

Supporting Information

From PDMS-based exposure profiling to machine learning-predicted serum concentrations: SVOC exposure disparities across occupational and environmental scenarios

Zihao Zhang ^a, Yan Wang ^{a,*}, Yubin Wu ^a, Ruize Chen ^a, Hongbo Zheng ^a

^a *Key Laboratory of Industrial Ecology and Environmental Engineering (MOE), School of Environmental Science and Technology, Dalian University of Technology, Dalian 116024, China*

* Corresponding author. E-mail: wangyandut@dlut.edu.cn

Twenty-three pages, including 13 tables and 2 figures.

Tables and Figures

Table S1 Sampling information.

Table S2 Full names, abbreviations, and properties of target SVOCs.

Table S3 Parameters for the GC-MS analysis.

Table S4 Blank levels and MDLs of SVOCs for the PDMS samplers.

Table S5 Surrogate recoveries for the PDMS samples.

Table S6 Parameters for the calculation of non-cancer and cancer risks to SVOCs.

Table S7 Ratios of SVOC concentrations between D_PS and S_PB, and S_PW and S_PB.

Table S8 Non-parametric Wilcoxon tests for SVOC concentrations in D_PS & S_PB, S_PW & S_PB, and W_PS & W_PB.

Table S9 Ratios of SVOC exposures between workers and students, and workshop and dormitory.

Table S10 Concentrations of SVOCs in the air (ng/m^3) calculated based on their concentrations in the PDMS and the sampling rates of PDMS (SR, $\text{ng}/\text{m}^3/\text{h}$).

Table S11 Non-cancer risks of SVOCs.

Table S12 Cancer risks of SVOCs.

Table S13 Comparison of SVOC concentrations in serum (C_{serum} , ng/L) from different studies.

Fig. S1 Correlations between mean concentrations of SVOC congeners in PDMS samples of university students and their $\log K_{\text{oa}}$ values.

Fig. S2 Correlations between mean concentrations of SVOC congener in PDMS samples of waste disposal workers and their $\log K_{\text{oa}}$ values.

Table S1 Sampling information.

Env. samples	Sampling sites	Individual samples	Type or place of activity	Gender
Solid waste disposal plant				
W_PS1	Sorting workshop	W_PB1	Sorting workshop	Male
W_PS2	Solid waste sifting workshop	W_PB2	Solid waste sifting workshop	Male
W_PS3	Waste chemical warehouse	W_PB3	Waste chemical warehouse	Male
W_PS4	Waste chemical warehouse	W_PB4	Waste chemical warehouse	Male
W_PS5	Solvent storage warehouse	W_PB5	Solvent storage warehouse	Male
W_PS6	Solvent storage warehouse	W_PB6	Solvent storage warehouse	Male
W_PS7	Fluid incinerator warehouse	W_PB7	Fluid incinerator warehouse	Male
W_PS8	Sewage treatment workshop	W_PB8	Sewage treatment workshop	Male
W_PS9	Sewage treatment workshop	W_PB9	Sewage treatment workshop	Male
W_PS10	Sewage treatment workshop	W_PB10	Sewage treatment workshop	Male
W_PS11	Central control room			
W_PS12	Central control room			
University campus				
D_PS1	Dormitory room	S_PW1/S_PB1	Biochemical experiment	Male
D_PS2	Dormitory room	S_PW2/S_PB2	Biochemical experiment	Male
D_PS3	Dormitory room	S_PW3/S_PB3	Biochemical experiment	Female
D_PS4	Dormitory room	S_PW4/S_PB4	Biochemical experiment	Female
D_PS5	Dormitory room	S_PW5/S_PB5	Library	Male
D_PS6	Dormitory room	S_PW6/S_PB6	Library	Male
D_PS7	Dormitory room	S_PW7/S_PB7	Library	Female
D_PS8	Dormitory room	S_PW8/S_PB8	Library	Female
D_PS9	Dormitory room	S_PW9/S_PB9	Physical experiment	Male
D_PS10	Dormitory room	S_PW10/S_PB10	Physical experiment	Male
D_PS11	Dormitory room	S_PW11/S_PB11	Physical experiment	Female
D_PS12	Dormitory room	S_PW12/S_PB12	Physical experiment	Female
		S_PW13/S_PB13	Welding experiment	Male
		S_PW14/S_PB14	Welding experiment	Male
		S_PW15/S_PB15	Welding experiment	Female
		S_PW16/S_PB16	Welding experiment	Female
		S_PW17/S_PB17	Vanishing mold casting	Male
		S_PW18/S_PB18	Vanishing mold casting	Male
		S_PW19/S_PB19	Vanishing mold casting	Female
		S_PW20/S_PB20	Vanishing mold casting	Female

Table S2 Full names, abbreviations, and properties of target SVOCs.

