Supporting Information

Occurrence and human exposure of *p*-hydroxybenzoic acid esters (parabens), bisphenol A diglycidyl ether (BADGE), and their hydrolysis products in indoor dust from the United States and Three East Asian Countries

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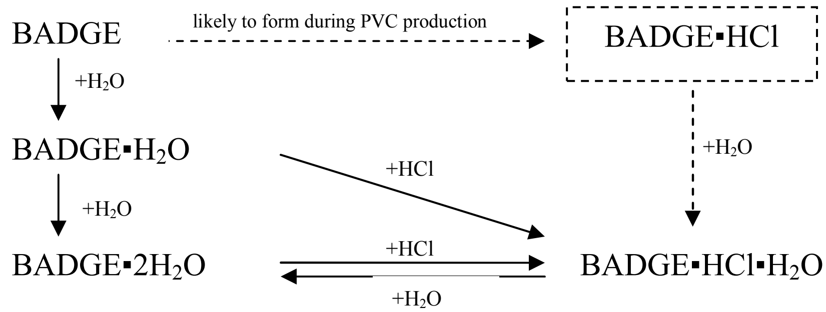

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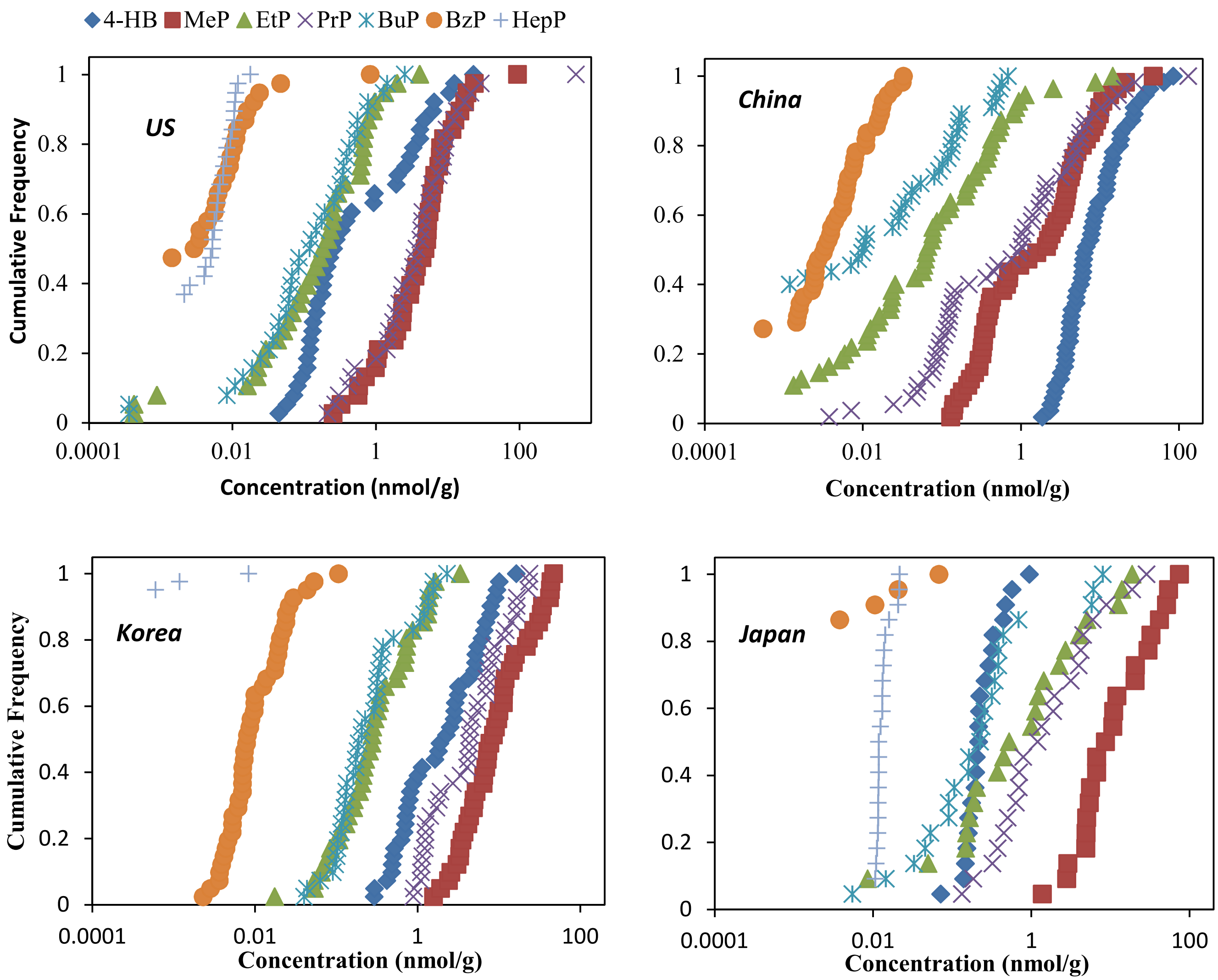
Figure S2



