Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

SUPPLEMENTARY INFORMATION

Evaluation and guidelines for using polyurethane foam (PUF) passive air samplers to assess semi volatile organic compounds (SVOCs) in non-industrial indoor environments

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Materials and Methods

Sample preparation

Prior to deployment, the PUF-PAS were pre-extracted for 8 hours in acetone and 8 hours in dichloromethane, dried under vacuum and stored in multiple layers of solvent-rinsed aluminum foil inside air tight polyethylene zip bags.

After exposure, PUF disks were wrapped in two layers of aluminum foil, labelled, placed into zip-lock polyethylene bags, and transported in a cooler at 5 °C to the laboratory where they were stored at -20°C until analysis.

Sample Cleanup and Analysis

PCBs, OCPs, PBDEs, nBFRs, PCDDs, and PCDFs

Extraction and clean-up of the chlorinated and brominated SVOCs followed the same procedure for PUF-PAS disks, active PUFs and QMFs. Samples were extracted with toluene using automated warm Soxhlet extraction (Büchi B-811, Switzerland). ^{13}C labelled BDE 28, 47, 99, 100, 153, 154, 183 and 209 congeners, ^{13}C dl-PCBs congeners and ^{13}C US EPA PCDDs/Fs congeners (Wellington, Canada) were added prior to the extraction. Extracts were cleaned-up using glass column (1 cm i.d.) filled with 5 g of H_2SO_4 modified silica (Merck, Germany), and eluted with 40 mL DCM:*n*-hexane mixture (1:1). Cleaned extracts were evaporated using nitrogen (TurboVap II, Caliper LifeSciences, USA) and further fractionated on a charcoal column (6 mm i.d.), filled with 50 mg silica, 70 mg charcoal (Sigma Aldrich, Czech Republic) /silica (1:40) and 50 mg of silica. The column was prewashed with 5 mL of toluene, followed by 5 mL of DCM:cyclohexane mixture (30%), then the sample was applied and eluted with 9 mL DCM:cyclohexane mixture (30%) for fraction 1 (mono-ortho dl-PCBs, PBDEs, nBFRs) and 40 mL of toluene for fraction 2 (PCDDs/Fs, non-ortho dl-PCBs). Each fraction was concentrated under nitrogen, solvent exchanged to nonane and transferred into a vial insert. ^{13}C labelled syringe standards were added (final volume 50 µL).

PCBs and OCPs were analyzed on GC-MS/MS system consisting of a 6890N GC (Agilent, USA), equipped with a 60 m x 0.25 mm x 0.25 µm DB5-MS column (Agilent J&W, USA) coupled to Quattro MicroGC MS (Waters, Micromass, UK). The MS was operated in positive electron ionisation impact mode (EI+) using multiple reaction monitoring (MRM). Injection was

splitless 1 μL at 280°C, with He as carrier gas at 1.5 mL min^{-1}. The GC temperature programme was 80°C (1 min hold), then 15°C min^{-1} to 180°C, and finally 5°C min^{-1} to 300°C (5 min hold).

Analysis of PBDEs and nBFRs (Table S3) were performed using GC/HRMS consisting of a 7890A GC (Agilent, USA) equipped with a 15 m x 0.25 mm x 0.10 μm DB5 column (Agilent J&W, USA) coupled to AutoSpec Premier MS (Waters, Micromass, UK). The MS was operated in EI+ SIM mode at the resolution of >10 000. For BDE 209, the MS resolution was set to >5 000. Injection was splitless 1 μL at 280°C, with He as carrier gas at 1 mL min^{-1}. The GC temperature programme was 80°C (1 min hold), then 20°C min^{-1} to 250°C, followed by 1.5°C min^{-1} to 260°C (2 min hold) and 25°C min^{-1} to 320°C (4.5 min hold).

dl-PCBs and PCDDs/Fs were analyzed on the same GC/HRMS but on a 60m x 0.25mm x 0.25μm DB5-MS column. The MS was operated in EI+ SIM mode at the resolution of >10 000. Injection was splitless 1 μL at 280°C, with He as carrier gas at 1.7 mL min^{-1}, and 1.9 mL min^{-1} for dlPCBs and PCDD/Fs respectively. The GC temperature programme for dl-PCBs was 130°C (1 min hold), then 40°C min^{-1} to 190°C, followed by 1.5°C min^{-1} to 240°C and 8°C min^{-1} to 310°C (3.42 min hold). The temperature programme for PCDDs/Fs was 135°C (1 min hold), then 15°C min^{-1} to 220°C, followed by 1°C min^{-1} to 240°C, 3.5°C min^{-1} to 260 °C and 6°C min^{-1} to 320°C (5 min hold).