Name	Abbr.	Cas number	$\log K_{ow}^a$	$\log K_{oa}^b$	S_w^c	MW ^d
PAEs						
Dimethyl phthalate	DMP	131-11-3	1.61 ¹	7.01 ¹	5220 ¹	194.19 ²
Diethyl phthalate	DEP	84-66-2	2.54 ¹	7.55 ¹	591 ¹	222.24 ²
Di- <i>iso</i> -butyl phthalate	DIBP	84-69-5	4.27 ¹	8.54 ¹	9.9 ¹	278.35 ²
Di- <i>n</i> -butyl phthalate	DNBP	84-74-2	4.27 ¹	8.54 ¹	4.18 ¹	278.35 ²
Butyl benzyl phthalate	BzBP	85-68-7	4.70 ¹	8.78 ¹	3.8 ¹	312.37 ²
Bis(2-ethylhexyl) adipate	DEHA	103-23-1	7.62 ²	10.8 ²	0.78 ²	370.57 ²
Di(2-ethylhexyl) phthalate	DEHP	117-81-7	7.73 ¹	10.53 ¹	2.49×10 ⁻³ ¹	390.56 ²
Di- <i>n</i> -octyl phthalate	DNOP	117-84-0	7.73 ¹	10.53 ¹	2.49×10 ⁻³ ¹	390.56 ²
Di(2-ethylhexyl) terephthalate	DEHT	6422-86-2	8.43 ²	11.7 ²	3.98 ²	390.56 ²
OPEs						
Tri-isobutyl phosphate	TIBP	126-71-6	3.60 ³	7.38 ²	3.72 ³	266.31 ²
Tri- <i>n</i> -butyl phosphate	TNBP	126-73-8	4 ⁴	8.03 ⁵	280 ³	266.31 ²
Tris(2-chloroethyl) phosphate	TCEP	115-96-8	1.44 ⁴	8.38 ⁵	7.00×10 ³ ³	285.48 ²
Tris(2-chloro-isopropyl) phosphate	TCIPP	13674-84-5	2.59 ⁴	9.77 ⁵	1.60×10 ³ ³	327.56 ²
Tris(1,3-dichloro-2-propyl) phosphate	TDCIPP	13674-87-8	3.80 ³	10.6 ⁵	1.5 ³	430.89 ²
Tris(2-butoxyethyl) phosphate	TBOEP	78-51-3	3.65 ⁴	11.4 ⁵	1.20×10 ³ ³	398.48 ²
Triphenyl phosphate	TPHP	115-86-6	4.59 ⁴	10.8 ⁵	1.90 ³	326.29 ²
2-Ethylhexyl diphenyl phosphate	EHDPP	1241-94-7	5.37 ⁴	11.0 ⁵	1.90 ³	362.41 ²
Tris(2-ethylhexyl) phosphate	TEHP	78-42-2	9.43 ²	11.7 ²	1.59 ²	434.64 ²
Triphenylphosphine oxide	TPPO	791-28-6	2.87 ⁴	10.9 ⁵	62.8 ⁴	278.29 ²
Tricresyl phosphate	TMPP	1330-78-5	5.11 ⁴	11.9 ⁵	0.36 ³	368.40 ⁶
Tris(2,4-di-tert-butylphenyl) phosphate	TDTBPP	95906-11-9	10.5 ²	11.7 ²	3.5 ²	662.94 ²
PAHs						
Naphthalene	NAP	91-20-3	3.30 ²	5.19 ²	31.66 ²	128.17 ²
Acenaphthylene	ACY	208-96-8	3.94 ⁷	6.34 ⁷	16.44 ²	152.20 ²
Acenaphthene	ACE	83-32-9	4.15 ⁷	6.52 ⁷	7.16 ²	154.21 ²
Fluorene	FLU	86-73-7	4.18 ⁷	6.90 ⁷	1.91 ²	166.22 ²
Phenanthrene	PHE	85-01-8	4.57 ⁷	7.59 ⁷	1.13 ²	178.23 ²
Anthracene	ANT	120-12-7	4.45 ⁷	7.62 ⁷	6.02×10 ⁻² ²	178.23 ²
Fluoranthene	FLA	206-44-0	5.22 ⁷	8.67 ⁷	0.25 ²	202.26 ²
Pyrene	PYR	129-00-0	4.88 ²	8.80 ²	0.13 ²	202.26 ²
Benz[a]anthracene	BaA	56-55-3	5.79 ⁷	10.20 ⁷	1.19×10 ⁻² ²	228.29 ²
Chrysene	CHR	218-01-9	5.73 ⁷	10.22 ⁷	2.78×10 ⁻³ ²	228.29 ²
Benzo[b]fluoranthene	BbF	205-99-2	6.11 ⁷	11.26 ⁷	2.37×10 ⁻³ ²	252.32 ²
Benzo[k]fluoranthene	BkF	207-08-9	6.11 ⁷	11.29 ⁷	8.07×10 ⁻⁴ ²	252.32 ²
Benzo[a]pyrene	BaP	50-32-8	6.13 ⁷	11.48 ⁷	2.12×10 ⁻³ ²	252.32 ²
Indeno[123-cd]pyrene	IND	193-39-5	6.72 ⁷	12.36 ⁷	1.91×10 ⁻⁴ ²	276.34 ²
Dibenz[ah]anthracene	DiB	53-70-3	6.50 ⁷	12.52 ⁷	1.20×10 ⁻³ ²	278.35 ²
Benzo[ghi]perylene	BghiP	191-24-2	6.90 ⁷	12.48 ⁷	2.60×10 ⁻⁴ ²	276.34 ²

^a octanol-water partition coefficient at 25°C.

^b octanol-air partition coefficient at 25°C.

^c solubility (mg/L) in water at 25°C.

^d MW=molecular weight.

Table S3 Parameters for the GC-MS analysis.

Chemicals	Retention time (min)	Quantifier ion (m/z)	Reference ion (m/z)
PAEs			
DMP	9.91	163	164/194
DEP	11.3	149	177
DIBP	13.8	149	223
DNBP	14.6	149	205/223
BzBP	17.6	149	206
DEHA	17.8	129	259
DEHP	18.8	279	149/167
DNOP	20.0	149	279/261
DEHT	20.1	261	149/167
OPEs			
TIBP	10.5	211	155
TNBP	11.8	211	155
TCEP	12.9	249	205/251
TCIPP	13.2	277	157/279
TDCIPP	17.4	381	209/321
TBOEP	17.9	299	226
TPHP	18.0	326	325
EHDPP	18.1	362	251/249
TEHP	18.2	323	221
TPPO	18.9	277	278/199
TMPP	20.0	368	367/165
PAHs			
NAP	7.00	128	129
ACY	10.1	152	153
ACE	10.4	153	154
FLU	11.5	166	165
PHE	13.4	178	179
ANT	13.5	178	179
FLA	15.8	202	203
PYR	16.2	202	203
BaA	18.6	228	226
CHR	18.7	228	226
BbF	20.6	252	253
BkF	20.70	252	253
BaP	21.2	252	253
IND	23.2	276	277
DiB	23.2	278	279
BghiP	23.6	276	277

Table S4 Blank levels and MDLs of SVOCs for the PDMS samplers.

Name	PDMS Blanks (ng/cm ²)		MDLs for PDMS samplers (ng/cm ²)
	Mean	Std	
PAEs	DMP	1.72E-03	6.44E-03
	DEP	4.85E-05	9.61E-05
	DIBP	2.52E-03	8.62E-03
	DNBP	7.08E-03	1.39E-02
	BzBP	3.61E-04	7.70E-04
	DEHA	7.77E-04	2.97E-03
	DEHP	4.94E-02	1.52E-01
	DNOP	6.86E-05	7.41E-05
	DEHT	2.92E-02	1.10E-01
OPEs	TIBP	2.27E-03	4.98E-03
	TNBP	1.20E-03	2.36E-03
	TCEP	5.76E-04	1.29E-03
	TCIPP	3.18E-03	4.12E-03
	TDCIPP	4.79E-04	1.87E-03
	TBOEP	2.14E-03	5.37E-03
	TPHP	3.78E-04	4.28E-04
	EHDPP	2.92E-03	6.60E-03
	TEHP	3.41E-03	1.44E-02
	TPPO	6.20E-04	6.90E-04
	TMPP	5.22E-04	1.79E-03
	TDTBPP	4.83E-03	5.79E-03
PAHs	NAP	1.71E-04	7.63E-04
	ACY	1.57E-05	5.19E-05
	ACE	3.41E-05	1.12E-04
	FLU	3.10E-05	6.41E-05
	PHE	1.01E-04	3.73E-04
	ANT	1.18E-05	2.82E-05
	FLA	9.17E-06	3.16E-05
	PYR	9.90E-06	3.29E-05
	BaA	3.73E-06	8.21E-06
	CHR	2.79E-06	1.01E-05
	BbF	5.37E-06	1.19E-05
	BkF	3.35E-06	4.64E-06
	BaP	5.66E-06	7.82E-06
	IND	3.48E-06	7.66E-06
	DiB	5.26E-06	7.24E-06
	BghiP	6.25E-06	1.38E-05

Table S5 Surrogate recoveries for the PDMS samples.