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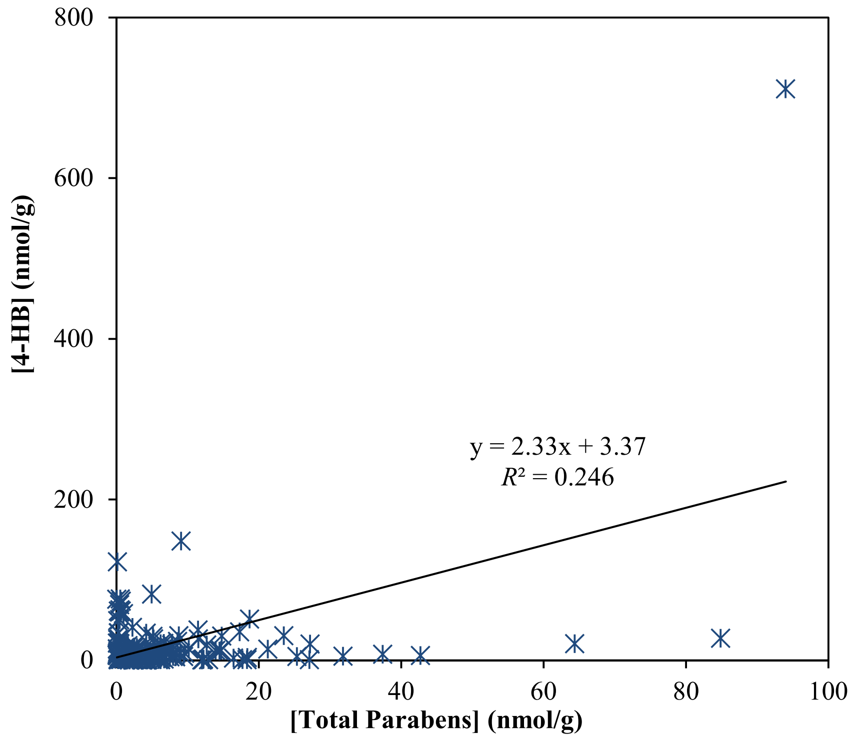

