

Occurrence of Phthalates in bottled drinks in Chinese market and its implications for dietary exposure

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Table S1. Detailed information of the 15 PAEs measured in this study.

full name	abbreviation	chemical formula	molecular weight	Log Kow
low molecular weight phthalates				
dimethyl phthalate	DMP	C10H10O4	194.2	1.6
diethyl phthalate	DEP	C12H14O4	222.2	2.47
dibutyl phthalate	DBP	C16H22O4	278.4	4.5
diisobutyl phthalate	DIBP	C16H22O4	278.4	4.11
bis(2-methoxyethyl) phthalate	BMEP	C14H18O6	282.3	1.11
diamyl phthalate	DAP	C18H26O4	306.4	5.62
bis(2-ethoxyethyl) phthalate	BEEP	C16H22O6	310.3	2.1
butyl benzyl phthalate	BBP	C19H20O4	312.4	4.73
dicyclohexyl phthalate	DCP	C20H26O4	330.4	6.2
dihexyl phthalate	DHP	C20H30O4	334.4	6.82
bis(4-methyl-2-pentyl) phthalate	BMPP	C20H30O4	334.4	
bis(2-n-butoxyethyl) phthalate	BBEP	C20H30O6	366.4	4.06
diethylhexyl phthalate	DEHP	C24H38O4	390.6	7.6
high molecular weight phthalates				
dinonyl phthalate	DOP	C24H38O4	390.6	8.1
dinonyl phthalate	DNP	C26H42O4	418.6	9.52

Table S2. Instrumental parameters on GC-MS conditions for phthalate analysis

<i>Parameter</i>	<i>Condition/setting values</i>		
Instrument	GC 6890B MS 5973 (Agilent Technologies)		
Column	DB-5MS (30 m × 0.25 mm × 0.25 µm; Agilent Technologies)		
Injection	Splitless mode, injection volume 2 µL, injection port temperature 280°C		
Carrier gas	Helium, flow rate 0.5 mL/min		
Oven temperature program	80 °C (hold 1 min), to 180 °C (12 °C/min, hold 1 min), to 230 °C (6 °C/min), to 270 °C (8 °C/min, hold 2 min), to 300 °C (20 °C/min, hold 15 min)		
Interface temperature	250 °C	Ion source temperature	230 °C
Ionization mode	EI, electron energy 70 eV	Monitoring mode	SIM

Table S3. Concentrations (ng/L) of the target phthalates in procedural blanks and their limits of detection (LOD) and limits of quantification (LOQ).

chemical	BLK ^a	LOQ ^b	relative recovery (%)		RSD(%) ^e
			low ^c	high ^d	
DMP	<LOQ	21	94.6±7.14	94.6±7.63	8.43
DEP	<LOQ	16	95.8±4.73	93.8±6.02	4.26
DIBP	<LOQ	214	104±8.03	104±6.03	5.06
DBP	<LOQ	113	107±8.47	103±4.80	5.37
BMEP	<LOQ	6	90.6±4.58	96.0±4.04	4.72
BMPP	<LOQ	3	93.4±5.39	94.6±5.04	4.08
BEEP	<LOQ	6	89.3±6.82	92.6±5.84	6.32
DAP	<LOQ	3	89.5±8.53	95.8±3.48	2.48
DHP	<LOQ	3	86.4±1.58	87.4±4.20	5.39
BBP	<LOQ	4	84.6±9.04	89.1±5.47	9.52
BBEP	<LOQ	9	90.6±11.2	95.2±8.65	9.58
DCP	<LOQ	5	94.8±10.3	93.8±6.32	6.04
DEHP	258±24	212	110.4±8.57	106±7.53	7.28
DOP	<LOQ	3	106±6.54	104±5.06	5.43
DNP	<LOQ	3	97.9±2.45	96.3±4.06	4.68

^a: BLK, procedural blank, calculated by analyzing the PAEs in the procedural blank samples (n=3); ^b: LOQ, limit of quantification; ^c: relative recoveries of PAEs in the analysis of bottled drink samples calculated using matrix spike of low amount chemicals (50 ng); ^d: relative recoveries of PAEs in the analysis of bottled drink samples calculated using matrix spike of high amount chemicals (500 ng); ^e: RSD, relative standard deviation, calculated using the replicates analysis of high amount chemical matrix spikes (n=3).

Table S4. Correlation coefficients between the new abstract principal components and the PAEs present in the bottled drinks.

variable	CAP1	CAP2	CAP3	CAP4	CAP5	CAP6
DMP	0.327	-0.102	0.19	-0.821	0.156	-0.072
DEP	0.147	-0.105	-0.128	-0.081	-0.092	-0.09
DIBP	0.358	0.283	0.363	0.222	-0.097	0.03
DBP	0.349	0.277	0.386	0.045	-0.058	0.029
BMEP	0.272	0.662	-0.625	-0.051	0.271	-0.01
DAP	0.28	-0.16	-0.273	-0.127	-0.428	-0.37
BEEP	0.333	-0.118	0.131	-0.028	0.271	0.095
BBP	0.345	-0.17	-0.195	0.147	-0.465	0.304
DCP	0.208	-0.042	-0.1	0.168	0.052	0.081
DHP	0.152	-0.141	-0.107	0.087	0.003	0.113
BMPP	0.255	-0.187	-0.059	0.024	-0.166	0.19
BBEP	0.247	-0.225	0.087	0.274	0.497	0.171
DEHP	0.051	0.316	0.315	0.158	-0.249	-0.341
DOP	0.131	-0.224	-0.108	0.167	0.118	-0.004
DNP	0.164	-0.241	-0.058	0.249	0.237	-0.738