75	NA	02/27/2012	NA
DWTP-43	GW	1.30	0.2	02/27/2012	NA
DWTP-44	RW	2.62	NA	02/27/2012	7 - 11.5
DWTP-45	GW	0.73	0.31	03/02/2012	11.9 - 16.1
DWTP-46	GW	0.51	0.26	03/02/2012	15 - 16
DWTP-47	R	2.35	0.4	03/02/2012	2 - 3
DWTP-48	GW	3.14	NA	03/09/2012	NA
DWTP-49	R	2.55	NA	03/09/2012	6.9 - 7.6
DWTP-50	GW	1.15	NA	03/09/2012	13.5 - 18
DWTP-51	R	NA	0.3	03/13/2012	NA
DWTP-52	RW	3.15	0.24	03/13/2012	6 - 6.5
DWTP-53	R	0.87	0.2	05/08/2012	NA
DWTP-54	R	2.45	0.22	05/15/2012	NA
DWTP-55	R	3.65	0.12	05/15/2012	10 - 10.8
DWTP-56	R	NA	NA	05/17/2012	NA
DWTP-57	R	4.01	NA	05/18/2012	NA
DWTP-58	R	4.51	NA	05/18/2012	14.3 - 14.8
DWTP-59	R	2.52	0.57	05/21/2012	7.4 - 14.6
DWTP-60	R	3.08	NA	05/24/2012	19.5 - 21.7
DWTP-61	R	2.86	NA	05/31/2012	NA
DWTP-62	R	2.46	NA	05/31/2012	NA

* R: reservoir; RW: river water; GW: groundwater.

TABLE S2. Multi-selected Reaction Monitoring (MRM) Conditions of the Target Analytes.

Substance	Dansyl Derivatives	MRM transition	Cone voltage (V)	Collision energy (eV)
E1	E1-dansyl	504>171	58	34
		504>156		60
E1-d4	E1-d4-dansyl	508>171	45	43
		508>156		60
2-chloro-E1	2-ClE1-dansyl	538>156	46	60
		538>171		55
4-chloro-E1	4-ClE1-dansyl	538>156	46	60
		538>171		55
dichloro-E1	diClE1-dansyl	572>171	40	50
		572>156		60
E2β	E2β-dansyl	506>171	50	45
		506>156		58
E2β-d3	E2β-d3-dansyl	509>171	65	35
		509>156		60
chloro-E2	ClE2-dansyl	540>171	55	41
		540>156		60
dichloro-E2	diClE2-dansyl	574>171	43	42
		574>156		60
BPA	BPA-$(dansyl)_2$	695>171	60	30
		695>156		40
d4-BPA	d4-BPA-$(dansyl)_2$	699>171	60	30
		699>156		55
monochloro-BPA	MCBPA-$(dansyl)_2$	729>171	52	50
		729>156		60
dichloro-BPA	DCBPA-$(dansyl)_2$	763>171	55	58
		763>156		60
trichloro-BPA	TCBPA-dansyl	566>171	45	55
		566>156		60
tetrachloro-BPA	TeBPA-dansyl	600>171	44	38
		600>156		58
NP	NP-dansyl	454>156	50	60
		454>171		45
4-n-NP	4-n-NP-dansyl	454>171	50	60
		454>156		60
chloro-NP	ClNP-dansyl	488>156	45	60
		488>171		60
dichloro-NP	diClNP-dansyl	522>156	40	60
		522>171		45

TABLE S3. Recoveries (%) of Target Analytes Employing Oasis HLB Extraction from Water Samples Eluting with Different Elution Solvents (n=3, spiked with 150 ng/L).

Substance	MeOH/MTBE (v/v 1:1)	MeOH	MTBE
E1	109 ± 2	89 ± 3	86 ± 6
E1-d4	117 ± 5	102 ± 4	116 ± 9
2-chloro-E1	119 ± 13	101 ± 4	68 ± 4
4-chloro-E1	100 ± 12	126 ± 6	76 ± 9
dichloro-E1	87 ± 5	76 ± 11	91 ± 13
E2β	117 ± 11	78 ± 8	78 ± 2
E2β-d3	119 ± 8	104 ± 2	97 ± 14
4-chloro-E2	99 ± 2	102 ± 11	62 ± 20
dichloro-E2	72 ± 13	73 ± 24	72 ± 12
BPA	123 ± 6	105 ± 5	51 ± 8
BPA-d4	115 ± 19	103 ± 1	46 ± 14
monochloro-BPA	113 ± 22	133 ± 2	42 ± 1
dichloro-BPA	115 ± 2	79 ± 3	54 ± 3
trichloro-BPA	92 ± 8	94 ± 13	56 ± 6
tetrachloro-BPA	97 ± 5	100 ± 12	85 ± 10
NP	100 ± 22	48 ± 12	108 ± 16
4-n-NP	91 ± 8	36 ± 21	86 ± 19
chloro-NP	83 ± 17	35 ± 2	100 ± 7
dichloro-NP	81 ± 15	24 ± 12	98 ± 5

TABLE S4. Concentrations (ng/L) of BPA, NP, Estrogens and Their Chlorinated By-products in Source Water and Drinking Water of DWTPs.