	PDMS brooch or sheet				PDMS wristband			
	Min	Max	Mean	Std	Min	Max	Mean	Std
DMP- d_4	70.3%	97.6%	83.1%	8.40%	70.6%	105%	85.0%	7.64%
DEP- d_4	71.9%	98.5%	85.5%	7.53%	73.2%	98.5%	86.7%	7.88%
DNBP- d_4	70.6%	108%	88.7%	8.62%	70.6%	105%	88.2%	8.97%
DEHP- d_4	70.9%	108%	90.1%	9.35%	70.9%	108%	88.5%	9.90%
TCEP- d_{12}	72.9%	106%	89.3%	9.26%	73.7%	106%	88.9%	10.2%
TPHP- d_{15}	72.5%	107%	92.0%	8.67%	72.5%	109%	92.8%	9.48%
NAP- d_8	72.4%	106%	81.9%	8.11%	74.0%	104%	83.8%	8.41%
ACE- d_{10}	71.7%	104%	86.3%	8.84%	71.5%	105%	86.6%	9.31%
PHE- d_{10}	71.3%	105%	86.6%	8.42%	71.0%	101%	85.0%	8.39%
CHR- d_{12}	70.6%	107%	91.6%	7.81%	77.6%	106%	91.2%	8.46%

Table S6 Parameters for the calculation of non-cancer and cancer risks to SVOCs.

Non-cancer risk				
	Workshop	Student dormitory	Worker	Student
Average age (year)	50.0	20.0	50.0	20.0
IR^8 (m ³ /d)	16	16.3	16	16.3
EF^9 (day/year)	83.3	75	83.3	75
ED^9 (year)	25	4	25	4
AT^9 (day)	9125	1460	9125	1460
BW^8 (kg)	89.5	Male: 77.3 Female: 65.9	89.5	Male: 77.3 Female: 65.9
Cancer risk				
	Workshop	Student dormitory	Worker	Student
Age (year)	50.0	20.0	50.0	20.0
IR^8 (m ³ /d)	16	16.3	16	16.3
EF^9 (day/year)	83.3	75	83.3	75
ED^9 (year)	25	4	25	4
AT^9 (day)	25550	25550	25550	25550
BW^8 (kg)	89.5	Male: 77.3 Female: 65.9	89.5	Male: 77.3 Female: 65.9

Table S7 Ratios of SVOC concentrations between D_PS and S_PB, and S_PW and S_PB.

times	PB/PS	PW/PB
DMP	0.73	1.67
DEP	1.06	3.99
DIBP	0.76	3.49
DNBP	0.65	4.32
BzBP	0.65	1.11
DEHA	0.90	13.84
DEHP	1.22	9.77
DNOP	0.80	12.41
DEHT	2.35	10.76
TIBP	0.63	1.69
TNBP	1.09	5.85
TCEP	0.69	2.42
TCIPP	1.02	3.53
TDCIPP	1.28	0.70
TBOEP	1.07	1.35
TPHP	0.71	9.55
EHDPP	0.56	2.96
TEHP	0.72	1.04
TPPO	0.03	1.50
TMPP	0.88	0.90
TDTBPP	0.73	0.73
NAP	0.74	1.14
ACY	0.50	2.15
ACE	0.74	2.05
FLU	0.62	1.81
PHE	0.67	2.09
ANT	0.64	1.85
FLA	0.81	2.82
PYR	0.70	3.00
BaA	0.51	1.40
CHR	0.97	1.53
BbF	0.99	3.36
BkF	1.49	2.87
BaP	0.82	2.14
IND	1.29	1.05
DiB	1.65	3.35
BghiP	0.94	1.39

Table S8 Non-parametric Wilcoxon tests for SVOC concentrations in D_PS & S_PB, S_PW & S_PB, and W_PS & W_PB.

<i>p</i> value	D_PS & S_PB	S_PW & S_PB	W_PS & W_PB
DMP	0.875	0.001	0.037
DEP	0.754	0.0001	0.028
DIBP	0.875	0.0001	0.386
DNBP	0.638	0.0001	0.093
BzBP	0.937	0.332	0.074
DEHA	0.182	0.0001	0.959
DEHP	0.272	0.0001	0.721
DNOP	0.530	0.0001	0.646
DEHT	0.480	0.0001	0.799
TIBP	0.695	0.015	0.959
TNBP	0.530	0.0001	0.022
TCEP	0.875	0.079	0.508
TCIPP	0.071	0.017	0.959
TDCIPP	0.117	0.296	0.959
TBOEP	0.814	0.550	0.646
TPHP	0.695	0.0001	0.203
EHDPP	0.583	0.012	0.114
TEHP	0.814	0.204	0.285
TPPO	0.530	0.025	0.445
TMPP	0.937	0.737	0.445
TDTBPP	0.695	0.008	0.646
NAP	0.937	0.852	0.169
ACY	0.003	0.0002	0.203
ACE	0.347	0.001	0.022
FLU	0.638	0.0001	0.013
PHE	0.937	0.0004	0.028
ANT	0.347	0.001	0.022
FLA	0.209	0.002	0.285
PYR	0.347	0.0001	0.285
BaA	0.239	0.502	0.646
CHR	0.530	0.145	0.508
BbF	0.084	0.0004	0.959
BkF	0.023	0.003	0.721
BaP	0.117	0.014	0.575
IND	0.008	0.232	0.445
DiB	0.050	0.0001	0.959
BghiP	0.084	0.086	0.241
PAEs	0.347	0.0001	0.285
OPEs	0.638	0.025	0.878
PAHs	0.937	0.001	0.047

p < 0.05: Significant difference at 0.05 level.

Table S9 Ratios of SVOC exposures between workers and students, and workshop and dormitory.

(times)	Workshop/dormitory	Worker/student
DMP	14.9	6.12
DEP	355	129
DIBP	2.33	1.21
DNBP	4.40	4.11
BzBP	0.074	0.192
DEHA	0.589	0.755
DEHP	2.04	2.21
DNOP	5.46	6.60
DEHT	1.05	1.84
TIBP	19.0	35.8
TNBP	12.2	8.90
TCEP	0.523	0.589
TCIPP	3.00	2.15
TDCIPP	103	80.0
TBOEP	0.589	0.704
TPHP	1.80	5.41
EHDPP	0.159	0.881
TEHP	4.92	4.84
TPPO	0.166	26.4
TMPP	26.7	36.6
TDTBPP	0.017	0.026
NAP	5.43	6.77
ACY	9.26	13.1
ACE	16.9	16.9
FLU	14.9	13.9
PHE	30.0	23.9
ANT	29.5	24.7
FLA	65.5	58.5
PYR	52.5	51.3
BaA	27.9	38.0
CHR	162	116
BbF	57.5	34.5
BkF	187	114
BaP	12.7	12.4
IND	36.5	16.6
DiB	6.48	2.37
BghiP	66.2	31.7

Table S10 Concentrations of SVOCs in the air (ng/m³) calculated based on their concentrations in the PDMS and the sampling rates of PDMS (R , m³/h/cm²).