PAHs

Samples for PAHs analysis were extracted using automated warm Soxhlet extraction with dichloromethane (DCM). The extract was fractionated on a silica column (5 g of activated silica 0.063 – 0.200 mm). The first fraction (10 mL *n*-hexane), containing aliphatic hydrocarbons, was discarded. The second fraction (20 mL DCM), containing PAHs, was collected and then reduced by stream of nitrogen and transferred into an insert in a vial. Terphenyl was added as syringe standard (final volume 200 μL).

PAHs were analyzed on GC-MS, 6890N GC (Agilent, USA), equipped with a 60m x 0.25mm x 0.25um DB5-MS column (Agilent, J&W, USA) coupled to 5973N MS (Agilent, USA). Injection was 1 μL splitless at 280°C, with He as carrier gas at constant flow 1.5 mL min^{-1}. The GC programme was 80°C (1 min hold), then 15°C min^{-1} to 180°C, followed 5°C min^{-1} to 310°C (20 min hold). The MS was operated in EI+ SIM mode.

QA/QC

Method performance for was tested prior to sample preparation by analyzing a reference material (soil). Recovery of native analytes measured in a reference material varied from 88 to 100% for PCBs, from 75 to 98% for OCPs, from 72 to 102% for PAHs. The results for PBDEs, dl-PCBs, and PCDDs/Fs samples were recovery corrected. The remaining analytes were not recovery corrected. Recoveries were higher than 75% and 70% for PCBs+OCPs and PAHs, respectively. 3 PUF-PAS, 2 active PUFs and 2 QMFs field blanks were analyzed within each set of PUF-PAS and high volume samples.

Applicability for human health risk assessment

The risk assessment involves predicting the frequency of these cancer risks in exposed populations (probabilistic approach). We applied the inhalation exposure model of the EPA baseline risk assessment approach (EPA, 1998; EPA, 2013). SVOCs specific risks (i.e. an estimate of the probability that an individual will develop cancer during their lifetime) were calculated using the linear low-dose cancer risk equation.

The chronic daily intake CDI was calculated using the following equation:

$$CDI = C_{air} \cdot IF$$

where Cair is a compound concentration (mg m^{-3}) and IF is an Intake Factor (m^{-3} kg^{-1} day^{-1}).

Intake Factor is derived from equation:

$$IF = \frac{(IR\text{–}A \cdot EF \cdot ED \cdot ET)}{BW \cdot AT}$$

where IR-A (Inhalation Rate) is a breathing rate (m^3day^{-1}), EF (Exposure Frequency) is a number of exposures per year, ED (Exposure Duration) is a duration of exposure in years, ET (Exposure Time) is a number of hours per exposure, BW (Body Weight) is a default weight of the receptor body (kg), and AT (Averaging Time) is an average exposure extent over a lifetime (35 500 day for carcinogenic exposure). Standard exposure parameters were obtained from EPA exposure handbook (EPA, 2013) [IR-A=20 m^3day^{-1}; EF=365 days; ED=70 years; ET=24 $hday^{-1}$; BW=70 kg]. CDI for carcinogenic substances is called Life Averaged Daily Dose (LADD).

Human health risk related to contaminated indoor air depends on the extent of exposure as well as on the toxicological properties of SVOCs chemicals. The chemical-specific risks were calculated from the LADD and slope factor (SF) using the linear low-dose cancer risk equation:

Cancer Risk = LADD . SF

Slope factor are a plausible upper-bound estimate of probability of the cancer response per unit chemical intake over the lifetime (EPA, 2013). The SF values were calculated from Inhalation unit risk IUR according to EPA approach (detail description in EPA 2013 and Čupr et al. 2013).The results are compared to the carcinogenic benchmark level, i.e. an exposure posing an upper-bound lifetime excess cancer risk of 1E−6 (i.e. one cancer occurrence over one million people in population). An exposure for which the risk factor exceeds 1E−6 is scored as significant. Cancer risks above 1E−4 are considered as unacceptable, and addressing such health problems is a high priority (EPA, 2013).

Table S1. Information from the reference active sampler during the 12 weeks sampling period: average air concentrations, gas/particle distribution (expressed as % in gas phase), and detection frequency (%).

