

## Supplementary data

### **A Pilot Study of Metabolites of Organophosphorus Flame Retardants in Paired Maternal Urine and Amniotic Fluid Samples: Potential Exposure Risks of Tributyl Phosphate to Pregnant Women**

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**Table S1**  
**Optimized MS/MS parameters for target organophosphate metabolites.**

Metabolites	Parent compounds	Precursor ion (Q1)	Product ion (Q3)	DP <sup>a</sup> (V)	EP <sup>b</sup> (V)	CE <sup>c</sup> (V)	CXP <sup>d</sup> (V)
<b>Native standards</b>							
bis(1,3-dichloro-2-propyl) phosphate (BDCIPP)	tris(1,3-dichloro-2-propyl) phosphate (TDCIPP)	318.9	35.0	-53	-4.5	-46	-11
bis(2-butoxyethyl) phosphate (BBOEP)	tris(2-butoxyethyl) phosphate (TBOEP)	305.0	79.0	70	-8	-40	-15
dibutyl phosphate (DBP)	tri- <i>n</i> -butyl phosphate (TNBP)	209.0	78.9	-80	-7	-30	-15
di- <i>o</i> -cresyl phosphate (DoCP)	tricresyl phosphate (TCP)	227.1	107.0	-80	-6	-33	-17
di- <i>p</i> -cresyl phosphate (DpCP)		227.1	107.0	-80	-8	-32	-15
diphenyl phosphate (DPHP)	triphenyl phosphate (TPHP) ethylhexyl diphenyl phosphate (EHDPP)	249.1	93.0	-100	-7	-45	-9
<b>internal standards</b>							
d <sub>10</sub> -BDCIPP		329.0	35.0	-90	-10	-60	-17
d <sub>8</sub> -BBOEP		305.0	79.0	-90	-7	-60	-10
d <sub>18</sub> -DBP		227.3	79.0	-80	-8	-50	-10
d <sub>14</sub> -DoCP		291.1	114.0	-90	-7	-40	-10
d <sub>14</sub> -DpCP		291.1	114.0	-120	-7	-36	-10
d <sub>10</sub> -DPHP		259.2	98.0	-90	-8	-32	-12

a DP = declustering potential.

b EP = entrance potential.

c CE = collision energies.

d CXP = collision cell exit potential.

**Table S2****Parameters Used for Calculation of Total Daily Intakes of OPs in China.**

	TPHP	TnBP
molecular weights of the parent OPs (MWp, g/mol)	326	266
molecular weights of the metabolite of OPs (MWm, g/mol)	250	210
$F_{UE}$ based on in vitro human liver microsome (HLM) experiment	0.09 <sup>a</sup>	0.18 <sup>b</sup>
$F_{UE}$ based on in vitro human liver S9 fraction experiment	0.04 <sup>a</sup>	0.18 <sup>b</sup>

<sup>a</sup>  $F_{UE}$  is the urinary excreted molar fraction of metabolite with respect to its parent compound, data from Van den Eede et al. <sup>b</sup>  $F_{UE}$  of TnBP was from TnBP metabolism experiment of male rats from Suzuki et al.