	R	W_PB		W_PS		S_PB		D_PS	
		Mean	Std	Mean	Std	Mean	Std	Mean	Std
DMP	3.28E-05	23900	17500	79900	137000	3910	3340	5350	2340
DEP	4.02E-04	687	517	1780	1260	5.32	4.15	4.99	3.13
DIBP	1.89E-04	597	5270	15200	27000	4950	3410	6530	3050
DNBP	4.93E-04	7560	7350	12400	11300	1840	2070	2830	1500
BzBP	8.35E-05	606	378	363	226	3160	3440	4880	2930
DEHA	2.98E-05	3960	1820	3440	1952	5250	7000	5840	3030
DEHP	1.26E-04	40400	29700	30600	16500	18300	33400	15000	9480
DNOP	6.00E-05	282	342	293	490	42.7	58.7	53.7	49.7
DEHT	7.84E-05	37500	61500	9120	7840	20400	52900	8680	5690
TIBP	3.43E-04	858	521	723	737	24.0	21.2	38.0	23.5
TNBP	1.92E-04	351	444	441	425	39.4	59.4	36.2	45.2
TCEP	5.51E-04	49.8	23.6	64.4	25.2	84.5	158	123	161
TCIPP	1.56E-03	50.1	44.4	68.8	67.3	23.4	23.4	22.9	14.0
TDCIPP	7.63E-05	3090	559	3110	783	38.6	38.3	30.1	17.1
TBOEP	8.62E-05	552	479	433	331	784	1280	736	738
TPHP	1.17E-04	287	288	134	146	53.0	111	74.6	145
EHDPP	4.07E-05	701	903	228	113	795	1460	1430	1610
TEHP	4.51E-05	2300	2190	3250	4870	475	513	661	476
TPPO	4.96E-05	4620	10800	914	1470	175	331	5510	12500
TMPP	1.07E-04	3390	5040	2820	5800	92.6	121	106	75.0
TDTBPP	8.66E-05	2260	1330	1990	1320	85400	90100	117000	103000
NAP	2.20E-05	2010	1940	2180	2280	296	309	402	191
ACY	2.41E-04	9.62	8.50	13.5	10.0	0.734	0.658	1.46	0.656
ACE	8.90E-05	102	105	137	105	6.02	9.85	8.10	4.84
FLU	5.38E-05	382	318	662	440	27.5	28.4	44.4	21.2
PHE	1.72E-04	356	174	665	483	14.9	14.2	22.2	11.0
ANT	5.85E-05	103	53.3	191	152	4.18	3.66	6.49	3.99
FLA	5.80E-04	27.5	22.5	38.0	41.3	0.471	0.458	0.581	0.286
PYR	3.92E-04	26.0	19.5	38.0	44.7	0.507	0.484	0.725	0.395
BaA	1.91E-05	91.0	105	132	265	2.40	2.46	4.72	2.97
CHR	4.95E-05	84.1	98.3	122	247	0.727	0.986	0.753	0.462
BbF	4.33E-05	49.7	74.4	83.8	191	1.44	2.08	1.46	0.722
BkF	1.74E-04	21.5	6.63	23.8	18.1	0.189	0.340	0.127	0.075
BaP	1.60E-06	535	756	665	1480	43.0	48.1	52.4	38.6
IND	1.26E-05	41.6	72.2	71.1	181	2.51	3.86	1.95	1.80
DiB	2.68E-05	6.04	10.0	10.0	23.0	2.55	5.62	1.54	2.05
BghiP	3.24E-06	209	386	462	1190	6.58	6.56	6.97	3.91

Table S11 Non-cancer risks of SVOCs.

	ADD (Non-carcinogenic, ng/kg/day)								RfD _o	HQ									
	Workshop		Dormitory		Worker		Student			Workshop		Dormitory		Worker		Student		Student	
	(daytime)		(nighttime)		(daytime)		(daytime)			(daytime)		(nighttime)		(daytime)		(daytime)		(total) ^a	
	50th	90th	50th	90th	50th	90th	50th	90th		50th	90th	50th	90th	50th	90th	50th	90th	50th	90th
DMP	829	12765	215	400	803	1997	131	348											
DEP	51.5	122	0.195	0.429	18.4	41.9	0.192	0.529	8.00E+05 ¹⁰	6.44E-05	1.52E-04	2.44E-07	5.37E-07	2.30E-05	5.24E-05	2.40E-07	6.61E-07	4.85E-07	1.20E-06
DIBP	256	868	323	472	164	342	208	452	1.00E+05 ¹¹	2.56E-03	8.68E-03	3.23E-03	4.72E-03	1.64E-03	3.42E-03	2.08E-03	4.52E-03	5.31E-03	9.24E-03
DNBP	301	1197	143	233	195	625	41.4	200	1.00E+05 ¹⁰	3.01E-03	1.20E-02	1.43E-03	2.33E-03	1.95E-03	6.25E-03	4.14E-04	2.00E-03	1.85E-03	4.32E-03
BzBP	13.4	20.1	270	432	19.5	44.5	72.0	356	2.00E+05 ¹⁰	6.70E-05	1.01E-04	1.35E-03	2.16E-03	9.75E-05	2.23E-04	3.60E-04	1.78E-03	1.71E-03	3.94E-03
DEHA	138	232	314	415	143	263	147	433	6.00E+05 ¹⁰	2.31E-04	3.87E-04	5.24E-04	6.91E-04	2.39E-04	4.38E-04	2.45E-04	7.22E-04	7.69E-04	1.41E-03
DEHP	1359	1996	706	1007	1322	2828	455	1222	2.00E+04 ¹⁰	6.80E-02	9.98E-02	3.53E-02	5.04E-02	6.61E-02	1.41E-01	2.28E-02	6.11E-02	5.81E-02	1.11E-01
DNOP	2.90	41.7	2.46	3.99	6.04	34.1	0.536	5.67											
DEHT	203	900	381	639	521	4946	230	1269											
TIBP	22.3	49.2	1.96	3.25	31.7	58.9	0.820	2.87											
TNBP	12.6	46.6	1.06	1.81	7.59	43.6	0.974	2.78	1.00E+04 ¹²	1.26E-03	4.66E-03	1.06E-04	1.81E-04	7.59E-04	4.36E-03	9.74E-05	2.78E-04	2.03E-04	4.59E-04
TCEP	2.71	3.82	2.15	14.2	1.68	3.53	2.05	7.84	7.00E+03 ¹²	3.88E-04	5.45E-04	3.07E-04	2.02E-03	2.41E-04	5.05E-04	2.93E-04	1.12E-03	5.99E-04	3.14E-03
TCIPP	1.52	6.61	0.989	1.94	1.44	4.23	0.809	2.81	1.00E+04 ¹²	1.52E-04	6.61E-04	9.89E-05	1.94E-04	1.44E-04	4.23E-04	8.09E-05	2.81E-04	1.80E-04	4.75E-04
TDCIPP	116	154	1.36	2.32	120	151	0.961	4.63	2.00E+04 ¹²	5.81E-03	7.71E-03	6.79E-05	1.16E-04	5.98E-03	7.55E-03	4.80E-05	2.31E-04	1.16E-04	3.47E-04
TBOEP	11.8	38.9	16.7	80.5	18.7	37.0	12.5	89.2	1.50E+04 ¹²	7.85E-04	2.59E-03	1.12E-03	5.36E-03	1.25E-03	2.46E-03	8.32E-04	5.95E-03	1.95E-03	1.13E-02
TPHP	2.92	14.0	1.72	3.33	6.28	29.7	0.637	4.50	7.00E+04 ¹²	4.17E-05	2.00E-04	2.45E-05	4.76E-05	8.97E-05	4.24E-04	9.09E-06	6.43E-05	3.36E-05	1.12E-04
EHDPP	9.07	14.8	32.3	146	8.82	92.4	14.6	68.6											
TEHP	57.8	419	28.6	58.2	52.2	245	8.43	63.9	1.00E+05 ¹²	5.78E-04	4.19E-03	2.86E-04	5.82E-04	5.22E-04	2.45E-03	8.43E-05	6.39E-04	3.70E-04	1.22E-03
TPPO	11.7	125	11.9	1302	28.6	308	3.42	12.8											
TMPP	16.5	435	4.37	7.31	23.9	474	1.79	13.2											