	C_{act} (pg m^{-3})/(ng m^{-3})*		Gas phase distribution (%)	Detection frequency (%)
	Average	Std	Average	
PCB 28	33.76	4.9	100	100
PCB 52	10.32	1.5	100	100
PCB 101	13.46	2.2	99	100
PCB 118	2.38	0.35	98	100
PCB 153	8.54	1.4	97	100
PCB 138	3.72	0. 6	95	100
PCB 180	1.52	0.24	87	100
Sum PCB-7	73.71		99	
PCB77	0.66	0.16	98	100
PCB81	0.03	<0.01	100	100
PCB126	0.01	<0.01	90	100
PCB169**	-	-	-	8
PCB105	0.68	0.19	97	100
PCB114	0.07	<0.01	100	100
PCB123	0.08	0.02	100	100
PCB156	0.44	0.16	93	100
PCB157	0.04	0.02	95	100
PCB167	0.25	0.08	96	100
PCB189	0.03	0.01	77	100
Sum dlPCB	7.50		98	
PeCB	4.07	0.69	100	100
HCB	65.99	8.1	100	100
α-HCH**	-	-	-	-
β-HCH**	-	-	-	-
γ-HCH**	-	-	-	-
δ-HCH**	-	-	-	-
Sum HCHs	-		-	
***o,p'*-DDE**	1.41	2.4	99	100
***p,p'*-DDE**	6.46	1.7	88	100
***o,p'*-DDD**	0.52	0.07	95	100

***p,p'*-DDD**	0.62	0.14	83	100
***o,p'*-DDT**	4.11	0.79	98	100
***p,p'*-DDT**	2.69	0.60	93	100
Sum DDTs	15.81		95	
BDE 28	2.15	0.49	100	100
BDE 47	3.03	0.85	94	100
BDE 66**	-	-	-	0
BDE 100	0.25	0.10	88	100
BDE 99	0.99	0.36	66	100
BDE 85**	-	-	-	0
BDE 153**	-	-	-	17
BDE 154	0.15	0.05	0	67
BDE 183	7.04	2.16	1	75
BDE 209**	-	-	-	-
Sum BDE w/o 209	13.61		40	
ATE	0.15	0.04	82	100
α,β,γ,δ-TBECH	68.99	21.81	99	100
BATE	0.04	0.01	100	92
TBCO	7.99	2.94	100	100
p-TBX	0.08	0.03	97	100
DPMA	0.06	0.03	97	83
PBEB	0.49	0.13	98	100
PBT	11.82	4.39	97	100
DPTE	1.97	0.80	95	100
HBB	9.41	2.55	95	100
HCDBCO**	-	-	-	0
EHTBB	0.20	0.06	81	100
BTBPE	0.60	0.81	20	100
s-DP**	-	-	-	-
a-DP**	-	-	-	-
BEHTBP	0.17	0.16	44	67
DBDPE	2.24	2.10	7	100
Sum nBFR	104		91	
Naphthalene	1.86*	0.83	88	83
Acenaphtylene	0.20*	0.12	83	92
Acenapthene	0.36*	0.16	99	100

Fluorene	1.47*	0.57	97	100
Phenanthrene	13.87*	4.89	96	100
Anthracene	0.47*	0.20	84	100
Fluoranthene	3.38*	1.65	72	100
Pyrene	2.88*	1.36	73	100
Benz(a)anthracene	0.71*	0.49	58	100
Chrysene	1.09*	0.68	48	100
Benzo(b)fluoranthene	1.84*	1.02	24	100
Benzo(k)fluoranthene	0.61*	0.35	26	100
Benzo(a)pyrene	1.07*	0.65	17	100
Indeno(123cd)pyrene	1.52*	0.88	0	100
Dibenz(ah)anthracene	0.09*	0.04	0	100
Benzo(ghi)perylene	1.15*	0.60	0	100
Sum EPA PAHs	32.55*		73	
2378-TCDD**	0.002	0.001	50	25
12378-PeCDD**	0.006	0.002	-	17
123478-HxCDD**	0.008	0.004	47	63
123678-HxCDD**	0.012	0.005	24	63
123789-HxCDD	0.013	0.003	24	63
1234678-HpCDD	0.121	0.044	14	100
OCDD	0.301	0.109	5	100
Sum PCDD	0.45		10	
2378-TCDF	0.010	0.005	80	63
12378-PeCDF	0.010	0.005	62	100
23478-PeCDF	0.019	0.008	50	100
123478-HxCDF	0.017	0.007	36	100
123678-HxCDF	0.017	0.007	40	100
234678-HxCDF	0.022	0.009	27	100
123789-HxCDF	0.010	0.005	45	83
1234678-HpCDF	0.064	0.027	22	100
1234789-HpCDF	0.018	0.007	33	100
OCDF	0.055	0.024	18	83
Sum PCDF	0.24		32	

116 *Air concentrations presented in ng m^{-3}.

