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Calculation of Passive Sampling Rates from Both Native PCBs and Depuration Compounds in Indoor and Outdoor Environments

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Abstract

Passive sampling has become a practical way of sampling persistent organic pollutants over large spatial and remote areas; however, its ease in use is also coupled with some uncertainty in calculating air concentrations from accumulated mass. Here we report a comparison study of polyurethane-foam-based passive samplers (PUF-PAS) for quantitatively determining the sampling rates of polychlorinated biphenyls (PCBs) from air. We measured both uptake of native PCBs and loss of depuration compounds and determined the sampling rates (R-values) for multiple samplers harvested at three different time periods. The uptake of native PCBs in the linear phase was similar to the loss of depuration compounds for indoor air and behaved as predicted. A single R-value of $2.6 \text{ m}^3\text{d}^{-1}$ was calculated from the mean of 12 samplers deployed indoors from three harvest dates with a range of 2.0 to $3.4 \text{ m}^3\text{d}^{-1}$ for both uptake of native PCBs and loss of depuration compounds. Loss of depuration compounds in outdoor air also followed the predicted linear behavior with a range of calculated R-value of $4.4 - 8.4 \text{ m}^3\text{d}^{-1}$. Uptake of native PCBs behavior was extremely variable, probably due to changes in ambient air concentrations and resulted in R-values of $1.6 - 11.5 \text{ m}^3\text{d}^{-1}$ with greater variation seen in higher chlorinated homolog groups.

Keywords

PUF; air quality; POPs; indoor air; sampler design

Introduction

The global and regional distribution of persistent organic pollutants (POPs) is now well understood, thanks in part to the development of passive samplers that are lightweight, uniform, inexpensive and unobtrusive (Farrar *et al.*, 2005; Gouin *et al.*, 2007; Kot-Wasik, *et al.*, 2007; Partyka *et al.*, 2007).

Passive samplers that use polyurethane foam, soils, and semi-permeable membranes (Law *et al.*, 1998; Migazweski *et al.* 1999; Shoeib and Harner, 2002; Harner *et al.*, 2004) have been used world-wide and have been particularly effective in remote areas, across large spatial areas, and indoors where high -volume samplers (Hi-Vols) are impractical (Shoeib and Harner, 2002).

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Currently, the comparison between Hi-Vol data and passive sampling data collected for specific compounds, such as PCBs, is difficult due to the difference in temporal resolution, low detection limits for Hi-Vol samples, and differences in calculating concentrations. Researchers, however, have already compared the differences in reported calculated concentrations between Hi-Vols and passive samplers (Gouin *et al.*, 2005a; Gouin *et al.*, 2005b; Harner *et al.*, 2006). Similar to Hi-Vol data and PAS-PUF data, PCB concentrations for PAS-PUFs are calculated in different ways as well. Researchers derive a sampling rate, or R-value (m^3d^{-1}), from either loss of depuration compounds or uptake of native compounds coupled with known air concentrations, yet these methods have never been compared side-by-side, to our knowledge, until this study.

Several studies have determined effective sampling rates of passive samplers by injecting depuration compounds onto the sampling media (Jaward *et al.*, 2004; Pozo *et al.*, 2004; Gouin *et al.*, 2005b). The sampling rate, R-value, is determined by measuring the loss rate (k_e) of these compounds. Alternatively, researchers have estimated R-values by correlating the mass of POPs on the passive sampler with the concentrations measured using Hi-Vols (Harner *et al.*, 2004; Motelay-Massei *et al.*, 2005; Klanova *et al.*, 2008; Hazrati and Harrad, 2007). The uncertainty of the relationship between Hi-Vol concentrations and PUF concentrations, which have distinctly different time resolutions, makes this method imprecise. Hi-Vol data collected in the field that is not continuous may also not be accurate in representing ambient air concentrations, especially when these concentrations are not constant.

One issue affecting the interpretation of passive sampling concentrations is that two different methods are used to derive R-values in order to calculate concentrations. The problem is the ability to relate concentrations from different studies using PAS-PUFs. The Hi-Vol method of calculating concentrations is straightforward and no groups deviate from each other when using this method to report ambient air concentrations of PCBs; however, with PAS-PUFs the different methods to calculate reported concentrations leave some uncertainty on how these two methods compare.