	Source Water				Drinking Water										
DWTP	E1	E2	BPA	NP	E1	2Cl-E1	E2	BPA	Cl-BPA	2Cl-BPA	3Cl-BPA	4Cl-BPA	NP	Cl-NP	2Cl-NP
1	1.6	0.2	64.6	309	0.2	ND	0.0	2.5	11.5	1.4	ND	ND	30.3	0.2	ND
2	0.6	0.1	9.9	123	0.1	0.1	ND	3.1	0.7	0.8	1.8	0.2	18.0	0.2	ND
3	2.8	0.7	97.2	421	0.2	ND	0.0	4.6	2.7	1.5	ND	ND	84.1	3.3	ND
4	1.0	0.2	26.1	81.7	0.4	0.1	0.1	5.4	1.0	0.3	0.2	0.0	8.3	0.3	ND
5	4.3	ND	81.3	87.7	1.2	ND	ND	28.8	14.4	1.1	ND	ND	11.3	1.1	ND
6	1.5	0.5	45.3	155	0.6	0.1	ND	5.4	1.6	0.9	5.0	0.3	50.0	0.1	ND
7	3.1	0.3	28.4	355	0.8	ND	0.0	9.9	1.7	0.2	0.1	ND	116	0.9	ND
8	0.9	0.1	25.3	113	0.1	ND	0.0	5.0	0.7	0.2	ND	ND	31.9	0.1	ND
9	0.5	ND	49.0	480	1.7	0.1	0.1	29.4	1.6	0.1	0.8	0.0	114	1.6	ND
10	2.6	0.3	47.0	257	0.8	ND	0.0	11.0	1.2	0.5	0.1	0.7	202	0.3	0.3
11	0.9	0.1	21.2	293	0.4	ND	0.0	6.2	3.0	1.9	1.6	0.6	58.6	5.5	0.4
12	1.7	0.2	46.5	592	ND	ND	ND	22.3	1.8	0.9	ND	0.3	558	13.3	ND
13	1.6	0.2	64.6	309	0.2	ND	0.0	2.5	11.5	1.4	ND	ND	30.3	0.2	ND

(continued)

14	2.7	0.1	80.6	134	0.9	0.1	0.1	18.5	1.4	2.5	ND	ND	57.6	0.2	ND
15	1.1	0.1	17.1	40.0	1.1	ND	0.0	9.2	2.9	1.9	ND	ND	20.6	0.3	ND
16	1.6	0.1	98.4	165	0.9	ND	0.0	20.7	4.1	1.0	2.2	ND	74.2	0.3	ND
17	0.4	ND	49.9	40.8	0.7	0.1	0.1	9.3	1.7	0.5	0.7	ND	25.5	ND	ND
18	0.5	ND	331	71.5	0.3	ND	ND	22.5	13.8	5.1	3.4	0.1	11.7	0.1	ND
19	0.6	0.1	41.4	45.3	0.1	ND	ND	5.4	1.2	0.5	1.7	0.3	16.8	3.2	ND
20	1.0	0.1	34.2	821	0.5	ND	0.1	16.2	1.3	1.9	2.1	0.4	446	4.3	ND
21	1.3	0.1	132.4	25.4	0.6	ND	0.1	22.0	9.0	6.3	4.5	0.1	9.3	0.5	ND
22	0.6	0.1	81.1	34.2	0.1	ND	0.1	10.0	2.2	3.5	4.4	1.0	23.2	0.3	ND
23	0.4	0.1	42.6	66.4	0.2	ND	0.0	10.1	3.6	0.9	1.6	ND	15.3	4.2	ND
24	0.4	ND	5.1	187	0.1	ND	0.0	ND	1.0	0.1	ND	ND	26.9	0.3	ND
25	2.0	0.0	20.5	751	0.3	ND	ND	7.6	4.9	2.2	ND	ND	297	0.7	ND
26	0.5	ND	15.8	165	0.1	ND	ND	5.5	2.0	0.2	0.7	0.1	22.9	3.0	ND
27	1.4	0.4	47.1	63.6	0.1	ND	0.1	11.3	3.1	1.2	1.3	0.2	15.1	3.6	1.6
28	1.8	0.6	82.6	277	0.9	0.1	0.1	22.6	6.1	0.6	7.7	4.8	74.4	ND	ND
29	1.4	0.1	89.2	112	0.3	0.1	0.1	33.7	10.3	0.9	1.2	0.2	101	1.0	ND

(continued)