117 **Excluded due to laboratory problems with detection.

Table S2. Three detection parameters for PUF-PAS; analytical limit of detection (LOD), method detection limit (MDL, from field blanks), and lowest detection concentration (LDC) at the sampling site during the calibration study.

	Analytical LOD (pg sample^{-1})	MDL (pg sample^{-1})	LDC (pg m^{-3}) 1 week exposure time	LDC (pg m^{-3}) 4 weeks exposure time	LDC (pg m^{-3}) 12 weeks exposure time
PCB 28	4.8	400	59.7	14.92	4.97
PCB 52	7.4	98	10.5	2.62	0.87
PCB 101	9.1	67	5.75	1.44	0.48
PCB 118	8.1	32	3.70	0.93	0.31
PCB 153	6.7	92	7.54	1.88	0.63
PCB 138	7.9	76	6.27	1.57	0.52
PCB 180	9.5	35	3.25	0.81	0.27
PCB77	0.3	7.1	0.99	0.25	0.08
PCB81	0.3	0.8	0.11	0.03	0.01
PCB105	0.4	6.7	0.94	0.23	0.08
PCB114	0.4	1.4	0.18	0.05	0.02
PCB123	0.4	0.9	0.09	0.02	0.008
PCB156	0.4	6.8	0.87	0.22	0.07
PCB157	0.4	0.8	0.09	0.02	0.008
PCB167	0.4	3.0	0.39	0.10	0.03
PCB189	0.4	0.9	0.12	0.03	0.01
PeCB	20.9	247	10.23	2.56	0.85
HCB	13.2	652	37.69	9.42	3.14
o,p'-DDE	5.0	18	1.93	0.48	0.16
p,p'-DDE	6.0	300	32.79	8.20	2.73
o,p'-DDD	4.7	49	4.95	1.23	0.41
p,p'-DDD	6.2	23	2.67	0.67	0.22
o,p'-DDT	16.9	38	4.70	1.18	0.39
p,p'-DDT	21.2	21	2.73	0.68	0.23
BDE 28	0.4	1.2	0.15	0.04	0.01
BDE 47	0.4	21	2.76	0.69	0.23
BDE 99	0.5	8.7	1.39	0.35	0.12
BDE 100	0.5	0	-	-	-
BDE 183	0.8	0	-	-	-
ATE	2.1	3.8	0.21	0.05	0.02

α,β,γ,δ-TBECH	2.4	100	0.24	0.06	0.02
BATE	1.0	1.0	0.09	0.02	0.008
TBCO	2.6	11	0.19	0.05	0.02
p-TBX	0.8	2.9	0.02	0.006	0.002
DPMA	0.8	0.8	0.11	0.01	0.009
PBEB	0.3	0.9	0.02	0.005	0.002
PBT	0.3	8.0	0.02	0.005	0.002
DPTE	11.0	11	0.74	0.18	0.06
HBB	0.2	11	0.02	0.004	0.001
EHTBB	10.0	10	1.53	0.38	0.13
BTBPE	1.3	25	0.05	0.01	0.004
BEHTBP	6.1	167	0.86	0.22	0.07
DBDPE	8.3	8.3	1.18	0.29	0.10
Naphthalene	0.2	400	3.07	0.77	0.26
Acenaphtylene	0.2	17	1.17	0.29	0.10
Acenapthene	0.2	14	0.13	0.03	0.01
Fluorene	0.2	47	1.22	0.31	0.10
Phenanthrene	0.2	95	8.25	2.06	0.69
Anthracene	0.2	3.0			
Fluoranthene	0.2	22	3.72	0.93	0.31
Pyrene	0.2	22	3.79	0.94	0.31
Benz(a)anthracene	0.2	0.6	0.60	0.15	0.05
Chrysene	0.2	1.4	1.13	0.28	0.09
Benzo(b)fluoranthene	0.2				
Benzo(k)fluoranthene	0.2				
Benzo(a)pyrene	0.2				
Indeno(123cd)pyrene	0.2				
Dibenz(ah)anthracene	0.2				
Benzo(ghi)perylene	0.2				
123478-HxCDD	0.4	0.7	0.04	0.01	0.004
123678-HxCDD	0.4	0.7	0.07	0.02	0.006
123789-HxCDD	0.4	0.7	0.04	0.01	0.004
1234678-HpCDD	0.5	1.2	0.36	0.09	0.03
OCDD	0.7	3.2	1.61	0.40	0.13
2378-TCDF	0.3	0.3	0.09	0.02	0.008
12378-PeCDF	0.3	0.3	0.04	0.01	0.003