Hazrati and Harrad (2007) and Klanova *et al.* (2008) have described the calculation of R-values and mass transfer coefficients by uptake in both indoor and outdoor environments respectively. However, to our knowledge, no study to date has examined both uptake of native congeners and loss of depuration compounds simultaneously for both indoor and outdoor environments in order to compare methods of deriving R values. In this paper we have calculated the sampling rates from both elimination (k_e) and uptake (k_u) for our PAS-PUF design to better understand how these different methods of deriving concentrations may differ and to understand the best practices of deriving R-values in the field. We will use the term “R-value” to distinguish the sampling rate from the correlation coefficient, r .

We have evaluated the reproducibility of sampling rates between indoor sites and calibrated the PAS-PUF for indoor sites in order to apply one constant R-value to all samples harvested from a specific design. We have also compared differences of calculated R-values for outdoor samplers. Finally, we compared the behavior of labeled PCBs used as depuration compounds to that of native PCBs in both indoor and outdoor environments.

The Sampling Rate

The mass of gas-phase PCBs (M_{PUF} , ng) accumulated on the PUF media is a function of a mass transfer coefficient as well as the concentration gradient between the air and the PUF disk (Bartkow *et al.*, 2005)

$$\frac{dM_{PUF}}{dt} = k_v \cdot A_s \cdot \left(C_{Air} - \frac{C_{PUF}}{K_{PUF}} \right)$$

Equation 1

where A_s is the PUF surface area (m^2), k_v is the mass transfer coefficient ($m \cdot s^{-1}$), C_{Air} is the analyte concentration in the air ($ng \cdot m^{-3}$), C_{PUF} is the PCB concentration on the PUF ($ng \cdot m^{-3}$) and K_{PUF} is the dimensionless PUF/air equilibrium partition coefficient. For PCBs, K_{PUF} is large and therefore the mass of PCBs on the PUF is a linear function of time. The concentration of PCBs in air, as measured by the passive sampler, can then be determined as in Equation 2, assuming that C_{Air} is a constant.

$$C_{Air} = M_{PUF} (k_v A_s t)^{-1}$$

Equation 2

The product $k_v \cdot A_s$ must be determined by experiment and is called the sampling rate, R-value.

R-values can be calculated from either the loss of depuration compounds from the PUF, or the uptake of native compounds onto the PUF.

The R-value calculated from the loss of depuration compounds is determined by calculating the mass transfer coefficient as a function of the first order elimination rate constant (k_e , sec^{-1}), and the stagnant air layer over the PUF surface (δ_{film} , m) as defined by Shoeib and Harner (2002):

$$k_v = k_e \cdot K_{PUF} \cdot \delta_{film}$$

Equation 3

where

$$k_e = \frac{\ln\left(\frac{m}{m_0}\right)}{t}$$

Equation 4

Alternatively, R-values may be derived from linear uptake curve of native congeners from ambient air of known concentration:

$$R = \frac{b}{C_{Air}}$$

Equation 5

where b is the slope of mass accumulated versus time.

In this study we calculated the R-value from both uptake and loss of PCB congeners for each sampler deployed.

Materials and Methods

Air Sampling

Passive samplers were deployed both indoors and outdoors at the Institute of Rural and Environmental Health (IREH) at the Oakdale Campus of The University of Iowa beginning the last week of August 2006 and ending in the first week of October 2006. Two indoor sites

were chosen; the first was an older laboratory that was built in 1960s and the second was a laboratory addition built in the 1990s. A third site was located outdoors approximately 150 meters from the IREH building. Twelve passive samplers (specifications: 18 cm lower bowl diameter, 23 cm upper bowl diameter, 3 cm gap between bowls, six ventilation holes in bottom) were deployed approximately 2.7 meters from the ground at each site, with three spiked and one unspiked PUF disks (specifications: 14 cm diameter, 1.35 cm thick, 365 cm² surface area, 4.40 g mass, 207 cm³ volume, 0.0213 g cm⁻³ density) harvested for each time frame (21, 28, and 46 days). A Hi-Vol sampler (Tisch Environmental, Cleves, OH) was deployed at each site and was equipped with quartz fiber filters and XAD Amber-lite 2 (Supelco, Inc) media. The Hi-Vols were operated for 8-hour periods at night on the three days that the passive samplers were harvested. A total of three Hi-Vol samples were collected at each site over the total deployment time for the PUF disks. PCB congeners were extracted and quantified using the same method as for the PAS-PUF. Because PCBs exist primarily in the gas-phase, PCBs were only measured in the XAD-2 and not in the quartz filters.

