

1 **Occurrence, Distribution and Ecological Risk of Bisphenol Analogues in the Surface Water**
2 **from a Water Diversion Project in Nanjing, China**

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53 2.3 Sample extraction and instrument analysis

54 Other instrumental parameters of UPLC/MS/MS were showed in Table S1 and Table S2.

55 Table S1

Time (min)	Composition of the mobile phase (%)	
Negative mode	Eluent A2 (0.01%Ammonium hydroxide)	Eluent B1 (Acetonitrile)
0	90	10
0.25	90	10
3.00	10	90
4.00	10	90
4.01	90	10
5.00	90	10

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57 Table S2

Compound	Retention time/min	Parent ion (m/z)	Daughter ions(m/z)	Dewll time(s)	Conevol tage (v)	Collision energy (v)
Bisohenol F	2.74	199.10	93.10	0.042	30	20
			105.10*			20
Bisphenol E	2.89	213.10	198.00*	0.042	40	22
			/			/
Bisphenol A	3.03	227.10	133.00	0.042	31	25
			212.00*			17
Bisphenol S	0.66	249.13	92.05	0.161	42	30
			108.07*			24
Bisphenol Z	3.45	267.22	93.02	0.042	56	32
			173.17*			30
Bisphenol AF	3.25	335.23	197.10	0.042	32	25
			265.16*			22
			419.92*			40

58 * represents quantification ion.

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60 2.4 Quality assurance and quality control

61 The strict QA/QC protocol was used to detect the extraction efficiency of BPs in the water

62 sample. The performance of the analytical method was evaluated in terms of linearity, limit of

63 detection (LOD) and limit of quantitative (LOQ) and recovery rate. When analyzing each group of
64 samples, running solvent, standar, and process blanks in turn to check background BPs, peak
65 identification, and quantification. Respectively, LOD and LOQ were determined to be the
66 minimum detectable amounts of the analyte with signal-to-noise (S/N) of 3 and 10. Through
67 injecting different concentrations of the standard solutions (seven-point calibration curve) into the
68 1.0-200 ng/mL range ($R^2 > 0.998$), the linearity of the target compounds was studied. In order to
69 evaluate the recovery, the spiked samples were prepared using ordinary surface water samples.
70 Prior to use, surface water samples used for recovery test were analyzed to detect the presence of
71 BPs. The recovery data for BPs had been corrected to take into account the fact that the average
72 blank peak area of BPs was subtracted from the average peak area of the other recovery points.
73 Six separate chromatographic runs were performed on each of the two concentration levels. The
74 analysis of the reagent blanks (n=3) showed that the analysis system and glassware did not contain
75 BPs.

76 Table S3

Compound	Recovery [%] (n = 6)				Quantitation limits (n = 3)	
	Water sample		SPM samples		Water (ng/L)	SPM (ng/g)
	10 ng/L	100 ng/L	10 ng/g	100 ng/g		
BPF	83.0±12.4	97.8±10.2	82.4±13.1	90.2±10.0	11.10	1.50
BPE	88.4±7.2	92.3±10.7	75.7±6.3	82.0±10.4	1.83	0.50
BPA	91.0±8.1	108±9.9	102±10.8	110±11.5	2.60	0.25
BPS	80.3±4.0	91.4±16.3	79.3±9.3	84.7±6.5	0.53	0.30
BPZ	70.3±5.6	85.6±10.0	73.5±7.4	80.2±7.1	7.07	1.00
BPAF	93.1±16.3	96.2±8.0	82.2±11.4	92.3±10.1	1.70	0.30

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78 2.5 Parameter measurement and statistical analysis

79 Using the risk quotient (RQ) to evaluate the risk assessment of the target compounds in the
80 urban water. The RQ_s was calculated as Eq (1).

81
$$RQ = \frac{MEC}{PNEC} = \frac{MEC}{EC_{50} \text{ or } LC_{50}/f} \quad (1)$$

82 MEC and PNEC are measured environmental concentrations and predicted no-effect
83 concentrations. According to the REACH guidance document, in order to estimate PNEC based on
84 toxicity data when only short-term/acute toxicity data EC_{50} or LC_{50} is available, PNEC is
85 calculated by the EC_{50} or LC_{50} that divides the safety factor (f) 1000. Once a long-term/chronic
86 NOEC value of one, two or three nutritional levels is available, using the f of the 100, 50, or 10
87 (ECHA, 2008). PNEC is derived from chronic and acute toxicity data in the literature and is 100
88 or $1000f$ in our study. Table 3 provides PNEC calculations for algae, daphnia and fish.

89 Calculation of the oestrogen equivalent concentration (EEQ) of a chemically determined
90 mixture is based on all measured xenoestrogens with a known oestrogen equivalency factor (EEF;
91 Table 3), as shown in the following equation (Eq. (2)). When $EEQ_{Total} > 1.0 \text{ ng } E_2/L$, the
92 contaminants are thought to affect the endocrine systems of organisms in the water bodies. So
93 EEQ is also used to assess the risk of BPs to human health.

