SUPPORTING INFORMATION FOR

Understanding the role of a specific microenvironment in personal exposure to semi-volatile organic compounds using silicone wristbands

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Reagents, chemicals and target SVOCs

All solvents (n-hexane, acetone, dichloromethane, methanol, ethyl acetate) used to extract samples were purchased as gas chromatography grade and silica gel and anhydrous sodium sulfate from Supelco (Merck KGaA, Germany). A mixture of 16 EPA-PAH compounds, PHE-d10 and perylene-d12 (PERY-d12), a mixture of 16 ortho-phthalate compounds, DEHTP and internal standards para-terphenyl and benzo(e)pyrene-d12 were purchased from Ehrenstorfer (LGC Labor GmbH Augsburg, Germany). Individual OPE standards, i.e., TPHP, TCEP, TCIPP, TBOEP, EHDPP, TDCIPP, TNBP, TEHP, and TEP, and deuterated phthalate standards, DMP-d4, DNBP-d4, and DEHP-d4, were purchased from AccuStandard (New Haven, CT, USA). OPE surrogate standards TCEP-d12 and TPHP-d15 were purchased from Wellington Laboratories (Guelph, ON, and Canada).

Method Validation and Verification

Before deployment of the SWBs, cleaning and conditioning was recommended using several techniques such as Soxhlet [1–3] and shaker extraction,[4–6] and conditioning in a vacuum oven.[7] Hence, the present study tested SWB precleaning via i) Soxhlet extraction with first 300 mL n-hexane:ethyl acetate mixture (1:1, v:v) for 24 hour, then 300 mL ethyl acetate:methanol mixture (1:1, v:v) for 18 hours, ii) shaker extraction with first 200 mL n-hexane:ethyl acetate mixture (1:1, v:v) and then 200 mL ethyl acetate:methanol mixture (1:1, v:v), each at 120 rpm for one hour, and iii) vacuum oven conditioning at 200 °C and 30 mbar for 24 hours.

For the extraction of deployed samples, ultrasonic and shaker extraction techniques were tested in this study using two different solvent mixtures, i) n-hexane:acetone (1:1) and ii) ethyl acetate. The techniques were adapted from previous SWB studies.[4,8] For both methods, surrogate standards, i.e. PHE-d_{10} and PERY-d_{12} for PAHs, TCEP-d_{12} and TPHP-d_{15} for OPEs, DMP-d_4, DNBP-d_4 and DEHP-d_4 for phthalates analysis were directly infused onto the SWBs. We applied two stage ultrasonic extraction using 30 mL of solvent in the first stage. After first extraction for two hours, SWBs were left in this solvent overnight. In the second stage, fresh solvents of 26 mL were added to the vials and second extraction was completed in another two hours. The solvents were combined in flasks and evaporated until one mL in a rotary evaporator (Büchi, Rotavap R-100). Shaker extraction was also achieved in two stages. In the first stage, 100 mL of solvent was added on top of SWBs in 250 mL bottles and shaken at 60 rpm for two hours. This stage was repeated, and solvents were combined in flasks and evaporated until one mL in the rotary evaporator.

Purification of extracts was achieved using activated silica gel. A chromatography column of 1 mm diameter involving five grams of silica gel was compared to a miniature version of it, i.e. glass Pasteur pipette column containing 0.5 g of silica gel. Both columns were topped with anhydrous sodium sulfate and conditioned using DCM. After elution of extracts, columns were eluted with first 20 mL DCM for chromatography and 2 mL DCM for Pasteur pipette columns and collected as the first fraction of eluate. Then, 7:3 (v:v) acetone:DCM mixture of same volumes was eluted from columns, and collected as the second fraction. Both fractions were evaporated until dryness and solvents were exchanged to 1 mL of hexane. The first fractions were spiked with p-terphenyl for PAH analysis, and the second fractions were spiked with benzo(e)pyrene-d_{12} for OPE and phthalates analysis. Due to occurrence of some OPE and phthalates in the first fraction, it was also spiked with benzo(e)pyrene-d_{12} and analyzed for OPEs and phthalates. The results were then combined.

Among the precleaning methods tested, Soxhlet extraction performed better revealing least number of peaks with less abundance in the GC-MS full scan analysis compared to shaker cleaning and vacuum oven (results not shown). Hence, Soxhlet cleaning was employed for all the samples used in the study. The results of extraction method validation experiments revealed that ultrasonic extraction using n-hexane:acetone (1:1) showed higher average surrogate recoveries (PHE-d_{10}, PERY-d_{12}, TCEP-d_{12}, TPHP-d_{15}, DMP-d_4, DnBP-d_4, DEHP-d_4: 59.5%, 61.2%, 134%, 84.4%, 109%, 60.6%, and 78.2%, respectively) than ultrasonic extraction using ethyl acetate (52.4%, 60.9%, 118%, 69.8, 114%, 56.7%, and 68.2%), shaker extraction using n-hexane:acetone (72.8%, 73.5%, 58.4%, 69.7%, 87.1%, 70.8% and 59.3%), and shaker extraction using ethyl acetate (47.1%, 44.9%, 55.2%, 50.7%, 36.2%, 18.0%, and 20.8%). The average recoveries for target compound groups are presented in Figure S2. Comparison of methods indicated that among the 37 compounds, 19 SVOCs had higher recoveries in the ultrasonic extraction method. One of the SVOCs, namely DEHP, showed 146% recovery in the shaker method, which was above the acceptable analyte recovery of 130% recommended by US EPA. Generally, ultrasonic extraction method performed better than the shaker extraction method for OPEs and phthalates, but otherwise was true for PAHs in this study. In fact, except for ACY, ANT, BaP, and IcdP, both methods demonstrated comparable and acceptable recoveries for PAHs. Hence, considering the efficiency of ultrasonic extraction method for OPEs and phthalates, and the smaller volume of solvents used in this method, ultrasonic extraction method was selected to be used in this study. We have also found that n-hexane:acetone mixture as the extraction solvent demonstrated higher recoveries than ethyl acetate for 30 SVOCs among 37 in the ultrasonic extraction method. An important observation in this study was that for several SVOCs and surrogate standards, recoveries were outside of the range recommended by US EPA, i.e. 70%-130%. For PAHs, the recovery range was 21.8% (ACY) to 88.6% (BbF), for OPEs it was 41.7% (TEHP) to 117% (TNBP), and for phthalates 49.6% (DNOP) to 142% (DEP) recoveries were observed. Previous studies using ultrasonic extraction of SWBs also demonstrated lower SVOC recoveries in their LCSs, such as 57.0±8.00% for ACY, and 58.0±17.0% for TEP [8].[8] S. Wang et al., (2019) reported a surrogate recovery range of 50-120% in all their samples, and 58.7%, 47.5%, 52.8% and 57.8% average recovery for ACY, TNBP, TCIPP, and TEP, respectively in their matrix spike samples.

Ultrasonic extraction yielded ~50% recoveries for TCEP and EHDPP, ~40% for an alternative plasticizer diethylhexyl adipate in their samples.[9] Another study employing ultrasonic extraction using n-hexane:dichloromethane demonstrated phthalate surrogate recoveries as low as 31.0% (DMP-d_4).[10] Therefore, it can be speculated that i) among PAHs, ACY showed consistently low recoveries, ii) OPE compounds demonstrated recoveries around 50%, in the literature as well, and iii) phthalate compounds and deuterated surrogate compounds revealed recoveries as low as 30%, while relatively more volatile DMP showed abnormally high recoveries possibly due to matrix effect. Considering the consistent results with the literature, ultrasonic extraction using n-hexane:acetone solvent mixture was used in the further analysis of samples. Furthermore, a recovery range of 50-120% was considered acceptable as the quality control criteria of this study.

