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Supporting Information

Exploring the Role of the Sampler Housing in Limiting Uptake of Semivolatile Organic

Compounds in Passive Air Samplers

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Figure S1. Experiment setup to study chemical distributions in the axially segmented passive sampling medium (XAD mesh cylinder) under wind and wind still conditions.

Class	Chemical	Target Ion	Qualify Ion	(Qual. /Targ.) *100%	LOD ^a (ng/sample)
Internal Standard	Mirex	272	274	81.1	n/a
Surrogate Standard	¹³ CPCB77	304	302	77.2	n/a
Surrogate Standard	¹³ CPCB101	338	340	64.8	n/a
Surrogate Standard	¹³ CPCB141	372	374	81	n/a
Surrogate Standard	¹³ CPCB178	406	408	97.2	n/a
Target Analyte	Tri-CB	256	258	98	0.5
Target Analyte	Tetra-CB	292	290	76.7	1
Target Analyte	Penta-CB	326	328	65.3	0.2
Target Analyte	Hexa-CB	360	362	81.4	1.5

Table S1. Target ions, quanlify ions and limit of detection (LOD) of the PCB homolog groups analyzed using GC-MS selected ion monitoring mode.

^a LOD calculated as the chemical amount of which the instrument detects a signal corresponding to three times of the noise level.



Figure S2. The blue, red and green bars indicate the amounts of PCBs accumulated in three axial segments of XAD-filled mesh cylinders of passive air samplers deployed in four indoor locations (L1-4), at indoor location 1 with lab generated wind (L1W), and at an outdoor location (OD). The yellow line indicates the amount of PCBs accumulated in a non-segmented XAD-filled mesh cylinder deployed at the same four indoor locations.



Figure S3. Distribution of PCBs in the three axially segmented XAD mesh cylinders in the normal housings (ODN), black housings (ODB) and housings shaded from sunshine (ODC).



Figure S4. Distribution of PCBs in the three axially segmented XAD mesh cylinders in the duplicated PASs blown with lab generated wind.



Figure S5. Distribution of PCBs in the three axially segmented XAD mesh cylinders in the duplicated PASs (a) under the quasi wind still condition (L); (b) under the lab generated windy condition (L1W); (c) in outdoor environment (ODN).

		ANOVA	on In-tr	ansform	ned PCB am	nount	S	Scheffé's Post Hoc Test			
Sample		SS	df	MS	F	p		В	М	т	
	PSM Segment	8.0	2.0	4.0	148.8	0.000	В		<0.001	<0. 001 <0	
L1	PCB Congener Segment *	63.6	14.0	4.5	169.2	0.000	М	<0.001		001	
	Congener	0.0	28.0	0.0	0.0	1.000	Т	<0.001	<0.001		
								В	М	T	
	PSM Segment	0.9	2.0	0.5	2.5	0.092	В		0.774	42	
L1_Wind	PCB Congener Segment *	64.4	14.0	4.6	24.9	0.000	М	0.774		0.1	
	Congener	0.0	28.0	0.0	0.0	1.000	т	0.342	0.1		
								В	м	T	
	PSM Segment	7.0	2.0	3.5	70.9	0.000	В		<0.001	<0. 001 <0.	
L2	PCB Congener Segment *	48.7	14.0	3.5	70.6	0.000	М	<0.001		001	
	Congener	0.3	28.0	0.0	0.2	1.000	т	<0.001	<0.001		
								В	м	Т	
	PSM Segment	1.2	2.0	0.6	9.9	0.000	В		<0.001	0.2 09 0.0	
L3	PCB Congener Segment *	42.7	14.0	3.1	49.1	0.000	М	<0.001		4	
	Congener	0.1	28.0	0.0	0.1	1.000	т	0.209	0.04		
								В	м	т	
	PSM Segment	2.4	2.0	1.2	36.6	0.000	В		<0.001	<0. 001	
L4	PCB Congener Segment *	39.9	11.0	3.6	111.4	0.000	М	<0.001		87	
	Congener	0.1	22.0	0.0	0.2	1.000	т	<0.001	0.787		
								В	м	т	
	PSM Segment	0.5	2.0	0.2	79.6	0.000	В		<0.001	<0. 001 <0	
OD	PCB Congener	42.5	14.0	3.0	1034.8	0.000	М	<0.001		<0. 001	
	Congener	0.0	28.0	0.0	0.3	0.999	т	<0.001	<0.001		
								В	М	Т	
	PSM Segment	2.7	2.0	1.4	197.1	0.000	В		<0.001	<0. 001 <0	
OD_Black	PCB Congener Segment *	42.2	14.0	3.0	432.4	0.000	М	<0.001		<0. 001	
	Congener	0.0	28.0	0.0	0.2	1.000	т	< 0.001	<0.001		

Table S2. Two-factorial ANOVA and Scheffé's post hoc test on the PCB congeners accumulated at the three axially segmented PSM.