TDTBPP	66.7	178	3962	12989	78.9	155	2654	9159											
NAP	54.9	166	17.7	30.6	43.1	174	8.12	43.5	2.00E+04 ¹⁰	2.74E-03	8.32E-03	8.86E-04	1.53E-03	2.15E-03	8.69E-03	4.06E-04	2.18E-03	1.29E-03	3.71E-03
ACY	0.508	0.849	0.076	0.100	0.225	0.810	0.021	0.081											
ACE	4.42	10.0	0.368	0.668	2.33	9.96	0.114	0.454	6.00E+04 ¹⁰	7.37E-05	1.67E-04	6.13E-06	1.11E-05	3.88E-05	1.66E-04	1.90E-06	7.57E-06	8.03E-06	1.87E-05
FLU	22.8	46.0	2.41	3.04	10.4	35.1	0.630	2.79	4.00E+04 ¹⁰	5.71E-04	1.15E-03	6.03E-05	7.61E-05	2.60E-04	8.78E-04	1.58E-05	6.98E-05	7.60E-05	1.46E-04
PHE	17.9	56.9	1.13	1.61	15.8	21.5	0.387	1.54	3.00E+05 ¹⁰	5.97E-05	1.90E-04	3.75E-06	5.35E-06	5.27E-05	7.17E-05	1.29E-06	5.14E-06	5.04E-06	1.05E-05
ANT	5.50	12.8	0.300	0.447	4.69	6.57	0.177	0.405	4.00E+04 ¹⁰	1.38E-04	3.19E-04	7.50E-06	1.12E-05	1.17E-04	1.64E-04	4.43E-06	1.01E-05	1.19E-05	2.13E-05
FLA	1.20	2.50	0.029	0.040	0.994	2.16	0.014	0.051	3.00E+04 ¹⁰	4.02E-05	8.32E-05	9.61E-07	1.33E-06	3.31E-05	7.21E-05	4.61E-07	1.71E-06	1.42E-06	3.03E-06
PYR	1.07	2.33	0.036	0.056	0.968	2.14	0.016	0.058											
BaA	0.855	10.1	0.262	0.383	2.38	11.2	0.045	0.287											
CHR	0.896	10.1	0.037	0.055	2.27	10.4	0.017	0.070											
BbF	0.070	6.66	0.076	0.100	0.899	7.18	0.017	0.158											
BkF	0.809	1.33	0.006	0.010	0.793	1.15	0.004	0.018											
BaP	0.695	61.2	2.42	4.24	8.92	72.1	0.774	4.64	3.00E+02 ¹⁰	2.32E-03	2.04E-01	8.06E-03	1.41E-02	2.97E-02	2.40E-01	2.58E-03	1.55E-02	1.06E-02	2.96E-02
IND	0.056	8.43	0.071	0.185	0.183	7.12	0.035	0.267											
DiB	0.032	1.26	0.031	0.230	0.064	0.863	0.037	0.150											
BghiP	0.378	51.3	0.276	0.591	0.532	37.3	0.208	0.829											

^a calculated as the sum of the *HQ* from dormitory residence and daytime exposure for students.

HQ values > 0.1 were bolded for emphasis.

All *HQ* values were below 1.

Table S12 Cancer risks of SVOCs.

