

Supporting Information

***p*-Phenylenediamine Derivatives in Drinking Water: Implication for Human Exposure**

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Table S1. List of *p*-Phenylenediamine Antioxidants Monitored in This Study and Their Abbreviation, Full Name, CAS Number, and Chemical Structure.

Abbreviation	Full name	CAS	Chemical structure
IPPD	N-isopropyl-N'-phenyl-1,4-phenylenediamine	101-72-4	
DPPD	N, N'-diphenyl-p-phenylenediamine	2687960-60-5	
CPPD	N-phenyl-N'-cyclohexyl-p-phenylenediamine	101-87-1	
6PPD	N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine	793-24-8	
7PPD	(1,4-dimethylpentyl)-N'-phenylbenzene-1,4-diamine	3081-01-4	
44PD	N, N'-Di-2-butyl-p-phenylenediamine	101-96-2	
77PD	N, N-Bis(1,4-dimethylpentyl)-p-phenylenediamine	3081-14-9	
DTPD	N, N'-di(o-tolyl)-p-phenylenediamine	15017-02-4	
DNPD	N, N'-di-2-naphthyl-p-phenylenediamine	93-46-9	

Table S2. Source of the Collected Drinking Water in Hangzhou and Taizhou.

Site		<i>n</i>	Source typology
Hangzhou city	Linping district	53	Tiaoxi River
	Xiaoshan district	31	Qiantang River
	Fuyang district	47	Fuchunjiang River
Taizhou city	Jiaojiang district	30	Lingjiang River

Table S3. MRM Transition Parameters for Analyzing PPDs and Internal Standard.

	Parent ion	Daughter ion	Cone voltage (eV)	Collision energy (eV)
IPPD	227	184	35	19
		107	35	24
DPPD	261	167	40	22
		107	40	31
CPPD	267	107	43	23
		84	43	35
6PPD	269	184	40	27
		166	40	27
DTPD	289	180	43	25
		92	43	35
DNPD	361	217	45	28
		234	45	20
7PPD	283	184	40	20
		93	40	35
44PD	221	135	37	20
		164	37	15
77PD	305	206	39	25
		135	39	41
¹³C₆-6PPD	275	190	40	27

Table S4. LODs and Extraction Recoveries of Target Analytes in Human Urine.

	LOD (ng/L)	Extraction Recovery (%)					
		Spiked at 0.1 ng/L		Spiked at 1 ng/L		Spiked at 10 ng/L	
		Mean	SD	Mean	SD	Mean	SD
IPPD	0.027	84	4	109	7	107	3
DPPD	0.044	100	5	81	5	106	9
CPPD	0.019	91	9	105	8	93	6
6PPD	0.055	82	9	96	7	100	7
7PPD	0.052	106	8	86	9	87	5
44PD	0.031	86	6	100	8	105	8
77PD	0.063	86	5	87	2	102	7
DTPD	0.048	85	8	92	7	106	10
DNPD	0.070	101	7	106	2	84	11

Table S5. Correlations among Concentrations (ng/L) of Various PPDs in Hangzhou Drinking Water.

		CPPD	IPPD	44PD	6PPD
CPPD	Spearman Correlation	1	0.249	0.149	0.320
	Sig. (2-tailed)		0.435	0.238	0.227
IPPD	Spearman Correlation		1	0.165	0.399
	Sig. (2-tailed)			0.672	0.190
44PD	Spearman Correlation			1	0.266
	Sig. (2-tailed)				0.404

Table S6. Correlations among Concentrations (ng/L) of Various PPDs in Taizhou Drinking Water.

		44PD	CPPD	7PPD
6PPD	Spearman Correlation	0.394	0.173	0.331
	Sig. (2-tailed)	0.381	0.891	0.469
44PD	Spearman Correlation	1	0.330	0.419
	Sig. (2-tailed)		0.279	0.084
CPPD	Spearman Correlation		1	0.409
	Sig. (2-tailed)			0.374

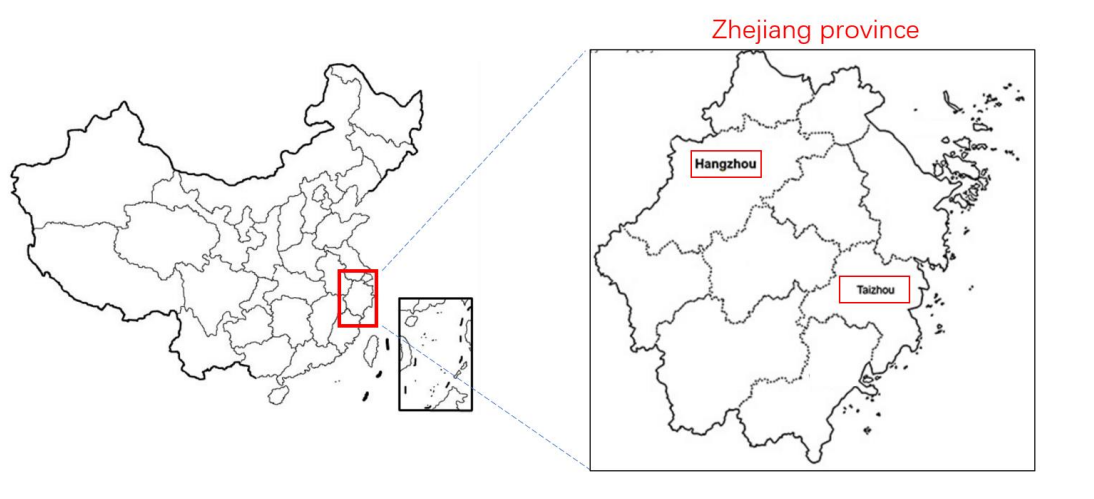


Figure S1. The map of sampling regions in this study, Hangzhou city and Taizhou city.

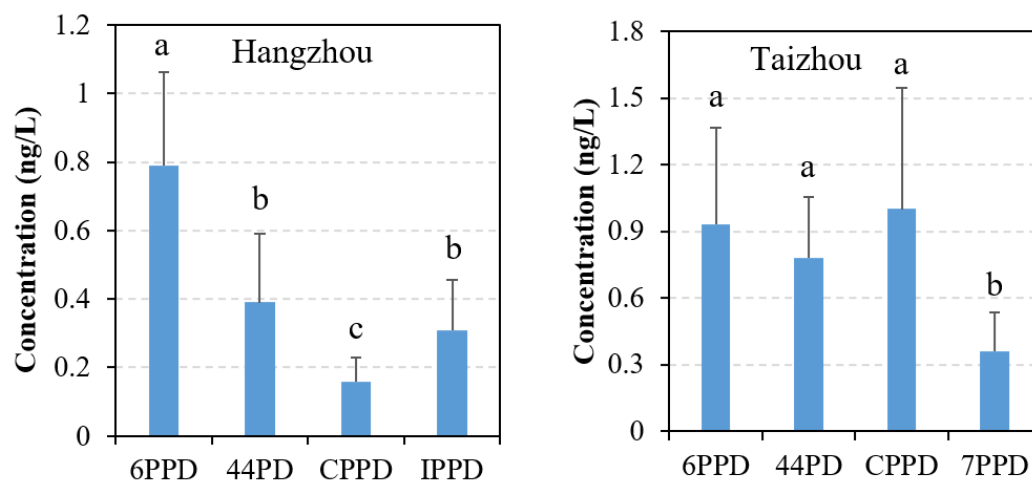


Figure S2. Concentrations (mean \pm SD) of detected PPDs in drinking water samples from Hangzhou and Taizhou. Different alphabets mean the significant difference in concentrations.