For the purification of extracts, chromatographic columns were commonly used in several SWB sample pretreatment procedures.[1,3] Instead of using higher amounts of adsorbent (i.e. silica gel in this study) and larger volumes of elution solvents, Pasteur pipette columns were prepared with 0.5 g of activated silica gel eluted with 2-5 mL of solvents. The SVOC recoveries when using Pasteur pipette columns were comparable to that of one millimeter diameter chromatographic columns (Figure S3). Hence, an economic and practical purification method has been employed in this study.

When reporting SWB concentrations, blank correction was performed for DEHTP. The average DEHTP concentration in blank samples were 224.1 ± 7.4 ng/sample. This concentration accounted for 0.16% of the worn SWB concentrations on average. On the other hand, the stationary office samples showed lower concentrations. The minimum DEHTP concentration in the office samples was the first week sample of the office, where we monitored SVOC accumulation (291 ng/sample). Hence, the blank accounted for 77% of this sample concentration. Other than the ones from the accumulation study, the blank DEHTP concentration was 52% of the 28-day office SWB concentrations on average. Hence the DEHTP amount found in the blank samples was subtracted from the concentration of deployed samples.

Equivalent air concentration and office air contribution calculations

The uptake of gas-phase chemicals by passive samplers is governed by molecular diffusion following Fick's Law and has been shown to be air-side controlled.[11–13] The uptake consists of three phases: linear uptake, curvilinear, and equilibrium. From the linear uptake phase, a sampling/uptake rate (R_s) can be found, and a partition coefficient (K_{sa}) can be calculated for chemicals that reach equilibrium with the air concentrations.

For the SVOCs identified to approach equilibrium, C_a was estimated using Eq. S1:

$$K_{sa} = \frac{N_s/V_s}{C_a} \qquad \text{Eq. S1}$$

Where $N_s$is the amount of SVOC measured in the office SWB (ng), V_s is the volume of SWB (L). The K_{sa} values were obtained following three separate approaches or models in the previous studies.[13–15] To consider all approaches and to take into account the temperature differences between these studies and ours, we followed three approaches individually and presented the mean and median values of the calculated C_a's.

K_{sa} values were available for most of our target SVOCs in Tromp et al. (2019) or were derived from Eq. S2 developed by Tromp et al. (2019), Eq. S3 by O'Connell et al. (2022), and Eq. S4 by Frederiksen et al. (2022):

$$logK_{sa} = 0.778logK_{oa} + 0.813 \qquad \text{Eq. S2}$$

$$logK_{sa} = 0.019BP(OPERA) + 0.829 \qquad \text{Eq. S3}$$

$$logK_{sa} = 0.46logK_{oa} + 3.34 \qquad \text{Eq. S4}$$

Where K_{oa} is the octanol-air partition coefficient calculated for PAHs using Parnis et al.,[16] for OPEs using Yaman et al. [17]at 21°C and obtained from EPI Suite KOAWIN v1.10 for 25°C for phthalates, $BP(OPERA)$ is the boiling point of SVOCs obtained from EPA Comptox Database [18] which gives the estimated BP values using open structure-activity/property relationship.[19] K_{sa} values were calculated for all compounds in this analysis.

For the SVOCs that could not reach equilibrium, i.e. having continuously increasing concentration profiles, Eq. S5 or Eq. S6 was used to estimate C_a:[15]

$$C_a = \frac{N_s}{V_s \times K_{sa} \times \left(1 - e^{(-k_e \times t)}\right)} \qquad \text{Eq. S5}$$

$$C_a = \frac{N_s}{V_s \times K_{sa} \times \left(1 - e^{(-(R_s \times t)/(V_s \times K_{sa}))}\right)} \qquad \text{Eq. S6}$$

Where $k_e$is the dissipation rate (d^{-1}), R_s is the sampling rate (m^3 d^{-1}), and t is the deployment time (d). R_s values proposed by Frederiksen et al. (2022); and Tromp et al. (2019) were utilized, while k_e is estimated by a model by O'Connell et al. (2022):[13–15]

$$logk_e = -0.009BP(OPERA) + 1.55 \qquad \text{Eq. S7}$$

After calculating C_a values for the SVOCs measured in the office air, the contribution of office exposure to personal exposure via SWBs was estimated by considering the time spent by the participants in their offices. The office SWBs were deployed for 28 days, and participants wore the SWBs for seven days, during which they spent an average of 8 hours/day for five days in their offices. Hence, a back-calculation was performed using Eq. S8,

$$N_{office} = R_{s,worn} \times C_a \times t \qquad \text{Eq.S8}$$

Where N_{office} is the amount of SVOC to be accumulated if the SWB was worn only in the office (ng), $R_{s,worn}$ is the sampling rate of worn wristbands. A generic $R_{s,worn} = 4.6\, m^3 dm^{-2} d^{-1}$, proposed by Frederiksen et al. (2022) for PCBs having log K_{oa} in the range

7.40 – 9.50 was utilized for all SVOCs measured. The sampling rate was shown to be influenced by the airflow on the SWB (i.e. arm movements), the exposure sources nearby the participants, and the ambient SVOC concentrations where the participant spent time.[20] Hence, the R_s for worn SWBs and stationary SWBs should vary. However, the $R_{s,worn}$ values are not available for all SVOCs. Hence, the unique sampling rate reported for the worn wristbands calculated on volume basis was used. We acknowledge that this might bring a limitation to the estimations. Lastly, $N_{office}$was divided by the amount of SVOC in the worn SWB by the corresponding participant and multiplied by 100 to find the percent contribution of the office air to total exposure.

Tables

Table S1. Semi-volatile organic compounds targeted in this study, their CAS numbers, and abbreviations used in this study

SVOC Class	Compoud Name	Abbreviation	CAS Number	Molecular weight	Log K_{oa}[a]
PAHs	Naphthalene	NP	91-20-3	128	5.04
	Acenaphthene	ACE	83-32-9	154	6.04
	Acenaphthylene	ACY	208-96-8	152	6.27
	Fluorene	FL	86-73-7	166	6.58
	Anthracene	ANT	120-12-7	178	7.09
	Phenanthrene	PHE	85-01-8	178	7.22
	Pyrene	PYR	129-00-0	202	8.19
	Fluoranthene	FLA	206-44-0	202	8.60
	Benzo(a)anthracene	BaA	56-55-3	228	9.07
	Chrysene	CHR	218-01-9	228	9.48
	Benzo(b)fluoranthene	BbF	205-99-2	252	10.4
	Benzo(k)fluoranthene	BkF	207-08-9	252	10.7
	Benzo[a]pyrene	BaP	50-32-8	252	10.8
	Benzo(g,h,I)perylene	BghiP	191-24-2	276	11.5
	Dibenz[a,h]anthracene	DahA	53-70-3	278	11.8
	Indeno(1,2,3-cd)pyrene	IcdP	193-39-5	276	11.5
OPEs	Triethyl phosphate	TEP	78-40-0	182	6.63
	Tri(n-butyl) phosphate	TNBP	126-73-8	266	8.24
	2-ethylhexyl diphenyl phosphate	EHDPP	1241-94-7	362	8.38
	Triphenyl Phosphate	TPHP	115-86-6	326	8.46
	Tris(2-chloroethyl) phosphate	TCEP	115-96-8	285	9.20
	Tris(2-chloro isopropyl) phosphate	TCIPP	13674-84-5	327	9.45
	Tris(1,3-dichloro-2-propyl) phosphate	TDCIPP	13674-87-8	431	10.6
	Tris(2-butoxyethyl) phosphate	TBOEP	78-51-3	398	13.1
	Tris(2-ethylhexyl) phosphate	TEHP	78-42-2	434	14.9
Ortho-phthalates	Dimethyl phthalate	DMP	131-11-3	194	6.69
	Diethyl phthalate	DEP	84-66-2	222	7.50
	Diisobutyl phthalate	DIBP	84-69-5	278	8.41
	Di-n-butyl phthalate	DNBP	84-74-2	278	8.63