23478-PeCDF	0.3	0.3	0.09	0.02	0.007
123478-HxCDF	0.4	0.6	0.11	0.03	0.009
123678-HxCDF	0.3	0.3	0.05	0.01	0.004
234678-HxCDF	0.3	0.3	0.04	0.01	0.004
123789-HxCDF	0.4	0.8	0.05	0.01	0.004
1234678-HpCDF	0.4	0.6	0.11	0.03	0.009
1234789-HpCDF	0.5	0.5	0.02	0.005	0.002
OCDF	0.6	1.1	0.10	0.03	0.008

RECOVERIES

The results for PCDDs/Fs, dl-PCBs, PBDEs, and NBFRs were recovery corrected using isotopically labelled standards. The recoveries of PCDDs/Fs were determined using 16 13C12 PCDDs/Fs - 2378-TCDD, 12378-PeCDD, 123478-HxCDD, 123678-HxCDD, 1234678-HpCDD, OCDD, 2378-TCDF, 12378-PeCDF, 23478-PeCDF, 123478-HxCDF, 123678-HxCDF, 123789-HxCDF, 234678-HxCDF, 1234678-HpCDF, 1234789-HpCDF and OCDF, and varied in the range of 55-90% (40% for OCDD and OCDF). For dl-PCBs, the average recoveries ranged between 60 and 90% based on 12 dl-PCBs 13C12 (77, 81, 105, 114, 118, 123, 126, 156, 157, 167, 169, 189). For PBDEs, recoveries were calculated using 8 13C12 BDEs (13C12 - 28, 47, 99, 100, 153, 154, 183, 209) and in the average ranged between 60 and 110% (45% for BDE 209). For NBFRs, the average recoveries varied from 50 to 125%. Following standards were used: 13C- HBB, sDP, aDP, DBDPE, BTBPE. Low-resolution MS was used for remaining analytes (PAHs, OCPs and indicator PCBs) and method recoveries were tested prior to the analyses. Recoveries of native analytes measured for a reference material varied from 88 to 100% for PCBs, from 75 to 98% for OCPs, from 72 to 102% for PAHs. Non-isotopically labeled recovery standards were added to all samples. Recoveries were higher than 75% and 70% for all samples for indicator PCBs+OCPs, and PAHs, respectively. Recovery factors were not applied to any of the data.

Table S3. Summary of linear regression analysis of compound fingerprints in PUF-PAS versus compound fingerprints in reference active sampler (bulk phase and gas phase).

		Reference active sampler	
		Bulk phase	**Gas phase**
PCB-7	R^2	0.95	0.94
	Slope	0.81	0.79
dlPCBs	R^2	0.98	0.98
	Slope	1.02	0.99
OCPs	R^2	0.91	0.90
	Slope	1.07	1.05
PBDEs	R^2	0.05	0.61
	Slope	0.27	0.72
nBFRs	R^2	0.62	0.57
	Slope	0.81	0.81
PAHs*	R^2	0.68	0.77
	Slope	1.02	0.83
PCDDs	R^2	0.87	0.04
	Slope	0.56	0.20
PCDFs	R^2	0.33	0.03
	Slope	0.64	0.41

*Naphthalene excluded from the fingerprints

126 **Table S4.** Exposure time specific R_S (m^3 day^{-1}) obtained by *Method 2*. Average of triplicates.