30	0.3	0.1	24.6	78.3	ND	ND	ND	6.6	2.6	0.4	0.6	0.2	ND	0.6	ND
31	1.2	ND	15.9	191	0.5	0.1	0.1	3.5	4.8	0.8	ND	ND	35.6	4.6	ND
32	0.9	0.1	18.7	726	0.2	ND	ND	3.8	3.7	0.4	1.5	0.7	91.7	0.2	ND
33	1.3	0.1	65.4	68.2	0.9	ND	0.1	33.1	1.9	0.2	ND	ND	35.5	0.2	ND
34	3.3	0.2	81.6	485	1.2	ND	ND	35.0	3.2	0.5	0.6	ND	67.2	0.9	ND
35	0.4	ND	59.2	534	ND	ND	ND	6.2	2.0	0.2	0.2	0.1	29.2	0.4	ND
36	0.5	0.0	18.6	122	0.2	ND	0.0	5.9	4.8	1.0	1.0	0.4	36.9	1.8	ND
37	0.7	ND	317	36.8	0.4	ND	0.1	68.1	9.5	3.2	1.9	1.2	16.0	ND	ND
38	0.3	0.0	378	12.5	ND	ND	ND	67.2	5.8	2.8	2.0	0.4	11.8	0.1	ND
39	0.2	0.0	4.7	10.2	0.1	ND	ND	6.1	1.0	0.3	0.4	0.1	10.3	ND	ND
40	1.9	0.1	71.0	47.2	0.6	ND	0.0	30.1	1.3	0.2	0.5	0.4	19.1	0.3	ND
41	0.0	ND	81.3	361	0.1	ND	ND	15.1	9.7	1.1	2.6	0.4	117	5.6	ND
42	0.3	0.1	72.9	178	0.4	ND	ND	51.1	6.0	0.4	0.4	0.2	ND	0.2	ND
43	2.4	ND	50.2	22.8	0.8	ND	0.1	16.0	6.5	1.2	3.3	0.7	ND	0.9	ND
44	3.3	ND	32.1	33.5	0.3	ND	ND	7.3	3.6	0.2	ND	ND	17.7	0.4	ND
45	9.9	3.1	79.0	122	0.1	ND	ND	3.1	7.5	2.2	ND	ND	ND	0.5	1.2

(continued)

46	5.0	ND	169	257	0.2	ND	0.04	14.4	1.1	0.3	ND	ND	95	ND	ND
47	0.1	0.03	178	33.2	ND	ND	ND	55.5	9.5	1	2.5	0.9	ND	0.1	ND
48	0.4	0.03	24.7	26.7	0.2	0.2	ND	5.7	1.7	0.8	ND	ND	6.9	1.4	ND
49	2	0.2	33.1	46.4	0.05	ND	ND	ND	1.0	0.6	ND	ND	ND	0.4	ND
50	0.3	0.03	59.6	83.4	0.2	ND	0.03	ND	7.5	0.5	1.1	0.2	9.2	0.6	ND
51	8.2	1.4	512	308	0.2	ND	ND	49.6	26.7	3.7	1.8	0.5	8.1	0.1	ND
52	1.2	ND	275	121	0.1	ND	ND	13.0	5.1	0.3	ND	ND	23.3	0.8	ND
53	1.6	ND	124	37.2	0.4	ND	ND	3.2	0.3	0.2	ND	ND	34.5	0.5	ND
54	7	ND	322	137	1.2	ND	ND	83.6	13.2	5.6	ND	ND	56.2	0.9	ND
55	0.7	ND	246	918	0.2	ND	ND	127.5	16.7	ND	ND	ND	245	1.7	ND
56	0.5	ND	38.4	217	0.4	ND	ND	20.9	4.9	1.7	0.8	ND	95.6	0.6	ND
57	2.3	ND	127	11.9	ND	ND	ND	16.3	1.2	0.3	0.4	ND	7.9	0.2	ND
58	3.4	ND	59.0	15.6	ND	ND	0.03	2.8	0.4	0.1	ND	ND	4	0.1	ND
59	0.2	ND	13.9	8.2	ND	ND	ND	2.6	0.2	0.06	ND	ND	9.5	0.6	ND
60	1.2	ND	10.6	259	0.08	ND	ND	4.7	0.8	0.08	ND	ND	ND	0.3	ND
61	1.9	ND	59.5	247	0.2	ND	0.03	30.1	2	0.6	ND	ND	17.8	0.4	ND
62	0.5	ND	21.1	154	0.2	ND	0.1	5.7	1.8	0.7	ND	ND	27	0.5	ND

Table S5. Pearson's Correlation Analysis Result of Correlations between Residual Chlorine, TOC or Temperature and Total Molar Concentration of Chlorinated BPAs or Chlorinated NPs.

	Residual Chlorine	TOC	Average Temp.
Chlorinated BPAs	$p = 0.355$	$p = 0.604$	$p = 0.966$
Chlorinated NPs	$p = 0.006$	$p = 0.449$	$p = 0.111$