	Benzyl butyl phthalate	BBP	85-68-7	312	9.02
	Dipentyl phthalate	DPP	131-18-0	306	9.67
	Bis(2-methoxyethyl)phthalate	DMEP	117-82-8	282	9.77
	Di-n-hexyl phthalate	DNHP	84-75-3	334	9.80
	Bis(2-ethoxyethyl) phthalate	DEEP	605-54-9	310	10.5
	Di-cyclohexyl phthalate	DCHP	84-61-7	330	11.6
	Bis(2-butoxyethyl) phthalate	DBEP	117-83-9	366	11.9
	di-n-octyl phthalate	DNOP	117-84-0	390	12.1
	Di-2-Ethylhexyl Phthalate	DEHP	117-81-7	390	12.6
	Dinonyl phthalate	DNP	84-76-4	418	12.6
Terephthalate	Bis(2-ethylhexyl) terephthalate	DEHTP	6422-86-2	390	11.7

[a] Log K_{oa} values were derived using EPI Suite KOAWIN v1.10 estimates for 25°C.

Table S2. Retention times, quantifier and qualifier ions in GC-MS analysis of target SVOCs

PAH	**RT**	**Quantifier/ Qualifier ions**	**OPE**	**RT**	**Quantifier/ Qualifier ions**	**Phthalates**	**RT**	**Quantifier/ Qualifier ions**
NP	5.33	127/128	TEP	4.01	99/155	DMP-d4	8.53	167/137
ACY	6.91	151/152	TNBP	11.1	99/155	DMP	8.58	163/77
ACE	7.09	153/154	TCEP-d_{12}	13.3	261/263	DEP	10.5	149/177
FL	7.66	165/166	TCEP	13.4	143/249	DIBP	15.4	149/150
PHE-d_{10}	8.95	188/189	TCIPP	13.9	99/125	DNBP-d4	16.6	153/207
PHE	8.99	178/176	TDCIPP	21.2	75/99	DNBP	16.7	149/150
ANT	9.07	178/176	TPHP-d_{15}	22.4	339/341	DMEP	17.9	149/85
FLA	11.2	202/200	TPHP	22.6	326/325	DEEP	18.0	149/85
PYR	11.7	202/200	TBOEP	22.8	85/125	DPP	19.0	149/237
BaA	14.7	228/226	EHDPP	23.1	251/250	DNHP	22.1	149/233
CHR	14.8	228/226	TEHP	23.8	99/113	BBP	22.2	149/91
BbF	17.6	252/250				DBEP	24.5	149/85
BkF	17.7	252/250				DCHP	25.3	149/167
BaP	18.4	252/250				DEHP-d4	25.7	153/207
IcdP	21.2	276/277				DEHP	25.7	149/167
DahA	21.3	278/279				DNOP	29.0	149/279
BghiP	21.9	276/277				DNP	31.3	149/293
						DEHTP	29.2	149/261

Table S3. The method detection limit (MDL) and limit of quantitation (LOQ) for SVOCs analyzed in silicone wristbands (ng/SWB), percent recoveries in the method validation study, SWB laboratory control samples- LCS (*n*=3, mean±standard deviation, %), solvent LCS (*n*=2, mean, %) for target SVOCs

	MDL	**LOQ**	**Recoveries in SWB LCS**	**Recoveries in Solvent LCS**
PAH				
NP	14.4	19.1	79.8±0.790	80.6
ACE	1.83	8.00	81.9±0.200	81.7
ACY	3.25	6.40	79.6±0.190	79.4
FL	1.90	4.76	93.0±11.0	91.2
ANT	0.890	1.68	78.8±5.02	82.0
PHE	1.87	5.94	79.7±10.9	91.6
PYR	0.300	0.940	85.9±6.89	92.5
FLA	0.190	0.680	81.7±6.78	88.4
BaA	0.690	2.19	92.3±8.01	97.5
CHR	0.0500	1.62	89.7±9.64	98.5
BbF	2.32	7.39*	104±16.5	86.7
BkF	1.26	4.02*	96.8±23.7	73.1
BaP	0.820	2.62	82.4±4.91	82.0
BghiP	4.35	13.8*	83.0±5.84	80.1
DahA	1.65	8.63	86.4±6.10	89.4
IcdP	2.37	7.54*	79.7±7.12	74.1
PHE-d_{10}	15.5	49.3*	82.1±4.50	84.8
PERY-d_{12}	112	357	75.0±12.5	60.9
OPE				
TEP	10.1	25.4	81.4±21.3	99.8
TNBP	3.91	12.4*	47.7±5.30	78.1
EHDPP	3.74	17.0	59.8±4.30	55.5
TPHP	7.18	22.8*	90.9±3.60	62.9
TCEP	2.82	54.0	78.1±30.1	87.4
TCIPP	4.29	22.2	43.7±0.200	46.3
TDCIPP	8.14	16.0	45.8±3.10	38.1
TBOEP	18.6	59.0*	54.5±4.78	57.2
TEHP	7.90	14.5	53.3±2.10	58.1
TCEP-d_{12}	5.53	17.6*	77.3±18.0	98.7
TPHP-d_{15}	10.8	34.5*	81.9±5.60	57.5
Phthalates				
DMP	3.27	28.1	139±22.2	77.6
DEP	3.42	35.6	80.9±14.4	66.2
DIBP	3.21	26.6	52.1±6.90	129
DNBP	2.57	37.2	51.0±23.1	68.7
BBP	6.92	22.0*	66.9±7.50	69.4
DPP	3.30	26.7	53.1±18.2	50.3
DEEP+DMEP	11.8	25.0	62.0±12.6	109
DNHP	5.54	21.5	84.2±14.3	65.7
DCHP	5.58	17.7*	55.8±18.1	122
DBEP	11.6	25.3	57.7±18.0	79.3
DNOP	5.36	17.1*	122±12.0	103
DEHP	17.4	55.4*	54.5±11.1	54.0
DNP	9.60	30.5*	76.0±5.30	112
DEHTP	12.7	40.4	68.2±10.1	66
DMP-d_4	3.71	11.8*	112±18.3	78.4
DNBP-d_4	2.66	8.46*	49.3±3.20	110
DEHP-d_4	14.6	46.5*	50.0±1.00	59.5

* The LOQs were calculated according to MDLx3.18.