	Exposure time (weeks)											
	1	2	3	4	5	6	7	8	9	10	11	12
PCBs												
PCB 28	5.3	3.5	2.3	1.7	1.6	1.3	1.3	1.4	1.3	1.1	1.2	1.4
PCB 52	4.2	3.1	2.6	1.9	2.0	1.6	1.9	1.7	1.6	1.3	1.5	1.7
PCB 101	4.7	3.4	2.7	2.2	2.4	1.9	2.2	2.0	1.9	1.5	1.7	2.1
PCB 118	3.4	2.7	1.9	1.8	1.6	1.4	1.4	1.3	1.4	1.1	1.2	1.7
PCB 153	6.2	4.3	3.3	2.8	2.9	2.3	2.6	2.2	2.1	1.7	1.9	2.4
PCB 138	6.6	4.3	3.3	2.9	2.9	2.3	2.5	2.2	2.2	1.8	1.9	2.4
PCB 180	6.9	4.4	3.5	2.7	2.9	2.3	2.5	2.0	2.2	1.6	1.9	2.2
PCB 77	4.7	2.5	1.8	1.7	1.2	1.2	1.1	1.2	1.2	1.2	1.1	1.6
PCB 81	4.2		1.4	2.0	1.3	1.2	1.1	1.0	1.1	1.3	1.2	1.5
PCB 105	3.8	2.3	1.7	1.6	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.5
PCB 114	3.6	2.0	1.6	1.5	1.1	1.0	1.1	0.9	1.1	1.1	1.1	1.4
PCB 123	3.1	2.2	1.7	1.6	1.5	1.2	1.2	1.0	1.6	1.4	1.4	1.5
PCB 156	2.4	1.8	1.4	1.5	1.2	1.2	1.1	1.0	1.3	1.1	1.2	1.6
PCB 157	0.6	0.9	0.9	1.1	0.9	1.0	0.8	0.7	1.0	0.8	0.9	1.4
PCB 167	3.5	2.1	1.6	1.6	1.2	1.2	1.1	1.1	1.2	1.1	1.2	1.1
PCB 189	3.9	2.9	2.1	1.8	1.4	1.5	0.9	1.0	1.3	1.0	1.4	1.2
OCPs												
PeCB	23.2	15.9	11.7	9.7	8.2	6.6	6.5	6.8	5.5	3.9	5.6	4.7
HCB	6.4	5.5	4.1	3.5	3.4	2.8	2.7	2.8	2.6	2.4	2.8	3.0
o,p′-DDE	3.5	2.8	2.4	2.0	2.1	1.6	1.9	1.6	1.5	1.3	1.3	1.8
p,p′-DDE		3.3	5.1	3.4	3.1	2.4	2.8	2.3	2.1	1.5	1.7	2.2
o,p′-DDD	3.5	6.1	3.2	3.5	3.4	2.9	3.1	2.7	2.9	2.1	2.1	2.3
p,p′-DDD	8.4	4.4	3.0	2.5	2.3	2.3	2.4	2.0	1.8	1.9	1.5	1.7
o,p′-DDT	4.3	3.0	2.4	2.0	2.2	1.6	2.3	1.5	1.5	1.4	1.2	1.5
p,p′-DDT	6.1	3.8	2.8	1.8	2.5	1.8	2.8	1.5	1.5	1.9	1.2	1.5
PBDEs												
BDE 28	2.2	2.0	1.3	1.3	1.2	1.0	1.2	1.1	1.2	1.1	1.2	1.5
BDE 47	3.3	2.4	1.8	1.7	1.3	1.2	1.1	1.2	1.2	1.2	1.4	1.5
BDE 100		3.9		2.0			0.8	1.2	1.2	1.6	1.3	1.8
BDE 99	4.5	2.7	1.3	1.3	1.2	1.3	0.9	1.0	1.0	1.3	1.5	1.1
nBFRs												
ATE	3.4	3.3	2.6	2.5	1.8	4.1	1.6	2.2	5.7	1.5	1.2	2.9
a,b,g,d-TBECH	2.0	1.9	1.7	1.5	1.5	1.4	1.5	1.5	1.4	1.1	1.5	2.0
BATE	3.0	2.6	2.7	1.7	1.2	2.0	1.7	1.8	2.9	1.3	1.1	2.9
TBCO	2.0	1.8	2.0	1.7	1.8	1.5	1.7	1.9	2.0	1.5	1.7	2.4
p-TBX	6.5	7.5	6.7	5.7	5.3	7.9	4.8	5.0	5.0	4.1	19.4	10.0
PBEB	3.5	3.1	2.5	2.5	2.2	2.4	2.2	2.2	2.3	1.6	1.4	2.8
PBT		2.9	3.2	3.0	2.6	2.7	1.9	2.0	2.0	1.7	2.9	2.9

