Supporting Information

Unexpectedly High Concentrations of a Newly Identified Organophosphate Ester, Tris(2,4-di-*tert*-butylphenyl) Phosphate, in Indoor Dust from Canada

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Table S1. Information on analyte name, abbreviations and CAS No.

Analyte name	Abbreviation	CAS
Tris(2-chloroethyl) phosphate	TCEP	115-96-8
Tris(1,3-dichloro-2-propyl) phosphate	TDClPP	13674-87-8
Triphenyl phosphate	TPHP	115-86-6
Tricresyl phosphate	TMPP	1330-78-5
2-Ethylhexyl diphenyl phosphate	EHDPP	1241-94-7
Tris(2-ethylhexyl) phosphate	TEHP	78-42-2
Tris(2,4-di-*tert*-butylphenyl) phosphate	AO168=O (T2,4D*t*BPP)	95906-11-9
Tris(2,4-di-*tert*-butylphenyl) phosphite	AO168	31570-04-4
Bis(2,4-di-*tert*-butylphenyl) phosphate	B2,4D*t*BPP	69284-93-1
2,4-Di-*tert*-butylphenol	2,4D*t*BP	96-76-4
Triphenylphosphate-d15	TPHP-d15	1173020-30-8

Table S2. Optimized multiple-reaction monitoring parameters in LC-MS/MS analysis.

Compounds	Precursor ion (*m/z*)	Product ion (*m/z*)	Cone potential (V)	Collision energy (V)	Inonization
TCEP	285.1	99.1	36	22	ESI+
		223.0		10	
TDClPP	429.2	99.1	32	20	ESI+
		209		14	
TPHP	327.2	77.1	68	32	ESI+
		152.2		32	
TMPP	369.2	91.2	72	36	ESI+
		165.2		42	
EHDPP	363.2	77.1	18	54	ESI+
		251.1		12	
TEHP	435.4	71.1	26	12	ESI+
		99.0		20	
AO168=O	663.3	327.1	54	54	ESI+
		495.3		32	
AO168	647.3	147.3	48	48	ESI+
		235.1		50	
B2,4D*t*BPP	475.5	251.2	4	34	ESI+
		363.3		18	
TPHP-d15	342.2	82.1	68	32	ESI+
2,4D*t*BP	205.3	149.2	50	26	ESI-
		189.2		24	

Table S3. Validation and performance data of the developed method.

Compounds	Recovery (%)	RSD (%)	Matrix effect (%)	MQL (ng/g)
TCEP	91	4.1	98	0.2
TDClPP	77	5.1	86	5.0
TPHP	95	5.4	96	0.4
TMPP	90	6.4	87	0.3
TEHP	82	4.1	83	1.0
EHDPP	76	1.7	87	0.8
AO168=O	77	12	81	0.5
2,4D*t*BP	91	5.4	90	12
B2,4D*t*BPP	57	13	99	3.0
AO168	88	12	93	0.6

Table S4. Comparison of OPE concentrations in indoor dust collected from North America.

Country	Environment	Number of samples	TCEP	TDClPP	TEHP	EHDPP	TPHP	TMPP	Reference
Canada	Offices	54	210 – 1.13e5 GM: 4.09e3 Median: 3.98e3	299 – 1.05e4 GM: 2.16e3 Median: 2.22e3	3.25 – 1.12e3 GM: 141 Median: 195	138 – 4.72e4 GM: 1.61e3 Median: 1.30e3	481 – 4.51e4 GM: 2.74e3 Median: 2.66e3	31.5 – 2.11e4 GM: 442 Median: 428	This study
Canada	Homes	30	174 – 5.79e3 GM: 621 Median: 535	146 – 1.05e4 GM: 982 Median: 1.12e3	2.94 – 316 GM: 105 Median: 128	130 – 2.92e4 GM: 742 Median: 673	484 – 4.66e4 GM: 1.42e3 Median: 1.08e3	7.79 – 3.14e3 GM: 66.0 Median: 302	This study
Canada	Homes	23	73.7 – 6.75e3 Median: 181	206 – 9.53e3 Median: 917	18.6 – 611 Median: 101	150 – 8.40e3 Median: 754	377 – 3.19e4 Median: 2.35e3	0.871 – 116 Median: 6.18	[1]
USA	Homes	49	-	197–39,530 GM: 1.39e3	-	-	99.5–40,350 GM: 1.02e3	-	[2]
USA	Homes	20	123 – 9.08e3 Median: 1.44e3	ND – 8.94e3 Median: 3.68e3	ND – 1.86e4 Median: 1.36e3	ND – 4.76e3 Median: 889	22.5 – 2.48e4 Median: 3.04e3	ND – 453 Median: 82.5	[1]
USA	Homes	16	330 – 1.10e5 Median: 2.70e3	920 – 4.40e4 Median: 2.10e3	ND – 340 Median: ND	140 – 1.50e3 Median: 560	-	180 – 1.00e4 Median: 680	[3]
USA	Children care centers	14	280 – 1.70e3 Median: 730	550 – 4.20e3 Median: 2.10e3	-	370 – 5.90e3 Median: 1.70e3	480 – 1.50e4 Median: 2.40e3	ND – 42.0 Median: ND	[4]

GM: geometric mean; ND: not detected; -: not investigated.