Table S4. Statistical terms

Term	Definition
R^2	Coefficient of determination; represents the proportion of variance in the dependent variable explained by the predictors.
Adjusted R^2	R^2 that adjusts for the number of predictors and sample size.
$F(x, y)$	F-statistic in linear regression; tests overall significance of the regression model with x as the number of predictors and y degrees of freedom for the residuals
p	Probability value indicating statistical significance
β	Standardized regression coefficient; used to compare the relative strength of predictors.
r_s	Spearman's rank correlation coefficient

Table S5. The statistical data regarding participants' characteristics and daily activities

The Variables of Participant Activities/ Characteristics	**Participants n = 12**
Gender	
Male	7 (58.3%)
Female	5 (41.7%)
The Time SW Covered with Clothes	
None	5 (41.7%)
Constantly during one or two days	5 (41.7%)
Daytime hours in every day	2 (16.7%)
Smoking	
None	10 (83.3)
One to three times a day	2 (16.7%)
Personal Care Products	
Shampoo	2 (16.7%)
Deodorant/perfume+shampoo	5 (41.7%)
All	5 (41.7%)
Nail polish use	
Yes	3 (25.0%)
No	9 (75.0%)
Avg Times SW Washed	
Once in 2 – 3 days	1 (8.33%)
Once in 3 – 4 days	1(8.33%)
Once in 4 – 5 days	1 (8.33%)
Once in everyday	3(25.0%)
More than one time everyday	6 (50.0%)
Home Cleaning (Times/7 days)	
0 – 0.75	4 (33.3%)
1 - 2	7 (58.3%)
> 2	1 (8.33%)
Cooking (Times/7 day)	
0 – 2	5 (41.7%)
2 - 4	2 (16.7%)
> 4	5 (41.7%)
Avg Hours/Day Spent in Office	
7	2 (16.7%)
7 - 8	1 (8.30%)
8	7 (58.3%)
8 - 9	1 (8.30%)
10	1 (8.30%)
Avg Hours/Day Spent in Home	
8 - 10	2 (16.7%)
11	1 (8.33%)
12	3 (25.0%)
12 - 13	1 (8.33%)
13	2 (16.7%)
13 - 14	2 (16.7%)
14 - 15	1 (8.33%)
Avg Mins/Day Spent in Car or Public Transportation	
30	1 (8.33%)
60	6 (50.0%)
90	3 (25.0%)
120	1 (8.33%)
240	1 (8.33%)
Avg Mins/Day Spent at Outdoor	

60	3 (25.0%)
120	6 (50.0%)
150	2 (16.7%)
180	1 (8.30%)
Waiting a Shuttle Bus (min)	
0 - 5	8 (66.7%)
5 - 10	2 (16.7%)
> 10	2 (16.7%)

Table S6. The statistical data regarding the building properties and location during the study

The Variables of Building Factors	**Participants n = 12**
Location	
Urban	8 (66.7%)
Suburban	4 (33.3%)
Age of Building (years)	
0 - 10	3 (25.0%)
10 - 20	1 (8.33%)
20 - 30	7 (58.3%)
> 30	1 (8.33%)
Floor Material	
Laminate flooring	8 (66.7%)
Woodblock/ varnished wood	4 (33.3%)
Using Carpet on the Floor	
Yes	7 (58.3%)
No	5 (41.7%)
Heating System	
Natural gas	5 (41.7%)
Electricity	4 (33.3%)
Coal	3 (25.0%)
Age of Mattress (months)	
0 - 12	2 (16.7%)
12 - 24	2 (16.7%)
24 - 48	2 (16.7%)
> 48	6 (50.0%)
Age of Sofa (months)	
24 - 36	3 (25.0%)
> 36	9 (75.0%)

Table S7. The descriptive statistics of PAH concentrations observed in SWBs worn by the study participants (n=12) (ng/g SWB)

	Median	**Mean**	**SD**	**Min**	**Max**	**Detection frequency**
NP	7.08	12.3	14.4	<LOQ	50.7	67%
ACE	5.11	6.43	6.62	<MDL	14.9	50%
ACY	215	213	95.7	92.3	383	100%
FL	3.21	4.07	4.21	<LOQ	16.7	92%
ANT	28.6	39.0	35.1	1.81	126	100%
PHE	35.7	35.6	34.4	2.93	86.7	100%
PYR	42.8	58.9	46.0	12.6	155	100%
FLA	7.51	16.5	19.0	0.810	59.4	100%
BaA	2.42	2.97	2.88	<MDL	9.32	83%
CHR	1.70	2.22	1.63	0.350	5.67	100%
BbF	8.95	19.3	90.2	3.45	50.8	100%
BkF	12.5	16.8	15.2	1.07	50.9	100%
BaP	28.9	33.9	22.0	9.68	66.3	100%
BghiP	2.49	3.31	3.18	<MDL	9.72	58%
DahA	21.6	31.8	51.7	<LOQ	76.9	75%
IcdP	19.7	28.7	22.3	<LOQ	65.7	92%

Table S8. The descriptive statistics of OPE concentrations observed in SWBs worn by the study participants (n=12) (ng/g SWB)

	Median	**Mean**	**SD**	**Min**	**Max**	**Detection frequency**
TNBP	20.9	45.7	59.3	3.56	202	100%
EHDPP	13.1	17.3	20.6	<LOQ	70.7	66.7%
TPHP	38.8	43.3	25.4	12.6	83.2	100%
TCEP	482	443	157	169	659	100%
TCIPP	32.3	49.7	38.4	15.7	129	100%
TDCIPP	20.9	35.3	34.8	7.50	116	100%
TBOEP	600	921	774	297	2450	100%
TEHP	15.6	17.6	11.0	6.03	43.6	100%

Table S9. The descriptive statistics of phthalate concentrations observed in SWBs worn by the study participants (n=12) (µg/g SWB)

	Median	**Mean**	**SD**	**Min**	**Max**	**Detection frequency**
DMP	0.0863	0.0887	0.0408	0.0250	0.159	100%
DEP	0.00628	7.39	6.07	0.671	19.2	100%
DIBP	1.58	1.61	0.510	0.642	2.72	100%
DNBP	0.602	0.811	0.749	0.168	2.94	100%
DNHP	0.0176	0.0181	0.0108	<LOQ	0.0391	92%
BBP	0.0272	0.0331	0.0219	0.0146	0.0929	100%
DPP	0.0150	0.0154	0.00411	0.0105	0.0235	100%
DEHP	10.7	10.5	3.18	4.14	14.1	100%
DNP	0.0515	0.0623	0.0372	0.0308	0.160	100%
DCHP	0.0359	0.0376	0.0125	0.0195	0.0583	100%
DNOP	0.0286	0.0352	0.0222	0.0151	0.0924	100%
DEHTP	27.0	28.9	12.6	14.4	57.8	100%

Table S10. The PAH concentrations in the office environment by using SWs (ng/g wristband, n=13)

	Median	**Mean**	**SD**	**Min**	**Max**	**Detection frequency**
NP	3.98	4.26	2.84	<MDL	12.7	69%
ACY	1.79	1.95	1.06	<LOQ	3.72	85%
ACE	3.87	4.06	1.80	1.86	8.51	100%
FL	5.95	6.05	2.08	2.34	9.30	100%
PHE	10.9	10.8	3.36	6.22	17.2	100%
ANT	1.66	2.01	1.15	0.680	3.88	100%
FLA	2.04	2.22	0.640	1.46	3.72	100%
PYR	2.49	2.54	0.900	1.29	4.55	100%

Table S11. The OPE concentrations in the office environment by using SWs (ng/g wristband, n=13)

	Median	**Mean**	**SD**	**Min**	**Max**	**Detection frequency**
TEP	22.2	45.7	46.7	13.5	146	100%
TNBP	57.1	71.9	53.5	43.3	248	100%
TCEP	71.1	75.8	40.3	34.8	190	100%
TCIPP	199	205	172	19.3	476	100%

Table S12. Ortho- and tere-phthalates observed in the SWBs deployed as the office indoor air sampler (ng/g SWB)