	<i>LADD</i> (Carcinogenic)								<i>OSF</i> ^{<i>a</i>}	<i>LCR</i>									
	Workshop		Dormitory		Worker		Student			Workshop		Dormitory		Worker		Student		Student	
	(daytime)	(nighttime)	(daytime)	(nighttime)	(daytime)	(nighttime)	(daytime)	(nighttime)		(daytime)	(nighttime)	(daytime)	(nighttime)	(daytime)	(nighttime)	(daytime)	(nighttime)	(total) ^{<i>b</i>}	(total) ^{<i>b</i>}
	50th	90th	50th	90th	50th	90th	50th	90th		50th	90th	50th	90th	50th	90th	50th	90th	50th	90th
DMP	296	4560	11.3	22.9	287	713	6.66	19.9											
DEP	18.4	43.5	0.010	0.025	6.58	15.0	0.009	0.030											
DIBP	91.5	310	16.1	27.0	58.7	122	11.9	25.9											
DNBP	108	427	7.61	13.3	69.7	223	2.37	11.4	1.90E-09	8.12E-07	2.53E-08	4.24E-07	2.17E-08	4.69E-08	1.90E-09	8.12E-07	2.53E-08	4.24E-07	2.17E-08
BzBP	4.78	7.18	13.8	24.7	6.96	15.9	3.51	20.4	1.20E-09	8.62E-09	2.96E-08	1.91E-08	2.44E-08	5.40E-08	1.20E-09	8.62E-09	2.96E-08	1.91E-08	2.44E-08
DEHA	49.4	82.9	15.3	23.7	51.2	93.8	7.51	24.7											
DEHP	485	713	39.1	57.6	472	1010	26.0	69.8	1.40E-08	6.80E-06	9.98E-06	5.47E-07	8.06E-07	6.61E-06	1.41E-05	3.64E-07	9.78E-07	9.12E-07	1.78E-06
DNOP	1.04	14.9	0.135	0.228	2.16	12.2	0.028	0.324											
DEHT	72.5	321	20.0	36.5	186	1767	13.1	72.5											
TIBP	7.95	17.6	0.095	0.185	11.3	21.0	0.043	0.164											
TNBP	4.50	16.7	0.060	0.104	2.71	15.6	0.051	0.159	9.00E-09	4.05E-08	1.50E-07	5.44E-10	9.32E-10	2.44E-08	1.40E-07	4.62E-10	1.43E-09	1.01E-09	2.36E-09
TCEP	0.969	1.36	0.120	0.809	0.601	1.26	0.100	0.448	2.00E-08	1.94E-08	2.73E-08	2.40E-09	1.62E-08	1.20E-08	2.52E-08	2.00E-09	8.95E-09	4.39E-09	2.51E-08
TCIPP	0.544	2.36	0.057	0.111	0.515	1.51	0.044	0.161											
TDCIPP	41.5	55.1	0.072	0.132	42.7	53.9	0.049	0.264											
TBOEP	4.20	13.9	0.872	4.60	6.70	13.2	0.653	5.10											
TPHP	1.04	4.99	0.090	0.191	2.24	10.6	0.031	0.257											
EHDPP	3.24	5.29	1.66	8.34	3.15	33.0	0.709	3.92											
TEHP	20.6	150	1.53	3.33	18.6	87.5	0.411	3.65	3.20E-09	6.60E-08	4.79E-07	4.89E-09	1.07E-08	5.97E-08	2.80E-07	1.31E-09	1.17E-08	6.20E-09	2.23E-08
TPPO	4.17	44.7	0.63	74.4	10.2	110	0.176	0.734											
TMPP	5.90	155	0.22	0.42	8.54	169	0.096	0.755											

TDTBPP	23.8	63.7	193	742	28.2	55.5	132	523											
NAP	19.6	59.4	0.92	1.75	15.4	62.0	0.464	2.49	1.20E-07	2.35E-06	7.13E-06	1.11E-07	2.10E-07	1.85E-06	7.44E-06	5.57E-08	2.98E-07	1.66E-07	5.08E-07
ACY	0.18	0.30	0.004	0.006	0.080	0.29	0.001	0.005											
ACE	1.58	3.59	0.018	0.038	0.83	3.56	0.007	0.026											
FLU	8.16	16.4	0.12	0.17	3.71	12.5	0.036	0.160											
PHE	6.40	20.3	0.059	0.092	5.65	7.68	0.022	0.088											
ANT	1.97	4.56	0.016	0.026	1.67	2.34	0.010	0.023											
FLA	0.43	0.89	0.002	0.002	0.35	0.77	0.001	0.003											
PYR	0.38	0.83	0.002	0.003	0.35	0.76	0.001	0.003											
BaA	0.31	3.59	0.014	0.022	0.85	3.99	0.002	0.016	1.00E-07	3.05E-08	3.59E-07	1.41E-09	2.19E-09	8.50E-08	3.99E-07	2.28E-10	1.64E-09	1.64E-09	3.83E-09
CHR	0.32	3.60	0.002	0.003	0.81	3.72	0.001	0.004	1.00E-09	3.20E-10	3.60E-09	1.86E-12	3.15E-12	8.09E-10	3.72E-09	9.42E-13	4.00E-12	2.80E-12	7.15E-12
BbF	0.025	2.38	0.004	0.006	0.32	2.56	0.001	0.009	1.00E-07	2.50E-09	2.38E-07	4.02E-10	5.73E-10	3.21E-08	2.56E-07	8.51E-11	9.05E-10	4.88E-10	1.48E-09
BkF	0.29	0.48	0.000	0.001	0.28	0.41	0.000	0.001	1.00E-08	2.89E-09	4.76E-09	3.29E-12	5.61E-12	2.83E-09	4.10E-09	1.86E-12	1.01E-11	5.15E-12	1.57E-11
BaP	0.25	21.9	0.12	0.24	3.19	25.8	0.040	0.265	1.00E-06	2.48E-07	2.19E-05	1.18E-07	2.43E-07	3.19E-06	2.58E-05	3.97E-08	2.65E-07	1.57E-07	5.08E-07
IND	0.020	3.01	0.004	0.011	0.065	2.54	0.002	0.015	1.00E-07	2.00E-09	3.01E-07	3.78E-10	1.06E-09	6.54E-09	2.54E-07	1.73E-10	1.52E-09	5.50E-10	2.58E-09
DiB	0.011	0.45	0.002	0.013	0.023	0.31	0.002	0.009	1.00E-06	1.15E-08	4.51E-07	1.51E-09	1.31E-08	2.28E-08	3.08E-07	2.00E-09	8.59E-09	3.51E-09	2.17E-08
BghiP	0.13	18.3	0.015	0.034	0.19	13.3	0.011	0.047											

^a (ng/kg/day)⁻¹. ¹³

^b calculated as the sum of *LCR* from dormitory residence and daytime exposure for students.

The pink highlighting indicates an unacceptable cancer risk.

Table S13 Comparison of SVOC concentrations in serum (C_{serum} , ng/L) from different studies.

Information of volunteers	This study (Median)			10 university students (6 males and 4 females) in Dalian, China ^a	207 precocious puberty females in China in 2011 ¹⁴	90 healthy puberty females in Korea in 2009 ¹⁵	60 policemen in Chongqing, China in 2013 ¹⁶
	Worker	Student		Median	Mean	Mean	Median
	Male	Male	Female				
DMP	91600	91600	35957	63900			108000
DEP	7200	5400	5408	11200			3460
DIBP	47500	47500	7478	53600	2400		79400
DNBP	71400	71400	10363	51400	2200	29000	168000
BzBP	43300	43300	8166	35900			17700
DEHA	12700	12700	3038	24700			
DEHP	66900	66800	14057	37200	32900	143820	177000
DNOP	56700	52800	7667	17300			21400
DEHT	32000	32000	6117	5280			
Information of volunteers	This study			10 university students (6 males and 4 females) in Dalian, China ^a	36 pregnant females in Mianyang, China in 2019 ¹⁷	319 females of childbearing ages from Tianjin, China from 2019 to 2020 ¹⁸	96 healthy adults from Anji, China in 2018 ¹⁹
	Worker	Student		Median	Median	Geometric means	Median
	Male	Male	Female				
TIBP	2810	2810	633	706		50.0	
TNBP	2590	2650	563	908	1100	120	869
TCEP	1920	1920	362	881	250	47.0	868
TCIPP	1260	1260	257		740	3190	494
TDCIPP	1200	1280	268	489	250	33.0	
TBOEP	2140	2140	336	1520		1440	280
TPHP	125	106	161	1470	1700		1826
EHDPP	848	848	327				