Analysis

PUF disks were cleaned (Soxhlet extraction 24 h in hexane followed by 24 h in acetone), dried in a desiccator, and spiked with 40 ng per congener of a mixture of EPA Method 1668A Labeled Toxics/LOC/Window defining solution (Cambridge Isotope Laboratories). PUFs were spiked by placing them in amber jars and then adding depuration compounds. PUFs were dried in the jars, then capped with Teflon lids, sealed in zip lock bags, and stored in a -20°C freezer until deployment. PAS-PUF sampling chambers were solvent-rinsed with hexane and acetone just prior to deployment. Exposed PUF disks were placed in amber jars with Teflon lids, sealed in zip lock bags and immediately transferred to a freezer. XAD Amberlite 2 resin was cleaned by using a comparable method (Peck and Hornbuckle, 2006).

All sample media were extracted with pressurized fluid extraction (Dionex ASE-200), using a 1:1 hexane: acetone mixture with parameters as follows: pressure 10.3 MPa (1,500 psi), 100 °C, 5 minutes static time, 1 static cycle, 60% of flush volume, and purge at 90 seconds. Extracts were concentrated to 1 mL (Caliper TurboVap II). Surrogate standards (50 ng each of PCB 14, 65, 166 from Accustandard) were added just prior to extraction. Internal standards (60 ng each of PCB 30 and 204 from Accustandard) were added just prior to analysis. All samples were analyzed using a modified EPA Method 1668A on Tandem Mass Spectrometry GC/MS/MS (Quattro MicroTM GC, Micromass MS Technologies) using a Supelco SPB-Octyl (30m × 0.25mm × .25µm) with GC inlet parameters of inlet temperature 270 °C, oven temperature ramp as initial temperature 75 °C, initial time 1 minute, ramp 15 °C/min to 150 °C, ramp 2.5 °C/min to 290 °C, with an interface temperature of 290 °C. Using this method we were able to identify 172 unique congeners, with an additional 37 congeners coeluting. Identification of 35 Carbon-13 labeled congeners (1, 3, 4, 9, 15, 19, 28, 37, 52, 54, 77, 81, 101, 104, 105, 111, 114, 118, 123, 126, 138, 155, 156, 157, 167, 169, 178, 188, 189, 194, 202, 205, 206, 208, 209) used as depuration compounds, was also achieved using this method.

Results and Discussion

Quality Control/Quality Assurance

Unspiked passive samplers (n=3) were deployed alongside passive samplers spiked with labeled PCBs to determine if labeled standards were re-depositing but none were detected. The average (± std dev.) recovery of the three surrogate standards were PCB 14, 82.4% ± 10.4; PCB 65, 98.0% ± 9.1 %; and PCB 166, 95. % ± 12.8%. A field blank was installed and removed at each site at the beginning of the study, and all were determined to be less than 10% of lowest calculated mass. Method blanks run with each extraction batch were also determined to be less than the detection limit (1 ng/mL mono-tri, 2 ng/mL tetra-hepta, and 3 ng/mL octa-deca). Three

spiked PUF disks were also extracted the day of deployment to measure any significant loss of spiked congener mass while stored in the freezer, but no significant loss was detected. Standard Reference Material, NIST 2274 PCBs in iso-octane, was run in triplicates on two separate dates. Our method is acceptable for congener-specific analyses. Standard Reference Material analysis is found in supplemental material.

Indoor Air Sampling Rates

In order to be able to deploy PAS-PUF in indoor environments without depuration compounds, the samplers must be calibrated with depuration compounds. Ideally, one R-value can be applied to all target compounds. A recent study by Hazrati and Harrad (2007) show that passive samplers used for indoor environments can be reliably calibrated and an R-value calculated for specific sampler designs. For our study, both the uptake of native compounds and loss of depuration compounds were measured. R-values were calculated from both methods. Samplers were calibrated, resulting in one R-value that could be confidently applied to all indoor samples acquired with this design, thus eliminating the need for depuration compounds at indoor sites.