	Median	**Mean**	**SD**	**Min**	**Max**	**Detection frequency**
DMP	17.5	17.8	2.45	14.2	22.8	100%
DEP	258	358	185	149	686	100%
DIBP	431	447	182	103	795	100%
DNBP	91.4	127	87.2	73.7	362	100%
BBP	15.0	20.6	14.7	6.10	49.9	100%
DEHP	35.1	50.6	32.9	22.4	134	100%
DEHTP	35.4	40.2	18.1	21.6	88.3	100%

Table S13. Estimation of equivalent air concentrations for the SVOCs measured in the office environment

SVOCs	(21°C-chamber) Tromp et al. 2019[13]	(25°C-chamber) O'Connell et al. 2022 [15]	(21°C-indoor) Frederiksen et al. 2022 [14]
ACY, FL, PHE, ANT, TNBP, TCEP, DMP, DEP, DIBP, DNBP	K_{sa} given for ACY, FL, PHE, ANT, DMP, DEP, DIBP For others*: $logK_{sa} = 0.778logK_{oa} + 0.813$ $logK_{oa} = A + B/T$	$logK_{sa} = 0.019BP(OPERA) + 0.829$	$logK_{sa} = 0.46logK_{oa} + 3.34$ $logK_{oa} = A + B/T*$
	$C_a = \frac{N_s/V_s}{K_{sa}}$		
All	R_s given for PHE, ANT, FLA, PYR, TNBP, TCEP, TCIPP, DMP, DEP, DIBP, DNBP, BBP, DEHP	$logk_e = -0.009BP(OPERA) + 1.55$	Generic R_s
	$C_a = \frac{N_s}{V_s \times K_{sa} \times (1 - e^{(-(R_s \times t)/(V_s \times K_{sa}))})}$	$C_a = \frac{N_s}{V_s \times K_{sa} \times (1 - e^{(-k_e \times t)})}$	$C_a = \frac{N_s}{V_s \times K_{sa} \times (1 - e^{(-(R_s \times t)/(V_s \times K_{sa}))})}$
All	$N_{office} = R_{s,worn} \times C_a \times t$		

*K_{oa} was calculated taking T= 21°C. A and B were obtained from previous studies for PAHs and OPEs. For phthalates K_{oa}'s were retrieved from EPI Suite (25°C).

Figures

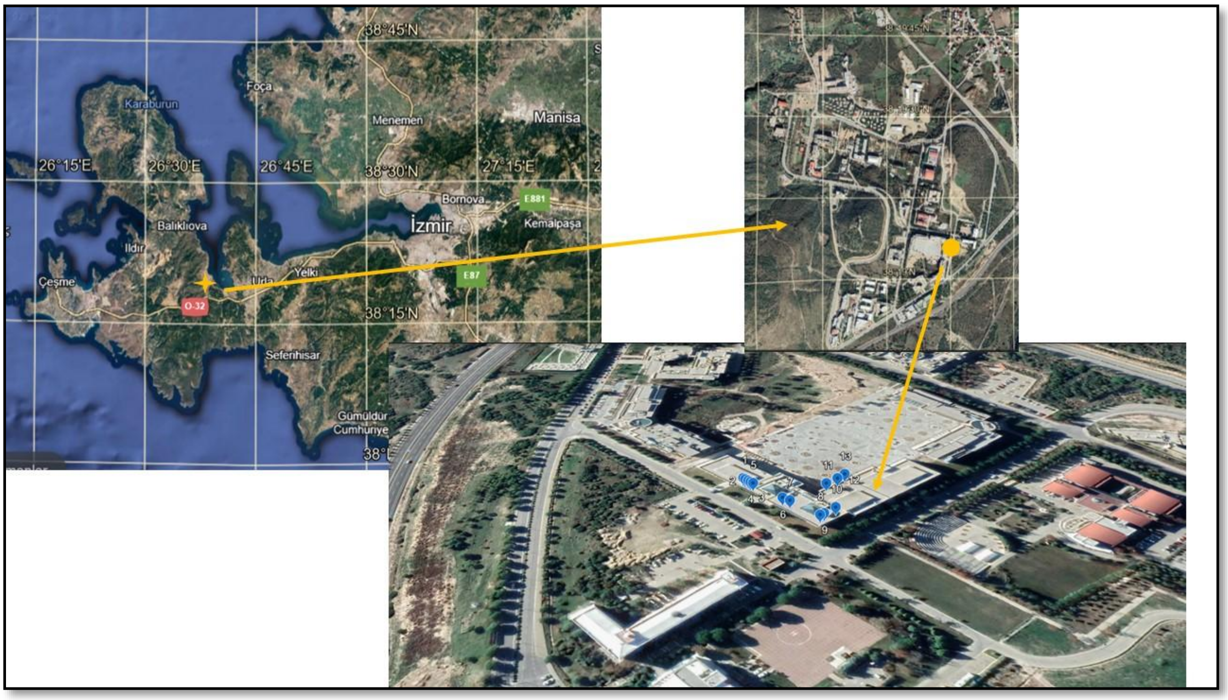

Figure S1. The coordinates of Izmir Institute of Technology Campus and the location of the offices sampled

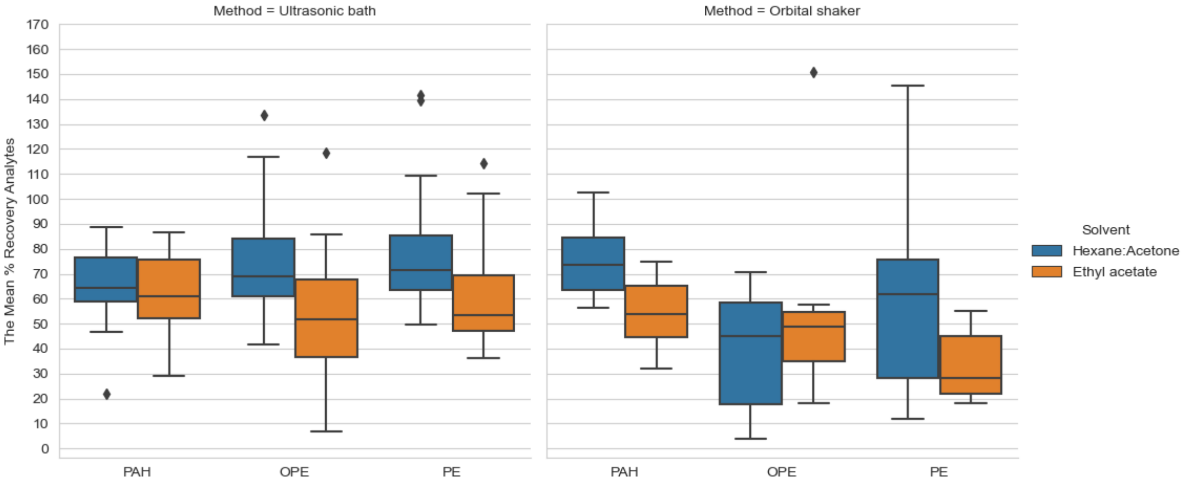

Figure S2. Percent recoveries of target analytes when extracted using ultrasonic bath and shaker using two solvent mixtures. Boxes show 25th and 75th percentiles with the horizontal line within the box showing median concentrations. Whiskers show 1.5*IQR (interquartile range), dots are the outliers.