								В	м	т
	PSM Segment	0.5	2.0	0.2	177.9	0.000	В		<0.001	<0. 001
OD_Covere d	PCB Congener Segment *	44.2	14.0	3.2	2428.6	0.000	М	<0.001		<0. 001
	Congener	0.0	28.0	0.0	0.3	0.998	т	<0.001	<0.001	

Table S3. Descriptive statistics on the temperature (°C) recorded by the temperature logger in the passive air samplers deployed outdoors.





Figure S6. Temperature differences in the normal, black, and shaded passive sampler housing.



Figure S7. Comparison of temperatures (°C) at different positions within the passive air sampling housing.

						Outo	door						
Sourc e	Sum of Squa res	d f	Mea n Squ are	F	Sig.	Outd	loor	Singl	e cylind	ler x 4	4	cylinde	ers
Corre cted Model	4.7	1 8	0.3	232.3	<0.0 01			Тор	Mid dle	Bott om	Тор	Mid dle	Bott om
Interc ept	116.8	1	116. 8	10284 5.4	<0.0 01		Тор			1			
PCB conge ner	4.5	1 3	0.3	306.7	<0.0 01	Single cylinder	Middle	0.17 5					
PSM segm ent	0.2	5	0.0	39.0	<0.0 01	x 4	Bottom	0.01 9	0.96 0				
Error	0.1	6 5	0.0				Тор	<0.0 01	<0.0 01	<0.00 1			
Total	121.6	8 4				4 cylindors	Middle	0.95 4	0.67 5	0.186	<0.0 01		
Corre cted Total	4.8	8 3				cymuers	Bottom	<0.0 01	0.10 0	0.496	<0.0 01	0.00 1	
						Ind							
	Туре					ma	001						
Sourc e	III Sum of Squa res	d f	Mea n Squ are	F	Sig.	Indo	oor	Singl	e cylino	ler x 4	4	cylinde	ers
Corre cted Model	9.8	1 8	0.5	3725.7	<0.0 01			Тор	Mid dle	Bott om	Тор	Mid dle	Bott om
Interc ept	744.7	1	744. 7	51194 73.2	<0.0 01		Тор						
PCB conge ner	8	1 3	0.6	4252	<0.0 01	Single cylinder	Middle	<0.0 01					
PSM segm ent	1.7	5	0.3	2357.6	<0.0 01	x 4	Bottom	<0.0 01	<0.0 01				
Error	0	6 5	0				Тор	<0.0 01	<0.0 01	<0.00 1			
Total	754.4	8 4				4 cylinders	Middle	<0.0 01	<0.0 01	<0.00 1	<0.0 01		
Corre cted Total	9.8	8 3				cymacr5	Bottom	<0.0 01	<0.0 01	<0.00 1	<0.0 01	<0.0 01	

Table S4. Randomized Block ANOVA and Scheffé's post hoc test on the PCB congeners accumulated in the three axially segmented PSM.



Figure S8. Distribution of PCBs in axially segmented XAD mesh cylinders of passive air samplers deployed in outdoor and indoor environment

Study Design of Hawaiian Samples: Pre-extracted XAD-resin was cleaned by Soxhlet extractions with acetone for 24 hours and subsequently with hexane for an additional 24 hours. Pre-cleaned mesh cylinders were filled with XAD-resin and suspended in a protective stainless steel tubes for transportation to the Big Island, Hawaii. Following the deployment period, the XAD-filled mesh cylinders were collected and stored in a freezer located in Hilo, Hawaii prior to being transported back to Toronto. Upon arrival in Toronto, the mesh cylinders were stored frozen at a temperature of -20 °C until extraction.

Hawaiian Sample Extraction. Before extraction, each sample was spiked with 100 μ L of isotope-labeled standards. The concentrations and identities of each isotope-labeled standard used are listed in Table S3. XAD-resin was transferred into 33 or 66 mL ASE cells for short and long mesh cylinders, respectively. They were subsequently extracted by pressurized liquid extraction using an Accelerated Solvent Extractor (ASE[®]) 350 (Dionex, Sunnyvale, CA, USA) with method previously used in our lab^{Zhang et al., 2012, Primbs et al., 2008}: 50:50 (%) acetone: hexane at 75°C, pressure 1500 psi; static time 5 min; static cycles 3; flush volume 100%; purge time 240 s. Extracts were then rotoevaporated to approximately 2 mL and eluted through approximately 1 g of anhydrous sodium sulphate (baked overnight at 400°C) column to remove moisture. The eluent was blown down to 1 mL with high purity nitrogen, solvent-exchanged to iso-octane, and further reduced to 0.5 mL in a GC vial. 10 μ L of 10 ng· μ L⁻¹ mirex was spiked as an internal standard for volume correction, and 20 μ L of 1 ng· μ L⁻¹ each of BDE-75, 116, 205 were added to quantify the recovery of the surrogates.