DPTE	2.1	1.5	1.6	1.5	1.4	1.6	1.6	2.4		1.2	1.1	1.0
HBB		2.5	2.3	2.2	2.0	1.9	1.6	1.6	1.6	1.5	1.4	2.1
EHTBB	4.9	2.9	2.2	1.6	1.4	1.1	1.8	1.4	1.2	1.4	1.0	1.0
PAHs												
Naphthalene	16.4	13.3	17.2	16.6	7.0	8.1	5.9	5.1	6.9	6.9	3.6	4.6
Fluorene	10.1	8.7	8.0	7.9	7.3	7.3	6.6	6.4	6.0	4.8	2.9	3.8
Phenanthrene	2.0	1.8	1.6	1.7	1.5	1.6	1.6	1.6	1.6	1.3	1.0	1.1
Fluoranthene	1.4	0.7	0.8	0.8	0.6	0.7	0.9	1.0	1.0	0.7	0.6	0.5
Pyrene	1.2	0.9	0.8	0.8	0.7	0.8	0.8	0.9	0.9	0.7	0.6	0.5
Benz(a)anthracene	1.2	0.9	0.1	0.1	0.1	0.1	0.1	0.2	0.2	0.1	0.1	0.1
Chrysene	0.5	0.1	0.1	0.1	0.1	0.1	0.2	0.2	0.2	0.2	0.1	0.1
Benzo(b)fluoranthene									0.06	0.05	0.05	0.03
Benzo(k)fluoranthene									0.05	0.05	0.04	0.03
PCDDs												
1234678-HpCDD					1.4		0.4			0.6	0.4	0.5
OCDD					0.6		0.3			0.4	0.3	0.3
PCDFs												0.5
2378-TCDF							1.0		0.9	0.8	0.7	
12378-PeCDF				1.4	1.2	1.1	1.0	0.7		1.2	0.8	0.4
23478-PeCDF				1.3	0.7	0.9	0.4	0.3	0.3	0.7	0.5	0.3
123478-HxCDF					2.2		0.9			1.2		0.7
123678-HxCDF					2.5		0.9			1.5	0.8	0.9
234678-HxCDF				1.8	2.7	0.9	0.5	0.3		0.8	0.6	0.5
123789-HxCDF					6.4					3.0		2.0
1234678-HpCDF			3.5	2.2	2.9	1.2	0.7	0.4		1.1	0.6	0.8
1234789-HpCDF		14.0	8.9	9.2	10.6	3.0	2.4			3.2	1.5	2.0
OCDF		10.4	6.4	5.6	3.4	2.3	1.5			2.1	0.9	1.5

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Table S5. Comparison of compound specific R_S to R_S for specific homologues (only PCBs and PAHs), SVOC classes, and generic SVOCs. Presented are the potential percentage errors added to the end point results (i.e. estimated air concentrations) when applying homologue or generic R_S instead of compound specific R_S.

	Homologue specific R_S	SVOC class specific R_S	Generic R_S for all SVOCs
PCBs	5-30% (15%)	5-40% (20%)	1-70% (30%)
OCPs	1-15% (7%)	15-50% (34%)	10-60% (30%)
PBDEs		5-60% (30%)	30-70% (50%)
nBFRs		5-60% (30%)	2-70% (20%)
PAHs	10-280% (60%)	20-2800% (920%)	10-5000% (1200%)
PCDD/Fs		5-160% (40%)	2-320% (90%)

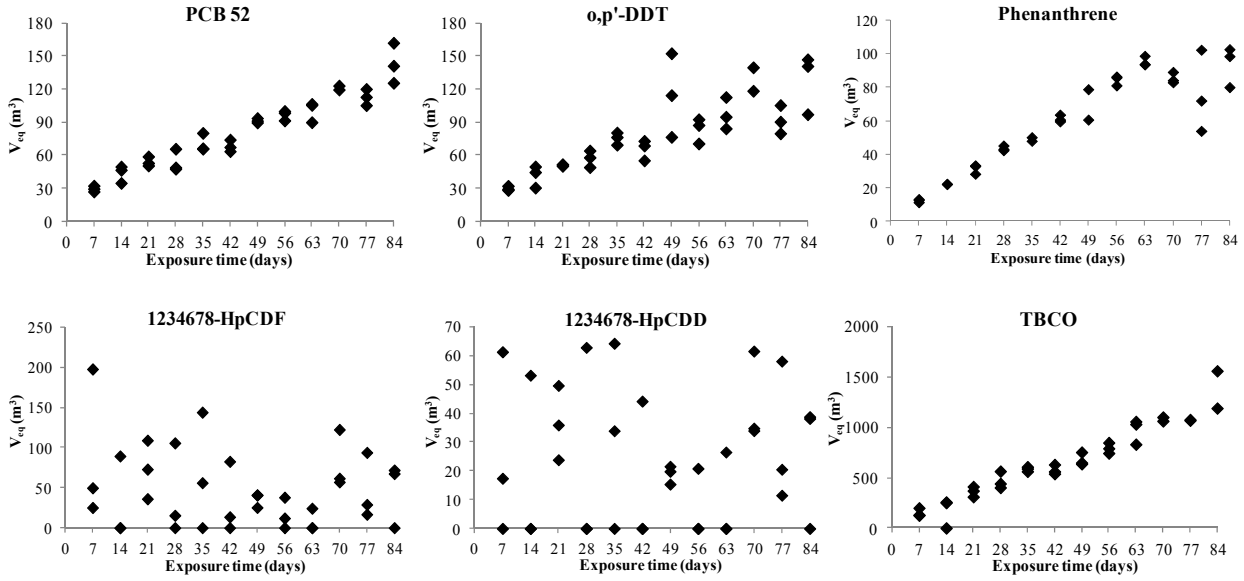

Figure S1. Accumulation pattern of compounds (Veq) in PUF-PAS used for determination of sampling rates with *Method 1*.