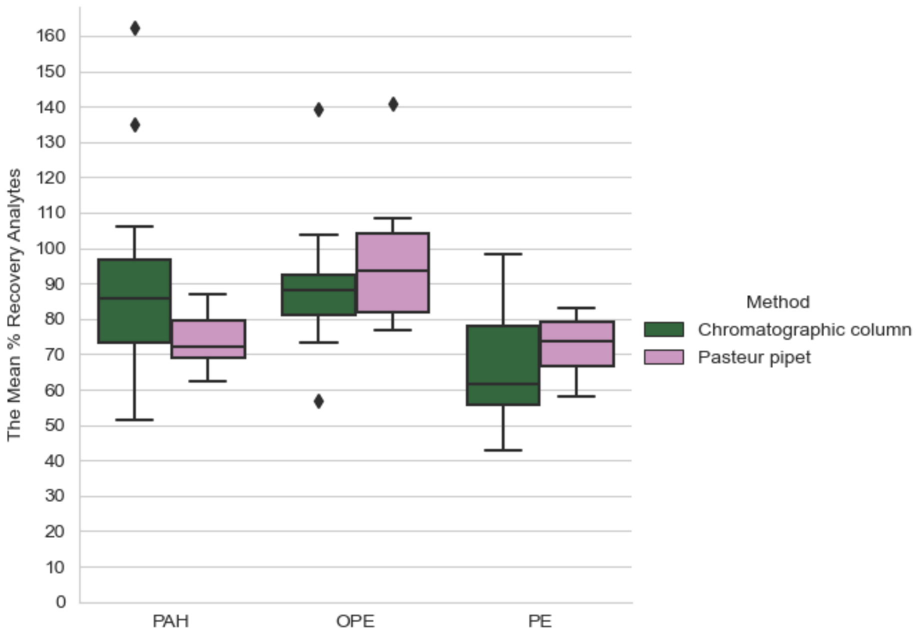

Figure S3. Percent recoveries of target analytes when the extracts were purified using 1 mm diameter chromatography columns and Pasteur pipette columns. Boxes show 25^{th} and 75th percentiles with the horizontal line within the box showing median concentrations. Whiskers show 1.5*IQR (interquartile range), dots are the outliers.

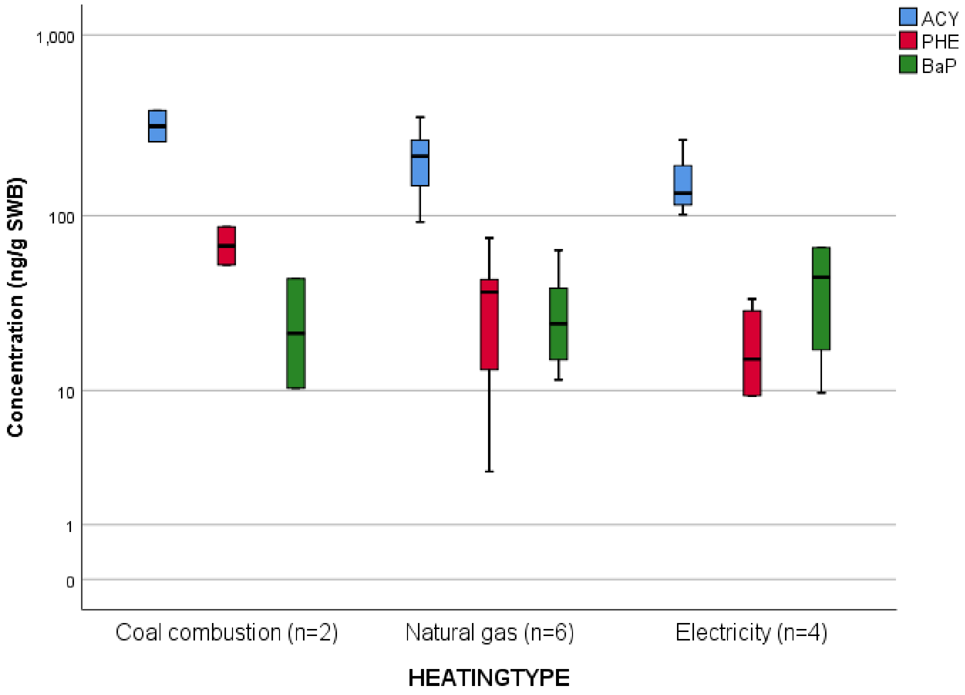

Figure S4. Comparison of ACY, PHE, and BAP concentrations in the personal SWBs with respect to heating types at homes of the participants.

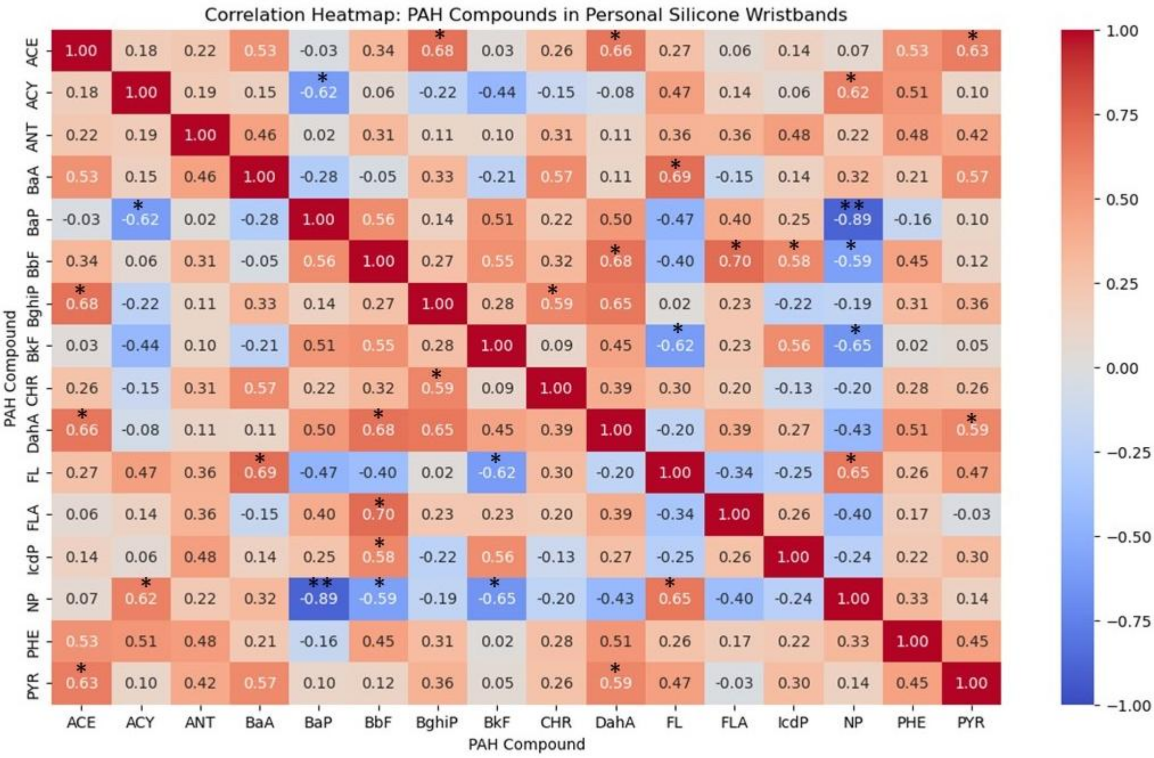

Figure S5. Correlations among PAH compounds measured in the worn SWBs (*: p<0.05, **: p<0.01)