Hawaiian Sample Analysis. Extracts were analyzed for selected PAHs, PBDEs, and pesticides using an Agilent 7890A gas chromatography (GC) coupled to an Agilent 7000A triple quadrupole mass spectrometry (MS/MS) with electron impact (EI) ion source and programmed on multiple reaction monitoring mode. To analyze for PAHs and pesticides, 1.0 μ L of extract was injected at 250 °C in splitless mode and separated by a HP-5MS capillary column (30 m length × 250 μ m ID x 0.25 μ m film thickness, J&W Scientific) with nitrogen (1.5 mL·min⁻¹) as the collision gas and helium (1.2 mL·min⁻¹) as the carrier gas. The GC temperature used to analyze PAHs was programmed at 90 °C for 1 min, to 250 °C at 10 °C·min⁻¹, to 300 °C at 5 °C·min⁻¹, and held for 3 min. The analysis of pesticides consist of programming the GC oven at 70 °C for 1 min, then to 150 °C increased at a rate of 50 °C·min⁻¹ for 0 min, then raised to 200 °C at 6 °C·min⁻¹ for 3 min and then to a final temperature of 300 °C at 10°C·min⁻¹ for 0 min. For analyses of PBDEs, a HP-5MS capillary column (1.5 mL·min⁻¹) and helium (1.8 mL·min⁻¹) to separate 2.0 μ L of extract injected in splitless mode (injector temperature 285 °C). The GC oven was programmed initially at 100 °C, then raised to 185 °C at 25 °C·min⁻¹, then 275 °C at 15 °C·min⁻¹.

and then to a final temperature of 315 °C at 45 °C·min⁻¹, and held for 6 min. For analyses of all compounds, the ion source and quadrupole temperatures were held at 230 °C and 150 °C, respectively. The ions monitors are listed in Table S4-S6.

QA/QC of Hawaiian Samples. 8 field blanks were collected by exposing mesh cylinders filled with XAD-resin to ambient air at the sampling site for 1 min and subsequently storing, transporting, extracting, and analyzing the field blanks with the identical procedure as the other Hawaiian samples. All field blanks contain less than 10% of the SVOCs amount in the samples, with 90% of the field blanks found with <5%. Due to low blank levels, the reported data were not blank corrected. Recoveries of the isotope labeled standards that were spiked prior to sample extraction ranged between 61-134% PAHs, 63-121% for PBDEs, 73-108% for pesticides.

Chemical	Concentration (ng/uL)	Chemical	Concentration (ng/uL)
¹³ C12 BDE28	0.2	D10 Acenaphthene	0.25
¹³ C12 BDE47	0.19	D8 Acenaphthylene	0.25
¹³ C12 BDE153	0.19	D10 Anthracene	0.25
¹³ C12 BDE209	0.84	D12 Benz[a]anthracene	0.25
		D12 Benzo[b]fluoranthene	0.25
¹³ C12 PCB77	0.2	D12 Benzo[k]fluoranthene	0.25
¹³ C12 PCB101	0.2	D12 Benzo[g,h,i]perylene	0.25
¹³ C12 PCB141	0.2	D12 Benzo[a]pyrene	0.25
¹³ C12 PCB178	0.2	D12 Chrysene	0.25
		D14 Dibenz[a,h]anthracene	0.25
D4 endosulfan	0.25	D10 Fluoranthene	0.25
D5 atrazine	0.25	D10 Fluorene	0.25
D10 chlorpyrifos	0.25	D12 Indeno[1,2,3-cd]pyrene	0.25
D14 trifluralin	0.25	D8 Naphthalene	0.25
¹³ C6 HCB	0.25	D10 Phenathrene	0.25
¹³ C6 α-HCH	0.25	D10 Pyrene	0.25
¹³ C6 γ-HCH	0.25		
¹³ C6 PeCB	0.25		
¹³ C4 dieldrin	0.25		
¹³ C10 trans chlordane	0.25		
¹³ C12 4,4 DDT	0.25		

Table S5. Details on surrogate standards spiked in samples.