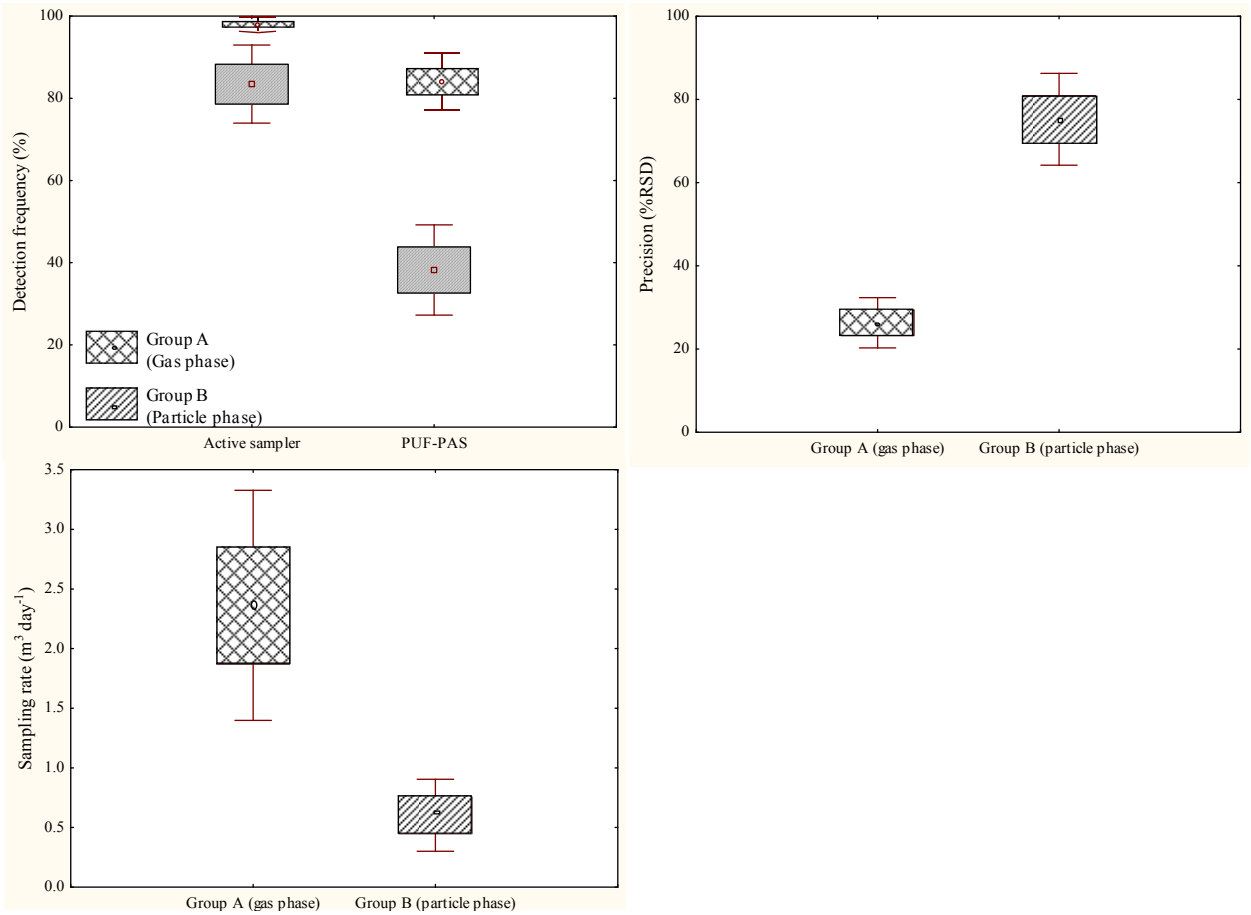

Figure S2. Comparison of two indicators for PUF-PAS performance (i.e. detection frequency and precision of replicates) as well as sampling rates for gas phase and particle associated compounds.