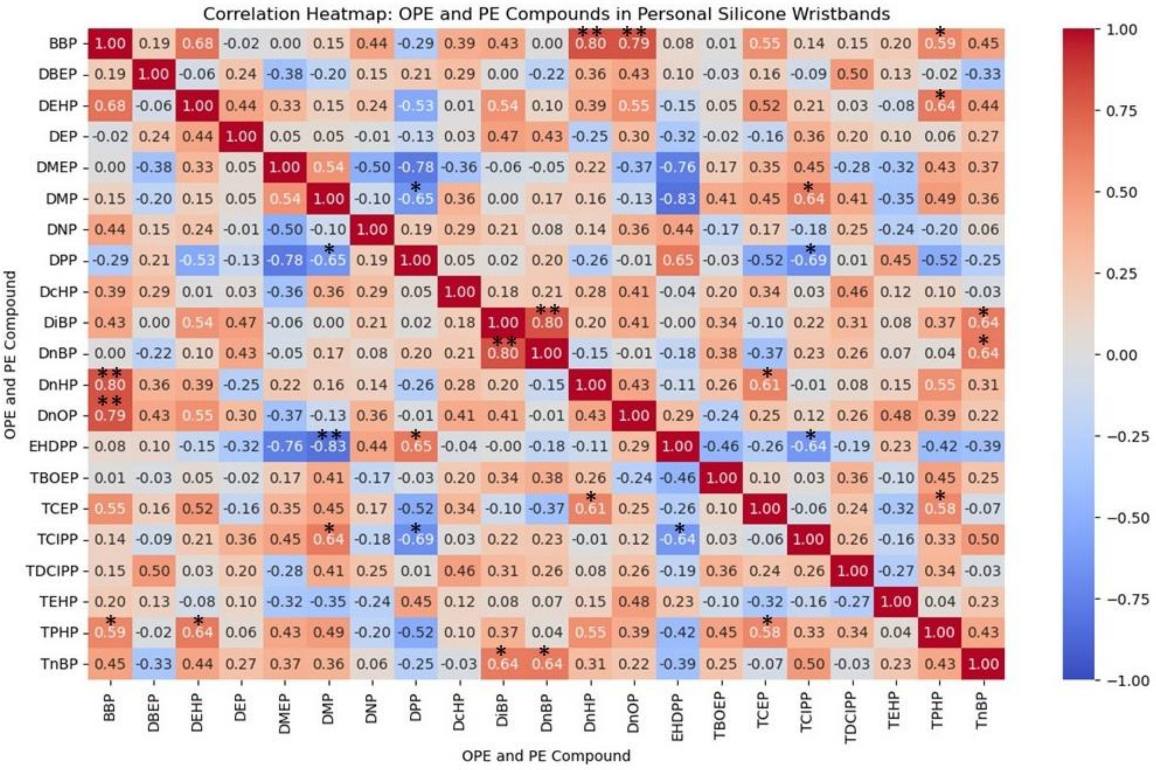

Figure S6. Correlations among OPE and ortho-phthalate compounds measured in the worn SWBs(*: p<0.05, **: p<0.01)

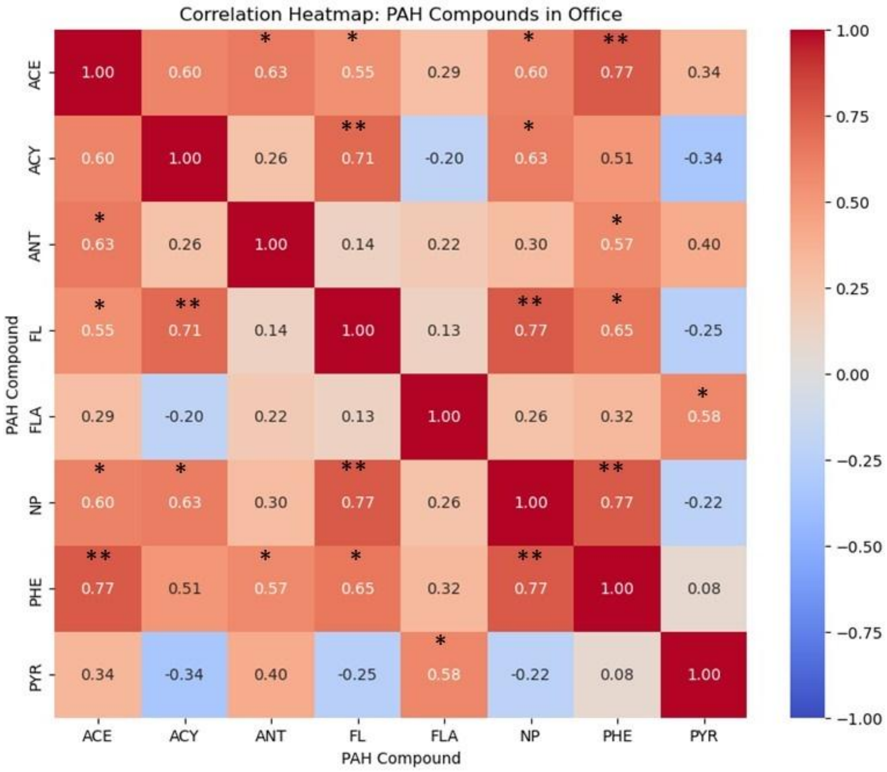

Figure S7. Correlations among PAH compounds measured in the office SWBs (*: p<0.05, **: p<0.01)

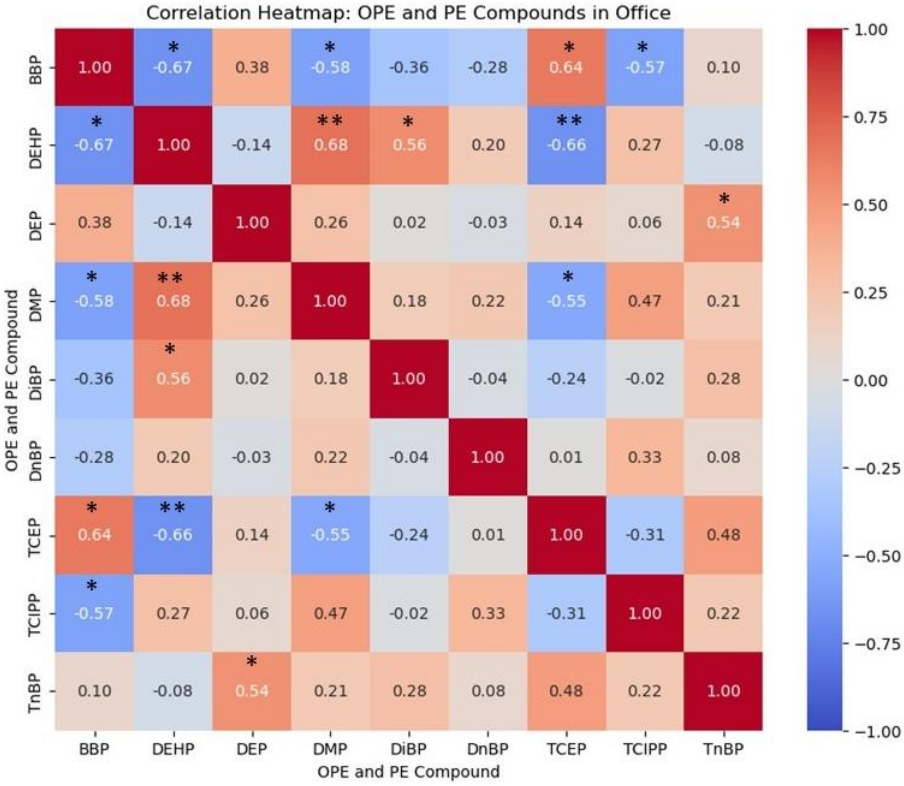

Figure S8. Correlations among OPE and ortho-phthalate compounds measured in the office SWBs (*: p<0.05, **: p<0.01)

References

1 Wang, S.; Romanak, K. A.; Stubbings, W. A.; Arrandale, V. H.; Hendryx, M.; Diamond, M. L.; Salamova, A.; Venier, M. Silicone Wristbands Integrate Dermal and Inhalation Exposures to Semi-Volatile Organic Compounds (SVOCs). Environ. Int. 2019, 132, 105104. https://doi.org/10.1016/j.envint.2019.105104.