TEHP	1220	1220	302	667	470		
TPPO	70.9	70.9	76.0	924			
TMPP	135	135	205	2720			
TDTBPP	1390	1390	340	1470			
Information of volunteers	This study			10 university students (6 males and 4 females) in Dalian, China ^a	114 people in the industrial complex area in Korea in 2010 ²⁰	98 pregnant females in Shengsi Islands, China from 2011 to 2012 ²¹	240 males and 240 females in Guangzhou, China in 2019 ²²
	Worker	Student		Median	Mean	Mean	Mean
	Male	Male	Female				
NAP	2130	2130	1890		3210	151	80
ACY	0.850	0.602	1.17	1.60		1.20	470
ACE	7.28	0.665	2.14	4.29		4.80	60
FLU	46.0	30.4	90.8	31.2	60.0	8.82	100
PHE	13.9	2.96	22.6	31.1	100	25.5	490
ANT	102	83.6	33.1	45.2	20.0	24.9	60
FLA	81.1	46.6	101	36.2	120	50.0	250
PYR	61.5	38.8	83.9	29.7	100	350	2020
BaA	16.4	7.98	18.8	33.0	20.0	21.9	30
CHR	15.3	10.8	17.5	16.5	20.0	30.2	10
BbF	9.58	0.779	1.00	1.03		27.6	
BkF	7.86	0.477	0.722	1.04		9.46	
BaP	9.17	5.80	10.7	9.6		54.5	1360
IND	1.23	0.914	1.27	1.07		29.1	550
DiB	1.16	1.17	1.73	1.70		16.8	470
BghiP	5.31	0.895	1.34	4.41		97.1	980

^a Data was predicted by the same machine learning method. ²³

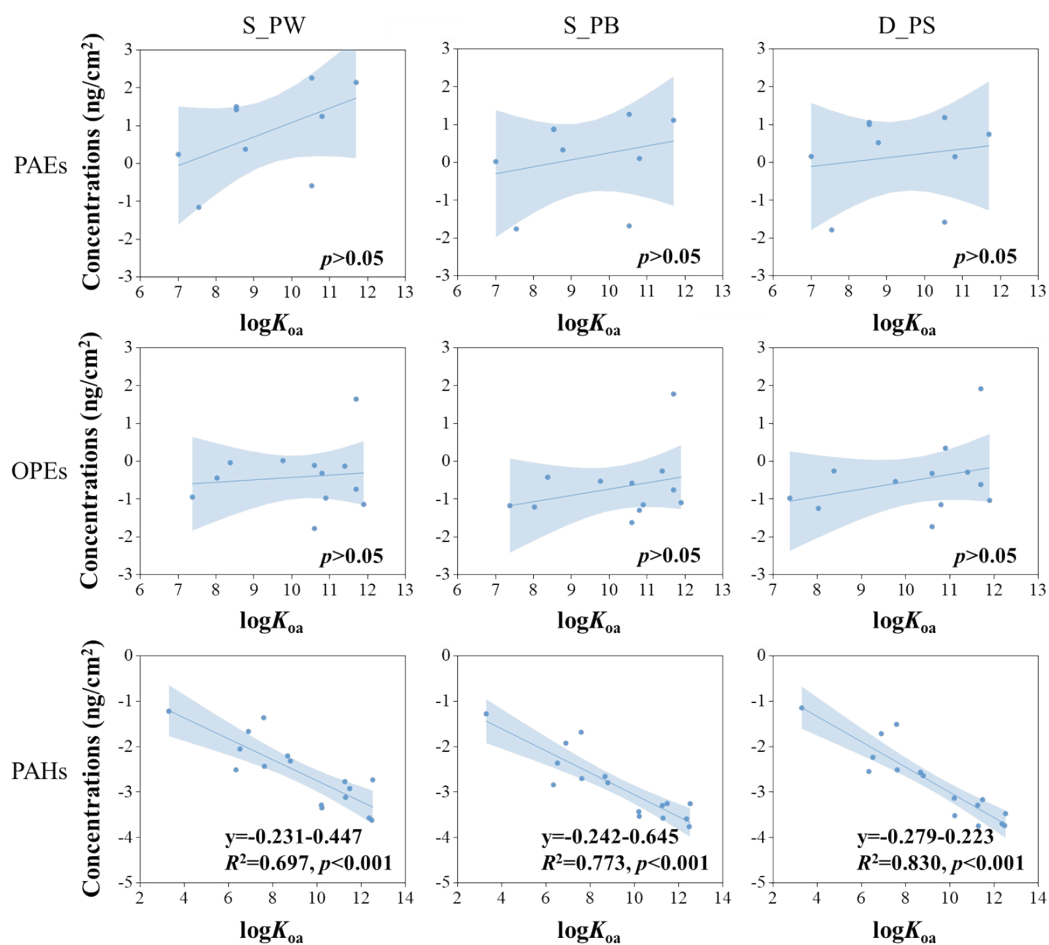


Fig. S1 Correlations between mean concentrations of SVOC congeners in PDMS samples of university students and their $\log K_{oa}$ values. (The shaded area represents the 95% confidence interval.)