Uptake of native PCB congeners over time was determined by deploying fifteen PAS-PUF samplers in one laboratory (Indoor 1) and fifteen in another laboratory (Indoor 2). At each location, a subset of one or four samplers was collected at four time intervals. The first sample was collected immediately (time = 0). A set of four samples was collected on day 21. Another set of four samples was collected on day 28 and also on day 46. PCB congeners were extracted and measured on each PUF. The mass accumulated is compared to the linear uptake described by Equation 1, and the results are shown in Figure 1. The linear regression resulted in r^2 values ranging from 0.97 to 0.99. The high coefficients of determination suggest that PCBs in indoor environments behave as predicted by the mathematical model for compounds where air side resistance dominates (Shoeib and Harner, 2002; Bartkow *et al.* 2005). By using uptake plots in Figure 1 and applying Hi-Vol data we derived R-values for indoor air (Table 1). The assumption that C_{Air} stays constant in indoor air seems to be valid as the uptake curve is linear and the resulting R-values show good agreement with R-values calculated from depuration compounds.

The congeners measured for the uptake experiment were also collected and measured from the Hi-Vol samplers operated at the same two laboratories. The concentration of total PCBs ranged from 0.05 to 10.5 ng/m³. The concentrations in the older laboratory were greater than the newer laboratory by one order of magnitude, possibly due to differences in building materials used (Table 1).

Loss of labeled PCB congeners was determined from the same samples as described for the uptake experiments. Each PUF media was spiked with four Carbon-13 labeled PCB congeners. The resulting loss of the four labeled PCBs from the thirteen deployed samples is shown in Figure 2. The linear regression resulted in coefficients of determination ranging from 0.73 to 0.99. As found for the uptake of native PCBs from indoor air, the loss is consistent with the first order uptake model (Equation 1).

Reproducibility of Indoor R-values

Using measurements from both uptake of native congeners and loss of depuration compounds, we calculated R-values for native homolog groups (Equation 5) as well as individual depuration compounds (Equation 4). R-values ranged from 2.0 m³d⁻¹ to 3.5 m³d⁻¹ for both native compounds and depuration compounds (Table 1), similar to R-values of 2.5 m³d⁻¹ for PBDEs calculated by Wilford *et al.* (2004). The calculated R-values are within the range of reported values from other indoor studies. For example Shoeib and Harner (2002) report R-values of

1.8 m³d⁻¹ to 8.3 m³d⁻¹ for many semivolatile compounds. Hazrati and Harrad (2007), report a slightly lower range of values: 0.57 m³d⁻¹ to 1.55 m³d⁻¹ for PCBs.

Outdoor Air Sampling Rates

Labeled PCBs in outdoor air, like indoor air, behave in a predictable manner with a good linear fit for each congener with the coefficients of determination ranging from 0.82 to 0.970 (Table 2 and Figure 3d).

Mass accumulated onto the PUF for seven homolog groups as a linear function of time. For mono-trichlorinated homolog groups, the coefficient of determination ranges from 0.64 to 0.93 (Table 2 and Figure 3a). However, a very poor correlation was observed for the higher chlorinated homolog groups tetra through hepta chlorinated, with the coefficients of determination ranging from 0.0001 to 0.33 (Table 2 and Figure 3bc). The data suggests that lower chlorinated PCBs will accumulate onto PUF disks in a predictable manner, but the accumulation of higher chlorinated PCBs onto PUF disks can vary significantly as a function of time harvested.

The high variability in the uptake of most native congeners over time is most likely caused by changes in the ambient air concentration (C_{Air}) during the study. Equation 1 assumes a constant C_{Air} ; however, the concentrations of PCBs in the ambient air during this study may vary, particularly as a function of the large temperature changes (Cortes *et al.*, 1998; Sun *et al.*, 2007; Sun *et al.*, 2006; and Simcik *et al.*, 1999) that occurred during our study of outdoor air. High variability in ambient air concentrations over a time frame of a single month at one site have been reported (Offenberg *et al.*, 1999; Wethington and Hornbuckle, 2005; Macleod *et al.*, 2007), and show that C_{Air} can vary two orders of magnitude (Offenberg *et al.*, 1999). Although the uptake of native congeners would be affected by temperature changes, the loss of depuration compounds would remain relatively constant since the loss mechanism is dominated by the large concentration gradient between spiked PUF and the ambient air. For this reason, uptake of higher chlorinated PCBs is extremely variable but loss of depuration compounds follows the linear trend.