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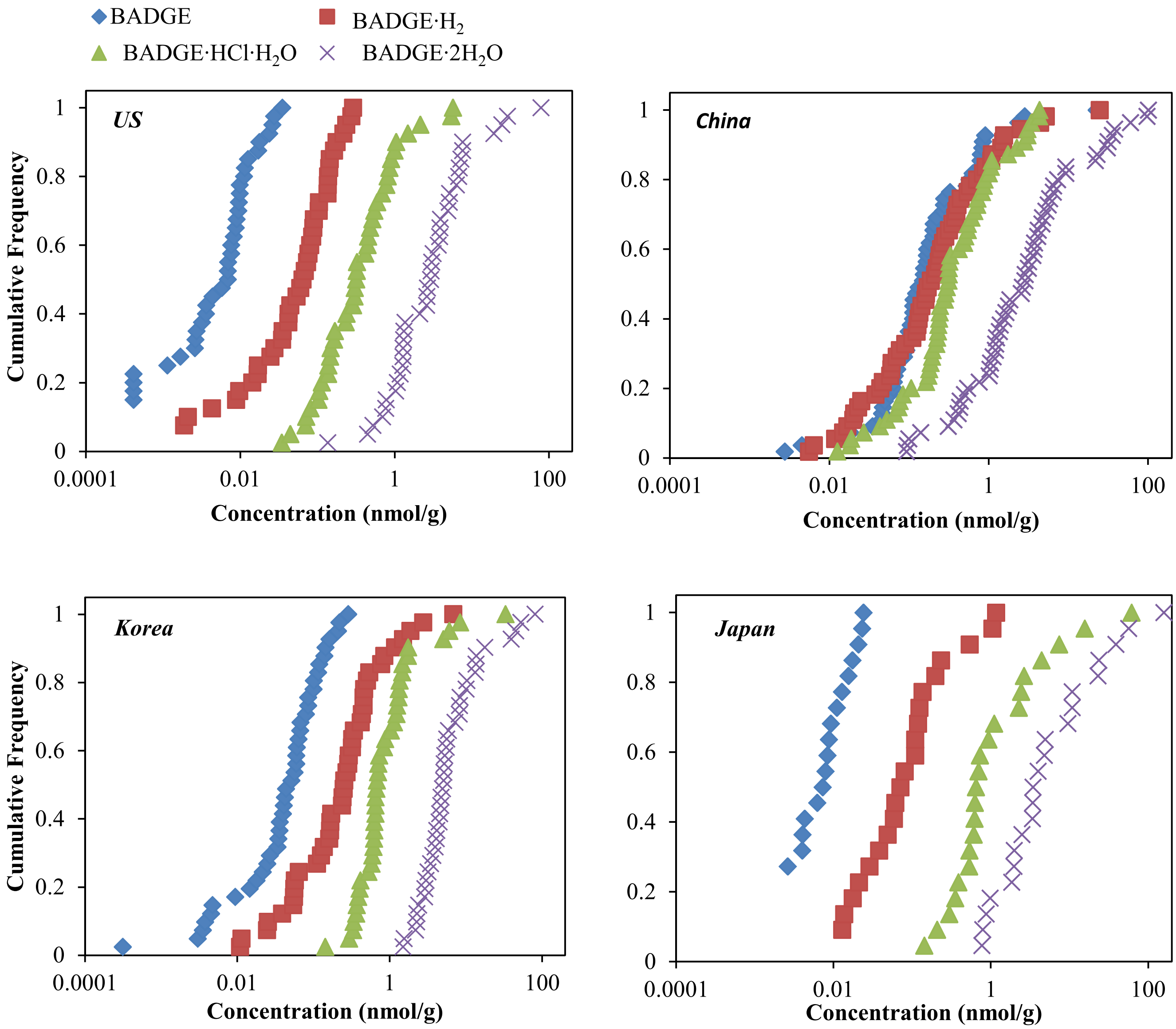

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Table S1 Gradient elution processes used in LC for parabens and BADGEs.

Parabens		BADGEs	
Time	Mobile B (%)	Time	Mobile B (%)
0.00	95	0.00	95
5.50	95	2.00	95
8.50	60	4.00	50
11.00	0	8.00	0
20.00	0	14.00	0
21.00	95	15.00	95
26.00	95	20.00	95

Note: The mobile phases were composed of methanol (A) and 10% methanol in Milli-Q water containing 2 mM of ammonium acetate (B); Flow rate = 200 µL/min.

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Table S2. Coefficients of MS/MS analysis for target analytes.

	Q1	Q3	DP (volts)	EP (volts)	CE (volts)	CXP (volts)
Negative [a]						
MeP ($^{13}C_6$-MeP)	151 (157)	92 (98)	-30	-8	-27	-10
EtP	165	92	-32	-10	-30	-5
PrP	179	92	-31	-10	-27	-10
BuP ($^{13}C_6$-BuP)	193 (199)	92 (98)	-30	-9	-28	-8
BzP	227	92	-30	-10	-27	-8
HepP	235	92	-35	-10	-33	-7
4-HB	137	92	-28	-10	-27	-10
Positive [b]						
BADGE	358	191	70	10	50	3
BADGE▪H_2O	376	209	50	5	30	1
BADGE▪HCl▪H_2O	412	227	70	10	50	3
BADGE▪$2H_2O$	394	209	50	5	30	1
$^{13}C_{12}$-BP-3	235	151	25	10	30	7

Note: DP=Declustering potential; EP=Entrance potential; CE= Collision energy; CXP: Collision cell exit potential.