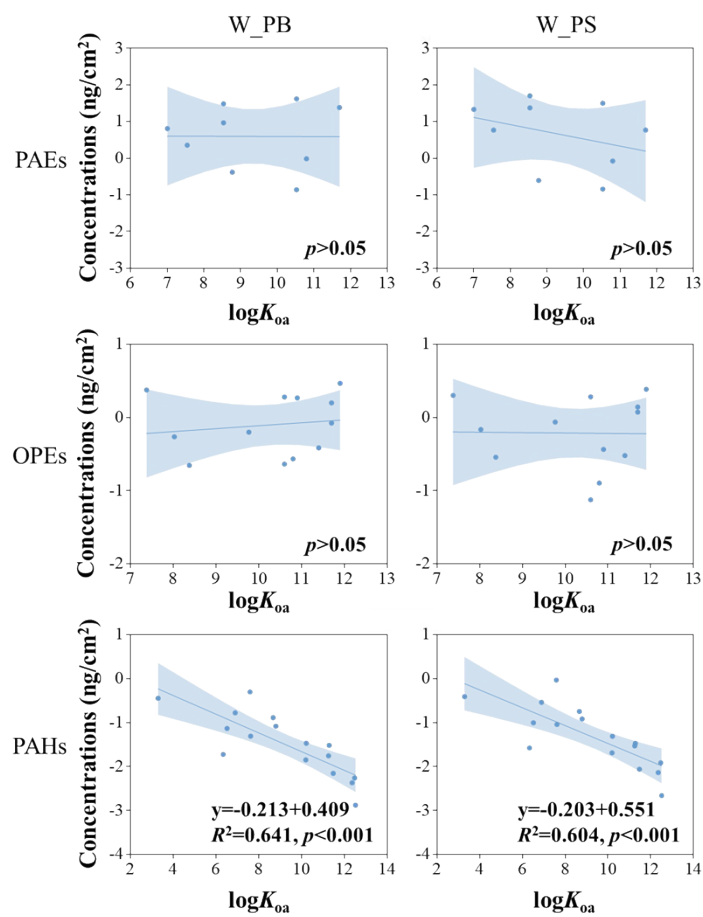


Fig. S2 Correlations between mean concentrations of SVOC congener in PDMS samples of waste disposal workers and their $\log K_{oa}$ values. (The shaded area represents the 95% confidence interval.)

References

1. S. Net, R. Sempéré, A. Delmont, A. Paluselli and B. Ouddane, Occurrence, fate, behavior and ecotoxicological state of phthalates in different environmental matrices, *Environ. Sci. Technol.*, 2015, **49**, 4019-4035.
2. USEPA, CompTox Chemicals Dashboard. <https://comptox.epa.gov/dashboard/>, 2023.
3. G.-L. Wei, D.-Q. Li, M.-N. Zhuo, Y.-S. Liao, Z.-Y. Xie, T.-L. Guo, J.-J. Li, S.-Y. Zhang and Z.-Q. Liang, Organophosphorus flame retardants and plasticizers: Sources, occurrence, toxicity and human exposure, *Environ. Pollut.*, 2015, **196**, 29-46.
4. I. Van der Veen and J. de Boer, Phosphorus flame retardants: Properties, production, environmental occurrence, toxicity and analysis, *Chemosphere*, 2012, **88**, 1119-1153.
5. Q. Wang, H. Zhao, Y. Wang, Q. Xie, J. Chen and X. Quan, Determination and prediction of octanol-air partition coefficients for organophosphate flame retardants, *Ecotox. Environ. Safe.*, 2017, **145**, 283-288.
6. NLM, National Library of Medicine. <https://pubchem.ncbi.nlm.nih.gov/>, 2023.
7. M. Odabasi, E. Cetin and A. Sofuoglu, Determination of octanol-air partition coefficients and supercooled liquid vapor pressures of PAHs as a function of temperature: Application to gas-particle partitioning in an urban atmosphere, *Atmos. Environ.*, 2006, **40**, 6615-6625.
8. USEPA, Exposure Factors Handbook (2011 edition). <https://www.epa.gov/expobox/about-exposure-factors-handbook>).
9. USEPA, Regional Screening Levels (RSLs) - Generic Tables. <https://www.epa.gov/risk/regional-screening-levels-rsls-generic-tables>).
10. USEPA, IRIS Assessments. https://iris.epa.gov/AtoZ/?list_type=alpha).
11. A. Kortenkamp and H. M. Koch, Refined reference doses and new procedures for phthalate mixture risk assessment focused on male developmental toxicity, *Int. J. Hyg. Environ. Health.*, 2020, **224**, 113428.
12. W. Li, Y. Shi, L. Gao, C. Wu, J. Liu and Y. Cai, Occurrence, distribution and risk of organophosphate esters in urban road dust in Beijing, China, *Environ. Pollut.*, 2018, **241**, 566-575.
13. RAIS, The Risk Assessment Information System, Toxicity Values and Physical Parameters Search. https://rais.ornl.gov/cgi-bin/tools/TOX_search?select=chemtox).
14. Z. P. Yang, Q. Jian, B. Zhou, S. Y. Liu, G. Q. Ding and Y. M. Zhu, Environmental endocrine disruptors in serum of sexually precocious girls, *J. Environ. Occup. Med.*, 2014, **31**, 331-335.
15. T. Yum, S. Lee and Y. Kim, Association between precocious puberty and some endocrine disruptors in human plasma, *J. Environ. Sci. Health Part A-Toxic/Hazard. Subst. Environ. Eng.*, 2013, **48**, 912-917.
16. L. Lu, H. Rong, C. Wu, B. Cui, Y. Huang, Y. Tan, L. Zhang, Y. Peng, J. M. Garcia and J.-a. Chen, Levels of phthalate acid esters and sex hormones and their possible sources in traffic-patrol policemen in Chongqing, *Environ. Sci.*

- Pollut. Res.*, 2019, **26**, 9005-9013.
17. W. W. Luo, Y. X. Liu, X. M. Yang, M. Aamir, X. X. Bai and W. P. Liu, Prenatal exposure to emerging and traditional organophosphate flame retardants: Regional comparison, transplacental transfer, and birth outcomes, *Environ. Pollut.*, 2023, **336**, 122463.
 18. Y. Liu, Y. Li, N. Xiao, M. Liu, Y. Wang, H. Luo, Y. Yao, Y. Feng and S. Wang, Serum organophosphate flame retardants and plasticizers in Chinese females of childbearing age: Association with serum reproductive and thyroid hormones, *Chemosphere*, 2023, **337**, 139237-139237.
 19. Q. Zhang, M. J. Chu, S. Lin, J. L. Lou and C. Wang, Partitioning behavior-oriented health risk assessment on internal organophosphorus flame retardants exposure, *Environ. Res.*, 2023, **216**, 114704.
 20. Y. G. Phee, O. Gon, B. Shon, K. Lee and H. Lim, Concentration levels and distribution characteristics of polycyclic aromatic hydrocarbons (PAHs) at ambient air in industrial complex area, *Clean Technologies*, 2011, **17**, 379-388.
 21. S. S. Yin, M. L. Tang, F. F. Chen, T. L. Li and W. P. Liu, Environmental exposure to polycyclic aromatic hydrocarbons (PAHs): The correlation with and impact on reproductive hormones in umbilical cord serum, *Environ. Pollut.*, 2017, **220**, 1429-1437.
 22. Z. Y. Yang, C. S. Guo, Q. Li, Y. Zhong, S. T. Ma, J. H. Zhou, X. T. Li, R. D. Huang and Y. X. Yu, Human health risks estimations from polycyclic aromatic hydrocarbons in serum and their hydroxylated metabolites in paired urine samples, *Environ. Pollut.*, 2021, **290**, 117975.
 23. Z. Zhang, Y. Wang, T. F. M. Rodgers and Y. Wu, Exposure experiments and machine learning revealed that personal care products can significantly increase transdermal exposure of SVOCs from the environment, *J. Hazard. Mater.*, 2025, **487**, 137271.