Reproducibility of outdoor R-values

Sampling rates vary much more in outdoor air than in indoor air. Our outdoor R-values for individual congeners ranged from 3.4 m³d⁻¹ to 9.3 m³d⁻¹ with an average of 6.5 m³d⁻¹ ± 2.4 m³d⁻¹ (Table 2). This is within the range of reported values. Jaward *et al.* (2004) found outdoor R-values ranging from 3.0 m³d⁻¹ to 4.0 m³d⁻¹. Others found average R-values between 3.0 m³d⁻¹ and 5.0 m³d⁻¹ (Harner *et al.*, 2006, 2004; Pozo *et al.*, 2004; Gouin *et al.*, 2005b; Motelay-Massei *et al.*, 2005). This large variation in R-values calculated from uptake rates could be attributed to the fact that R-values are dependent on short-term Hi-Vol measurements that may not reflect the integrated average concentration captured by the PUF.

For outdoor deployment, R-values determined from depuration compounds vary less than R-values calculated from the native PCB congeners. The calculations derived from depuration compounds reflect the current literature that states outdoor air concentrations of POPs between Hi-Vol and PAS-PUF could be off by a factor of 2 (Shoeib and Harner, 2002; Gouin *et al.*, 2005b; Tuduri *et al.*, 2006; Yao *et al.*, 2007), which would be a more conservative calculation than concentrations derived from using R-values derived from uptake curves.

Due to the variations in C_{Air} in outdoor air, as well as the variation between homolog groups studied, we chose to look at qualitative aspects of PCB masses collected on the PUF as well. Although PCB mass accumulated onto PUF varied depending on the date harvested, congener distribution had little variation with exception to the mono chlorinated PCBs which were seen

at 21 and 46 days, but were not detected at 28 days (Figure 4). The similarity in the congener distribution histograms suggest that the PUF is sampling from the same ambient air source, but physical factors such as temperature and wind effects are changing the rate of uptake from this ambient air source and therefore the magnitude of the mass quantified.

Recommendations

For indoor air, the average R-value of $2.6 \text{ m}^3 \text{ d}^{-1}$ calculated from both uptake and loss of PCBs is recommended for application to samples using this passive sampler design for indoor sites. For outdoor applications using this passive sampler design, we suggest using depuration compounds to reduce the uncertainty by nearly a factor of 2. Since PCB concentrations are not constant in outdoor air, uptake of native congeners was not linear. The Hi-Vol data collected was not continuous and therefore was not representative of the changes in C_{Air} . The inconsistency in C_{Air} leads to large variation in derived uptake R-values derived concentrations when compared to depuration derived concentrations. Comparing PCB concentrations derived from uptake of native congener to those derived from loss of depuration compounds is difficult, as uptake derived R-values are dependent on C_{Air} which may vary greatly, where depuration compound loss is independent of this variability.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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Figure 1. Mass uptake of native PCB homolog groups for indoor site 1 (a) and site 2 (c) onto PUF disks for 0, 21, 28, and 46 days.

Figure 2. Loss of depuration compounds for indoor site 1 (a) and site 2 (c) onto PUF disks for 0, 21, 28, and 46 days.

Figure 3.

Mass uptake and loss of PCB congeners for PUF-PAS deployed outdoors. Uptake of mono- and di-chlorinated PCBs shown in (a). Uptake of tri- and tetra-chlorinated PCBs shown in (b). Uptake of penta-, hexa-, and hepta-chlorinated PCBs shown in (c). Loss of depuration compounds from PUF-PAS shown in (d).

Figure 4.

Congener distributions from outdoor air for 21 (a), 28(b), and 46(c) days. High concentrations of PCB 153/168 were detected in all samples; the possible source is the indoor air ventilation system from labs where PCB 153 may be used for toxicological studies.

Table 1

Calculated R-values, coefficients of determination (r^2), linear equations used, and hi-vol concentration averages over the PUF deployment time for native uptake and depuration loss for indoor sites.