2 Kassotis, C. D.; Herkert, N. J.; Hammel, S. C.; Hoffman, K.; Xia, Q.; Kullman, S. W.; Sosa, J. A.; Stapleton, H. M. Thyroid Receptor Antagonism of Chemicals Extracted from Personal Silicone Wristbands within a Papillary Thyroid Cancer Pilot Study. Environ. Sci. Technol. 2020, 54 (23): 15296–15312. https://doi.org/10.1021/acs.est.0c05972.

3 Hendryx, M.; Wang, S.; Romanak, K. A.; Salamova, A.; Venier, M. Personal Exposure to Polycyclic Aromatic Hydrocarbons in Appalachian Mining Communities. Environ. Pollut. 2020, 257, 113501. https://doi.org/10.1016/j.envpol.2019.113501.

4 O’Connell, S. G.; Kincl, L. D.; Anderson, K. A. Silicone Wristbands as Personal Passive Samplers. Environ. Sci. Technol. 2014, 48 (6): 3327–3335. https://doi.org/10.1021/es405022f.

5 Travis, S. C.; Aga, D. S.; Queirolo, E. I.; Olson, J. R.; Daleiro, M.; Kordas, K. Catching Flame Retardants and Pesticides in Silicone Wristbands: Evidence of Exposure to Current and Legacy Pollutants in Uruguayan Children. Sci. Total Environ. 2020, 740, 140136. https://doi.org/10.1016/j.scitotenv.2020.140136.

6 Baum, J. L. R.; Bakali, U.; Killawala, C.; Santiago, K. M.; Dikici, E.; Kobetz, E. N.; Solle, N. S.; Deo, S.; Bachas, L.; Daunert, S. Evaluation of Silicone-Based Wristbands as Passive Sampling Systems Using PAHs as an Exposure Proxy for Carcinogen Monitoring in Firefighters: Evidence from the Firefighter Cancer Initiative. Ecotoxicol. Environ. Saf. 2020, 205, 111100. https://doi.org/10.1016/j.ecoenv.2020.111100.

7 Anderson, K. A.; Points, G. L.; Donald, C. E.; Dixon, H. M.; Scott, R. P.; Wilson, G.; Tidwell, L. G.; Hoffman, P. D.; Herbstman, J. B.; O’Connell, S. G. Preparation and Performance Features of Wristband Samplers and Considerations for Chemical Exposure Assessment. J. Expo. Sci. Environ. Epidemiol. 2017, 27 (6): 551–559. https://doi.org/10.1038/jes.2017.9.

8 Romanak, K. A.; Wang, S.; Stubbings, W. A.; Hendryx, M.; Venier, M.; Salamova, A. Analysis of Brominated and Chlorinated Flame Retardants, Organophosphate Esters, and Polycyclic Aromatic Hydrocarbons in Silicone Wristbands Used as Personal Passive Samplers. J. Chromatogr. A 2019, 1588: 41–47. https://doi.org/10.1016/j.chroma.2018.12.041.

9 Gómez, Ó.; Ramírez, N.; Vallecillos, L.; Borrull, F. Determining Personal Exposure to High Production Volume Chemicals (HPVCs) and Polycyclic Aromatic Hydrocarbons (PAHs) with Silicone Wristbands: A Pilot Study. Environ. Res. 2024, 263. https://doi.org/10.1016/j.envres.2024.120107.

10 Young, A. S.; Herkert, N.; Stapleton, H. M.; Cedeño Laurent, J. G.; Jones, E. R.; MacNaughton, P.; Coull, B. A.; James-Todd, T.; Hauser, R.; Luna, M. L.; Chung, Y. S.; Allen, J. G. Chemical Contaminant Exposures Assessed Using Silicone Wristbands among Occupants in Office Buildings in the USA, UK, China, and India. Environ. Int. 2021, 156. https://doi.org/10.1016/j.envint.2021.106727.

11 Bartkow, M. E.; Booij, K.; Kennedy, K. E.; Müller, J. F.; Hawker, D. W. Passive Air Sampling Theory for Semivolatile Organic Compounds. Chemosphere 2005, 60 (2):

170–176. https://doi.org/10.1016/j.chemosphere.2004.12.033.

12 Shoeib, M.; Harner, T. Characterization and Comparison of Three Passive Air Samplers for Persistent Organic Pollutants. Environ. Sci. Technol. 2002, 36 (19): 4142–4151. https://doi.org/10.1021/es020635t.

13 Tromp, P. C.; Beeltje, H.; Okeme, J. O.; Vermeulen, R.; Pronk, A.; Diamond, M. L. Calibration of Polydimethylsiloxane and Polyurethane Foam Passive Air Samplers for Measuring Semi Volatile Organic Compounds Using a Novel Exposure Chamber Design. Chemosphere 2019, 227: 435–443. https://doi.org/10.1016/j.chemosphere.2019.04.043.

14 Frederiksen, M.; Andersen, H. V.; Ovesen, S. L.; Vorkamp, K.; Hammel, S. C.; Knudsen, L. E. Silicone Wristbands as Personal Passive Samplers of Exposure to Polychlorinated Biphenyls in Contaminated Buildings. Environ. Int. 2022, 167. https://doi.org/10.1016/j.envint.2022.107397.

15 O’Connell, S. G.; Anderson, K. A.; Epstein, M. I. Determining Chemical Air Equivalency Using Silicone Personal Monitors. J. Expo. Sci. Environ. Epidemiol. 2021, No. 1. https://doi.org/10.1038/s41370-021-00332-6.

16 Parnis, J. M.; Mackay, D.; Harner, T. Temperature Dependence of Henry’s Law Constants and KOA for Simple and Heteroatom-Substituted PAHs by COSMO-RS. Atmos. Environ. 2015, 110: 27–35. https://doi.org/10.1016/j.atmosenv.2015.03.032.

17 Yaman, B.; Dumanoglu, Y.; Odabasi, M. Measurement and Modeling the Phase Partitioning of Organophosphate Esters Using Their Temperature-Dependent Octanol-Air Partition Coefficients and Vapor Pressures. Environ. Sci. Technol. 2020, 54 (13): 8133–8143. https://doi.org/10.1021/acs.est.0c02823.

18 US EPA. CompTox Chemicals Dashboard. https://comptox.epa.gov/dashboard/ (accessed 2024-12-01).

19 Mansouri, K.; Grulke, C. M.; Judson, R. S.; Williams, A. J. OPERA Models for Predicting Physicochemical Properties and Environmental Fate Endpoints. J. Cheminform. 2018, 10 (1). https://doi.org/10.1186/s13321-018-0263-1.

20 Miller, J. D.; Herkert, N. J.; Stapleton, H. M.; Hsu-Kim, H. Silicone Wristbands for Assessing Personal Chemical Exposures: Impacts of Movement on Chemical Uptake Rates. Environ. Sci. Process. Impacts 2025, 27(3):670-681. https://doi.org/10.1039/D4EM00440J.