[a]: Curtain gas (CUR): 20;Collision gas (CAD): 7; Ionspray voltage (IS): -4500; Temperature (TEM): 400; Ion source gas 1 (GS1): 50; Ion source gas 2 (GS2): 60;

[b]: CUR: 10; CAD: 4; IS: 4700; TEM: 615; GS1: 68; GS2: 69;

Table S3. Recoveries (%) of parabens, 4-HB, BADGEs, and its hydrolysis products from spiked procedure blank and spiked matrices (*n*=6) of indoor dust.

Analytes	Analytes concentration in spiked procedure blank (ng/mL)	spiked procedure blank (%)	spiked matrix corrected by internal standard (%)
MeP	<LOQ	78.44	96.5
EtP	<LOQ	82.9	107.9
PrP	<LOQ	85.7	99.0
BuP	<LOQ	83.2	101.3
BzP	<LOQ	86.7	103.1
HepP	<LOQ	87.1	114.6
4-HB	0.27	85.3	80.2*
BADGE	<LOQ	96.7	104.9
BADGE▪H_2O	<LOQ	90.5	98.4
BADGE▪HCl▪H_2O	<LOQ	91.3	101.5
BADGE▪$2H_2O$	<LOQ	87.2	85.6

*spiked recovery of 4-HB was not corrected by internal standard.

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Table S4 Factor of the indoor dust ingestion rate (m_{di}) and body weight (BW) used in daily intake of analytes via dust ingestion of indoor dust.

	m_{di} (mg)	BW (kg)	Source of factors
US			
infants	30	7.5	Ages of infants, toddlers, children, and teenagers are defined as 1 m-1 yr, 1-3 yr, 3 - 11 yr, and 11-21 yr in this study. Factors of m_{di} and BW come from *USEPA's hand book* (*2011*). The body weight (BW) of US children was also assigned to those of three East Asian countries, because the BW factors for the same age are unavailable for these countries, and the difference of BW is not significant for children.
toddlers	60	12.6	
children	60	25.2	
teenagers	60	64.2	
adults	30	80	
China			
Children	59	25.2	BW comes from the *Chinese National Physique Monitoring Communique 2010*. The m_{di} factors of korea was used because there's no available data of them for China.
adults	30	62.9	
Korea			
children	59	25.2	Adults' BW and soil ingestion of children were reported by *Jang et al. (2008)*. Children's m_{di} was assumed to be half of soil ingestion *(Stanek & Calabrese, 1992)*. Adults' m_{di} were assumed to be half of m_{di} of children (*USEPA, 2011*).
adults	30	62.8	
Japan			
children	59	25.2	BW come from *Japanese Exposure Factors Handbook* (*2012*), while the m_{di} factors of korea was used here because there's no suitable data of them for Japan.
adults	30	58.4	

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Human Exposure to Parabens and BADGEs via Dermal Absorption of Dust

Daily intake of parabens and BADGEs via dermal absorption of indoor dust can be estimated using eqs (S1) as follows (*USEPA, 2011; Guo and Kannan, 2011*),

$$EDI_{du} = \frac{C \times A \times f_{das} \times f_{absorb}}{BW} \quad \text{(S1)}$$

where A is the body surface area (cm^2), f_{das} is the dust adhered to skin per day (mg/ cm^2/day), and f_{absorb} is the fraction of analytes abosrbed by the skin. ($A \times f_{das}$) can be calculated using eqs (S2)

$$A \times f_{das} = \left(p_{face} \times f_{das,face} + p_{arms} \times f_{das,arms} + p_{hands} \times f_{das,hands} + p_{legs} \times f_{das,legs} + p_{feet} \times f_{das,feet}\right) \times A \quad \text{(S2)}$$