Chemica	Precursor	Product	Collision	Chemical	Precursor	Product	Collision
	lon	lon	Energy	chennear	lon	lon	Energy
Fluo	166.0	165.0	30	D10-Fluo	176.0	174.0	30
Phe	178.0	152.0	20	D10-Phe	188.0	160.0	34
Ant	178.0	152.0	20	D10-Ant	188.0	184.0	34
Flu	202.0	201.0	30	D10-Flu	212.0	210.0	30
Pyr	202.0	201.0	30	D10-Pyr	212.0	210.0	30
Chry	228.0	226.0	38	D12-Chry	240.0	236.0	38
BaA	228.0	226.0	38	D12-BaA	240.0	236.0	38
BbF	252.0	250.0	42	D12-BbF	264.0	260.0	42
BkF	252.0	250.0	42	D12-BkF	264.0	260.0	42
BeP	252.0	250.0	42				
BaP	252.0	250.0	42	D12-BaP	264.0	260.3	42
IP	276.0	274.0	42	D12-IP	288.0	284.0	42
DBA	278.0	276.0	38	D14-DBA	292.0	284.0	40
BghiP	276.0	274.0	30	D12-BghiP	288.0	284.0	38
Mirex	274.0	274.0	0				

Table S6. Precursor ions, product ions and collision energies for the multiple reaction monitoring mode for PAH analysis.

Fluo: fluorene; Phe: phenanthrene; Ant: anthrancene; Flu: fluoranthene; Pyr: pyrene; Chry: chrysene; BaA: benzo(a)pyrene; BbF: benzo(b)fluoranthene; BkF: benzo(k)fluoranthene; BeP: benzo(e)pyrene; BaP: benzo(a)pyrene; IP: Indeno(1,2,3-c,d)pyrene; DBA: Dibenzo(a,b)anthracene; BghiP: Benzo(g,h,i)perylene

Table S7. Precursor ions, product ions and collision energies for the multiple reaction monitoring mode for PBDE analysis.

Chamical	Precursor	Product	Collision	Chamical	Precursor	Product	Collision
Chemical	lon	lon	Energy	Chemical	lon	lon	Energy
BDE-17	247.9	139.0	30	¹³ C-BDE-28	259.9	150.1	30
BDE-28	247.9	139.0	30	¹³ C -BDE-47	497.7	337.9	25
BDE-47	485.7	325.8	55	¹³ C -BDE153	655.7	495.7	25
BDE-66	325.9	138.0	55	¹³ C -BDE209	811.4	651.1	55
BDE-71	325.9	138.0	55				
BDE-100	565.7	405.7	55	BDE-75	325.9	138.0	55
BDE-99	565.7	405.7	55	BDE-116	403.7	137.1	25
BDE-138	643.6	483.6	25	BDE-205	801.5	641.6	25
BDE-153	643.6	483.6	25				
BDE-154	643.6	483.6	25				
BDE-181	561.6	454.6	30				
BDE-183	561.6	454.6	30				
BDE-190	561.6	454.6	30				
BDE-209	799.7	639.6	55				

Chemical	Precursor Ion	Product Ion	Collision Energy	Chemical	Precursor Ion	Product Ion	Collision Energy
Trifluralin	306.1	264.0	5	Chlorpyrifos	196.9	168.9	15
Phorate	231.0	174.9	10	Dacthal	300.9	222.9	25
α-ΗCΗ	181.0	145.0	15	Trans-Chlordane	372.9	265.9	20
НСВ	283.9	248.8	25	Endosulfan I	240.9	205.9	15
Dazomet	161.9	89.1	5	Cis-Chlordane	372.9	265.9	40
Dimethoate	124.8	78.8	5	trans-Nonachlor	408.8	301.8	30
Carbofuran	163.9	149.1	10	Dieldrin	262.9	192.9	40
β-НСН	181.0	145.0	15	Endosulfan II	195.0	159.0	10
ү-НСН	181.0	145.0	15	Endosulfan Sulfate	271.9	236.9	20
Quintozene (PCNB)	236.9	118.9	25				
Diazinon	179.1	137.2	20				
Disulfoton	88.1	60.0	5				
δ-ΗCΗ	181.0	145.0	15	α -HCH- ¹³ C6	224.9	152.0	20
Chlorthalonil	265.9	133.0	40	HCB- ¹³ C6	289.9	254.9	20
Metribuzin	197.9	82.0	10	γ-HCH- ¹³ C6	229.9	155.7	20
Malathion	173.1	99.0	15	Trans- Chlordane- ¹³ C10	384.9	276.0	20
Aldrin	262.9	192.9	40	Dieldrin- ¹³ C12	269.8	199.7	30

Table S8. Precursor ions, product ions and collision energies for the multiple reaction monitoring mode for pesticides analysis.