Table S5. Pearson's correlation matrix for the concentrations of AO168 and related transformation products in indoor dust.

	AO168	AO168=O	B2,4D*t*BPP
AO168	1		
AO168=O	-.0.122	1	
B2,4D*t*BPP	0.044	0.566**	1

** Correlation is significant at the 0.01 level (2-tailed).

Table S6. Estimated daily intakes (EDI, ng/kg bw/day) of OPEs by ingestion of indoor dust for toddlers and adults in Canada.

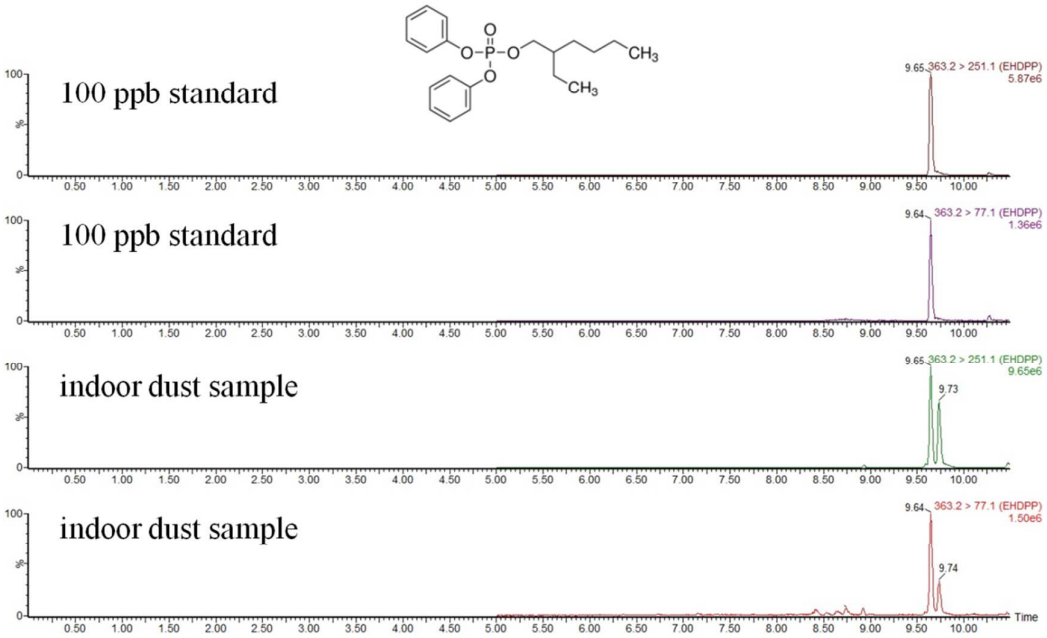
Compounds	Adults				Toddlers	
	Office		Home		Home	
	GM	95th percentile	GM	95th percentile	GM	95th percentile
TCEP	0.57	1.78	0.25	0.62	4.78	12.0
TDClPP	0.30	0.51	0.39	1.04	7.55	20.0
TPHP	0.38	0.95	0.57	2.62	10.9	50.5
TMPP	0.06	0.26	0.03	0.17	0.57	3.37
TEHP	0.02	0.05	0.04	0.07	0.81	1.33
EHDPP	0.22	0.84	0.30	1.50	5.70	29.0
AO168=O	0.28	0.50	0.77	1.31	14.8	25.3
∑OPEs	2.62	4.20	3.23	6.09	62.3	118

The estimated daily intake (EDI) was calculated from the equation as below:

$$EDI = C \times DIR \times IEF / BW$$

Where "C" is is the concentration of target analyte, "DIR" is the dust ingestion rate (g/day), "IEF" is indoor exposure fraction, and "BW" is the body weight (kg). The body weights for toddlers and adults were 13 and 80 kg,[5] respectively, and "DIR" of 0.1 and 0.05 g/d was used for toddlers and adults,[5] respectively. The IEFs were 63.8% and 22.3% for home and office for adults in literature.[6] For toddlers, the IEFs were 100% and 0% for home and office.

Figure S1. MRM chromatograms of EHDPP (the first peak) and an unknown peak (the second peak).



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