The mean indoor dust adhered to skin of body part ($f_{das,i}$) were 0.0041 (arms), 0.0011 (hands), 0.0035 (legs), 0.010 mg/cm^2 (feet) for both US children and US adults, which come from (*USEPA, 2011*). Value of f_{ads} on arms (0.0041) was assigned to f_{ads} of face, because there's no available data of it. For US children, mean percent of total body area (p) were 3.5% (face, equal to half of the head area), 14% (arms), 4.8% (hands), 27.2% (legs), and 6.6% (feet), with a mean total body surface area (A) for children of 9200 cm^2 (*USEPA, 2011*). For US adults, values of p were 3.2% (face, equal to half of the head area), 14% (arms), 5% (hands), 32.7% (legs), and 6.6% (feet), with a mean total body surface area (A) for children of 19500 cm^2 (*USEPA, 2011*). Therefore, the values of $A \times f_{das}$ were calculated to be 22 and 50 mg for US children and adults, according to equation S2.

Values of the fraction of analytes on dust absorbed by skin per day (f_{absorb}) for parabens were 0.050 (MeP), 0.066 (EtP), 0.056 (PrP), 0.056 (BuP), 0.026 (BzP), and 0.026 (HepP) (Table S5), which were calculated based on the data as follows. All parabens can easily absorbed through percutaneous process (*Jewell et al., 2007*). The daily dermal uptake rate of parabens for human skin in 24 h 33.4% (MeP), 44.1%(EtP), 37.0% (PrP), 37.4% (BuP), and 17.0% (BzP) (*Jewell et al., 2007*). There are no available uptake rate of HepP for human dermal exposure, so 17.0% was also assigned to the dermal uptake rate of HepP. A coefficient of 15% was also used to reduce the matrix of soil and dust (*Hawley, 1985*). For infants, toddlers, and children, the skin permeability is twice high as that of teenagers and adults (*Hawley, 1985*).

For BADGE, uptake through human skin is lower than through mouse skin by a factor of 3 (Boogaard et al., 2000). Therefore, a daily dermal uptake rate of 1% for BADGE was obtained since 3.0±0.8% of BADGE penetrated the skin of mouse in 24 h. Besides, the matrix of soil and dust reduces the uptake of chemicals to about 15% (*Jewell et al., 2007*), which led to an uptake rate of 0.0015 for BADGE dermal exposure by dust/soil to human teenagers and adults. There are no available uptake rate for hydrolysis products of BADGE. However, the logarithm of the apparent permeability constant for aromatic glycidyl ether chemicals was found to be negatively related to their log Kow. Therefore, the daily uptake rate of BADGE▪H2O, BADGE▪HCl▪H2O, and BADGE▪$_2$H2O were >0.0015. For infants, toddlers, and children, the skin is twice as permeable as the skin of teenagers and adults (*Jewell et al., 2007*), and the daily dermal uptake rate of BADGE and its hydrolysis products by dust/soil contact were 0.0030 and >0.0030, respectively.

According to factors selected and calculated above, human exposure to parabens and BADGEs via dermal absorption of indoor dust for children and adults of U.S, which was shown in (Table S5).

Table S5. Human exposure to parabens and BADGEs via dermal absorption of indoor dust for U.S. children and adults.

	Parabens							BADGEs				
	MeP	EtP	PrP	BuP	BzP	HepP	∑Parabens	BADGE	BADGE ▪H_2O	BADGE ▪H_2OHCl	BADGE ▪$2H_2O$	∑BADGEs
U.S. children												
f_{absorb}	0.10	0.13	0.11	0.11	0.05	0.05		0.003	>0.003	>0.003	>0.003	
EDI_{ddu}	0.04	0.002	0.05	0.002	1.71e-5	1.95e-5	0.09	2.75e-6	>4.41e-5	>2.73e-4	>0.002	>0.002
U.S. adults												
f_{absorb}	0.05	0.07	0.06	0.06	0.03	0.03		0.0015	>0.0015	>0.0015	>0.0015	
EDI_{dda}	0.02	0.001	0.02	6.11e-4	6.83e-6	7.76e-6	0.04	1.10e-6	>1.76e-5	>1.09e-4	>8.78e-4	>0.001

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