94
$$EEQ_{Total} = \sum EEQ_i = \sum (C_i \times EEF_i) \quad (2)$$

95 The C_i refers to the compound i with a concentration of C in the traditional dissolved phase.

96 EEQ_{Total} is the total estradiol equivalent and EEF_i is the estradiol equivalent.

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111 **Table S4**

Sampling locations	Time	Concentrations (ng/L) in traditionally dissolved phase				Reference
		BPA	BPS	BPF	BPAF	
Study area	2018 ^a	290 (244)	43.6(42.1)	2.53 (2.23)	6.68 (4.51)	This study
	(07)	133-576	5.87-83.5	ND-5.44	1.62-17.8	
Wujin district	2018	217 (157)	60.5(32.1)	7.13 (4.61)	2.70 (2.05)	[1]
	(08)	73.5-678	7.80-319	1.14-40.1	0.30-17.7	
Taihu Lake	2013	8.5 (7.9)	6.0 (2.0)	0.83 (0.5)	0.28 (0.2)	[2]
	(09)	4.2-14	0.28-67	ND-5.6	0.13-1.1	
Taihu Lake	2015	9.7 (7.3)	2.6 (0.94)	1.24 (1.1)	0.27 (0.1)	[3]
	(05)	3.9-33.2	0.32-27.3	0.5-3.28	0.06-2	
Taihu Lake	2015	92.6 (53.2)				[4]
	(11)	28-565				
Taihu Lake	2016	97	120	140	8.2	[5]
	(04)	28-560	4.5-1600	ND-1600	0.7-23	
Taihu Lake	2016	25.7 (23.8)	15.9 (6.6)	78 (30)	114 (111)	[6]
	(11)	19.4-68.5	41.-157	25.6-723	110-140	
Luoma Lake	2016	86	21	6.8	17	[5]
	(04)	49-110	ND-94	3.5-14	12-84	
Liaohhe River	2013	47 (29)	14 (8.9)		1.9 (1.0)	[2]
	(09)	5.9-141	0.22-52	ND ^b	0.5-9.6	
Hunhe River	2013	40 (42)	11 (8.4)		2.4 (0.94)	[2]
	(09)	4.4-107	0.61-46	ND	0.61-11	
Pearl River	2013	73 (73)	135 (135)	773 (757)		[7]
	(07)	ND-98	ND-135	448-1110	ND	
West River	-2014	43 (43)		64 (64)		[7]
	(03)	ND-43	ND	ND-105	ND	
20 source water China	2017	12.8 (10.5)	1.1 (0.4)	2.2 (ND)	3.0 (0.1)	[8]
	(11)	ND-34.9	ND-5.2	ND-12.6	ND-10.8	
Several Rivers, Bay (Japan)		104	5.3	638		[7]
	2013	ND-431	ND-15	ND-2850	ND	
Several Rivers (Korea)	(07)	105.7	41	633		[7]
	-2014	1.0-272	ND-42	ND-1300	ND	
Several Rivers, Lake (India)	(03)	551	2174	91.5		[7]
		ND-1950	ND-7200	ND-289	ND	

112 ^a Year (Month).113 ^b ND: not detected.

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117 **Table S5**

Compound	Non-target organism	Test Endpoint	Toxicity data (mg/L)	PNEC (ng/L)	Reference	EEF Ref. [17]
BPA	Algae	72h-EC50	2.2 (Growth)	2200	[9]	1.07×10 ⁻⁴
	Daphnias	48h-EC50	3.9 (Immobility)	3900	[10]	
	Fish	48h-EC50	3.6 (Pigmentation)	3600	[11]	
BPS	Algae	96h-EC50	6.9	6900	[13] ^a	1.06×10 ⁻⁶
	Daphnias	48h-EC50	55 (Immobility)	55000	[14]	
	Fish	72 hpf-EC50	155 (Mortality)	155000	[15]	
BPF	Algae	72h-IC50	22.1 (Growth)	22100	[11]	1.08×10 ⁻⁴
	Daphnias	21d-NOEC	0.84 (Reproduction)	8400	[11]	
	Fish	48h-EC50	1.1 (Pigmentation)	1100	[11]	
BPAF	Algae	72h-IC50	3.0 (Growth)	3000	[11]	7.23×10 ⁻⁴
	Daphnias	21d-NOEC	0.23 (Reproduction)	2300	[11]	
	Fish	72hpf-EC50	0.92 (Mortality)	920	[15]	
BPE	Daphnias	48h-EC50	18	18000	[14]	5.92×10 ⁻⁵
	Fish	EC50	0.0579	57.9	[16]	

118 ^a The toxicity data was calculated from the ecological structure activity relationships (ECOSAR)
 119 model.

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