Site	Homolog or Congener	R-value (m^3d^{-1})	r^2	Equation for linear range	C_{Air} HI-vols Average (ng/m^3)
Indoor 1 Native	Monochlorinated	2.5	0.97	$y = 0.4696x - 3.91$	0.19
	Dichlorinated	3.1	1.00	$y = 2.2256x - 10.181$	0.72
	Trichlorinated	2.9	1.00	$y = 3.9789x - 33.462$	1.36
	Tetrachlorinated	2.4	1.00	$y = 20.215x + 58.052$	8.55
	Pentachlorinated	3.5	1.00	$y = 36.508x - 259.47$	10.5
	Hexachlorinated	2.7	0.99	$y = 8.0818x - 7.6742$	3.00
	Heptachlorinated	2.0	0.99	$y = 0.6529x - 6.5037$	0.32
	PCB 3	3.4	0.96	$y = 0.5296x - 11.036$	0.16
	PCB 73	2.4	0.85	$y = 7.8215x - 75.615$	3.26
	PCB 101/113/90	2.9	0.82	$y = 16.414x - 222.31$	5.66
Depuration	PCB 141	3.3	0.99	$y = 1.7013x - 31.447$	0.52
	^{13}C PCB 3	2.2	0.81	$y = -0.142x + 1.140$	ND
	^{13}C PCB 15	2.1	0.99	$y = -0.114x + 1.086$	ND
	^{13}C PCB 28	2.7	0.96	$y = -0.132x + 1.079$	ND
	^{13}C PCB 118	2.4	0.73	$y = -0.226x + 1.226$	ND
Indoor 2 Native	Monochlorinated	2.3	0.89	$y = 0.2072x - 3.3027$	0.09
	Dichlorinated	2.8	0.62	$y = 0.1413x + 4.2812$	0.05
	Trichlorinated	2.7	0.98	$y = 0.8011x - 1.302$	0.29
	Tetrachlorinated	2.2	0.99	$y = 6.5104x + 145.21$	3.01
	Pentachlorinated	2.9	0.99	$y = 9.2099x - 24.787$	3.21
	Hexachlorinated	2.0	0.56	$y = 1.5591x + 64.776$	0.77
	Heptachlorinated	2.4	0.97	$y = 0.4001x - 5.0823$	0.17
	PCB 3	3.3	0.93	$y = 0.4399x - 9.7248$	0.13
	PCB 73	2.8	0.96	$y = 3.7413x - 49.795$	1.34
	PCB 101/113/90	2.5	0.47	$y = 2.5771x - 18.861$	1.03
	PCB 141	2.7	0.99	$y = 0.2795x - 4.2532$	0.10

Site	Homolog or Congener	R-value ($\text{m}^3 \text{d}^{-1}$)	r^2	Equation for linear range	C_{Air} HI-vols Average (ng/m^3)
Depuration	^{13}C PCB 3	2.1	0.75	$y = -0.117x + 1.017$	ND
	^{13}C PCB 15	2.3	0.94	$y = -0.116x + 1.063$	ND
	^{13}C PCB 28	2.2	0.97	$y = -0.136x + 1.090$	ND
	^{13}C PCB 118	2.6	0.84	$y = -0.231x + 1.191$	ND

Table 2

Calculated R-values, coefficients of determination, linear equations used, and hi-vol concentrations from native uptake and depuration loss for outdoor sites.

Site	Congener	R-value (m^3d^{-1})	r^2	Equation for linear range	C_{Air} Hi-vols Average (ng/m^3)
Outdoor Native	Monochlorinated	5.3	0.84	$y = 0.1067x - 2.3134$	0.02
	Dichlorinated	3.9	0.93	$y = 2.3138x - 54.175$	0.60
	Trichlorinated	4.2	0.64	$y = -3.8003x + 164.59$	0.91
	Tetrachlorinated	11.5	0.25	$y = -1.0346x + 84.787$	0.09
	Pentachlorinated	1.6	0.33	$y = 0.1096x + 9.7431$	0.07
	Hexachlorinated	7.9	0.01	$y = -0.3646x + 93.924$	0.05
	Heptachlorinated	-	0.0001	$y = -0.0013x + 3.6028$	0.00
Depuration	PCB 73	7.8	0.32	$y = 0.0508x + 2.5467$	0.007
	PCB 101/113/90	8.0	0.16	$y = 0.0642x + 2.2393$	0.008
	PCB 153	3.4	0.77	$y = 0.0136x + 0.0622$	0.004
	PCB 163	9.3	0.02	$y = -0.2518x + 82.41$	0.027
	^{13}C PCB 3	8.4	0.82	$y = -0.238x + 1.065$	ND
	^{13}C PCB 15	4.4	0.91	$y = -0.166x + 1.077$	ND
	^{13}C PCB 28	4.8	0.92	$y = -0.164x + 1.096$	ND
	^{13}C PCB 118	6.2	0.97	$y = -0.225x + 1.193$	ND