

# Effects of Salinity, pH and Temperature on the Octanol-Water Partition Coefficient of Bisphenol A

Siriporn Borriukwisitsak, Helen E. Keenan, and Caroline Gauchotte-Lindsay

**Abstract**—Bisphenol A (BPA) has been widely used as an industrial plasticizer and is considered an endocrine disrupting chemical (EDC). BPA can be released into the aquatic environment and magnify in the food chain, resulting in human exposure. To understand and predict the environmental fate and toxicity in the aquatic environment, the octanol-water partition coefficient ( $K_{ow}$ ) was determined at various salinity, pH and temperatures using the OECD guideline 107 shake flask method. With increasing salinity the log  $K_{ow}$  of BPA at 25°C increased from 3.44 to 3.55. The log  $K_{ow}$  also changed at different pH, it decreased at pH > pK<sub>a</sub>, at pH between 6 and 8 a small increase (from 3.39 – 3.47) was observed which was then followed by a decrease at pH 10 (to 2.99). Increasing temperatures (between 25°C and 45°C) affect log  $K_{ow}$  leading to decreased log  $K_{ow}$  values (3.42 to 3.18). The log  $K_{ow}$  for the natural seawater (salinity 29 psu and pH 8) was also determined at 3.52. The experimental and the default values were input into the prediction program EPI Suite™, which was used to assess environmental fate and toxicity of BPA. Using the experimental values enables a more accurate model for site specific samples can be defined. The model using the experimental  $K_{ow}$  values of natural seawater indicated higher bioaccumulation and higher sediment adsorption but slightly lower aquatic toxicity than the default values. These findings imply that BPA in the marine environment is more bioaccumulative therefore has a greater biomagnification potential in fish species, particularly benthic feeders. This may adversely impact on human health and prove detrimental to humans that consume these marine species compared to similar species from a freshwater environment.

**Index Terms**—Bisphenol A, Octanol-water partition coefficients, salinity, pH and temperature effects, EPI Suite™

## I. INTRODUCTION

Bisphenol A (BPA) or 4,4'-isopropylidenediphenol (CAS number 80-05-7) is used as a monomer and plasticizer, adding strength and flexibility, in the production of polycarbonate plastic (PC) and epoxy resins. BPA is an emerging pollutant in the aquatic environment which may adversely affect both the environment and human health. It is considered an endocrine disrupting chemical (EDC) because it can mimic the action of oestrogen and interfere with the function of various hormone systems [1]-[5]. BPA tolerable daily intake (TDI) was determined at 0.05 mg of BPA kg<sup>-1</sup> of body weight day<sup>-1</sup> [6]. However, recent studies found that

BPA may provoke adverse effects even at very low doses (i.e. <TDI) [7], thus, public and scientific community have shown increasing concern over possible human health effects of BPA.

BPA has molecular weight (MW) of 228 g mol<sup>-1</sup>. It is a moderately hydrophobic (water solubility 120-300 mg L<sup>-1</sup>) and a very weak acid pK<sub>a</sub> 9.6 - 10.2. It is readily degraded in aerobic conditions but less so under anaerobic conditions. Although BPA is expected to have low persistence and low bioaccumulation (bioconcentration factors (BCFs) 5 - 68), it has been commonly detected in the environment due to its continuous release [1], [6], [8].

The octanol-water partition coefficient ( $K_{ow}$ ) is the equilibrium ratio of concentration of a dissolved chemical between octanol and water at a specified temperature [9]. The  $K_{ow}$  represents the membrane lipid-water barrier because octanol (C<sub>7</sub>H<sub>15</sub>CH<sub>2</sub>OH) represents lipids in living organisms due to the similar carbon to oxygen ratio. Hence, it is used as an indicator of the bioconcentration and bioaccumulation [10]-[15]. The  $K_{ow}$  is related to water solubility (S), soil/sediment adsorption coefficients ( $K_{oc}$ ), and bioconcentration factors (BCFs) for aquatic life [16], [17]. The examples of correlations between those coefficients are shown in (1) – (3) [18].

$$\text{Log } S \text{ (mol L}^{-1}\text{)} = 0.796 - 0.854 \text{ Log } K_{ow} - 0.00728 \text{ MW} \quad (1)$$

$$\text{Log } K_{oc} \text{ (L kg}^{-1}\text{)} = 0.8679 \text{ Log } K_{ow} - 0.0004 \quad (2)$$

$$\text{Log BCF (L kg}^{-1}\text{)} = 0.6598 \text{ Log } K_{ow} - 0.333 \quad (3)$$

Previous studies have indicated that salinity, pH and temperature have influence on the  $K_{ow}$  values [14], [19]-[24]. Also, previous work found that BPA can persist longer in seawater than in freshwater without any degradation (~30 days) and possibly accumulate higher in marine organisms than in freshwater organisms [25].

Estimation Program Interface Suite™ program (EPI Suite™) is a common environmental modeling program which predicts the environmental fate and toxicity of chemicals from the partition coefficients and also provides physico-chemical properties of substances. However, in order to improve the resulting model, experimental values are preferred. The models generated from experimental values are considered to have greater accuracy and are site specific [18], [26].

Therefore, in this study, the experimental  $K_{ow}$  values were determined based on the Organisation for Economic Co-operation and Development (OECD) guideline 107 shake flask method. The  $K_{ow}$  values of BPA were investigated at

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various salinity, pH, and temperatures to assess their effects on aquatic environments. Firstly, the  $K_{ow}$  value of a natural Scottish coastal seawater was determined to predict the environmental fate, transport and toxicity of BPA in the marine environment. The  $K_{ow}$  obtained from this experiment and subsequent program calculations from the Estimation Programs Interface (EPI) Suite™ (version 4.1) [18] were compared to the default  $K_{ow}$  generated by the program (2 default values were generated). The experimental  $K_{ow}$  was also used as the input for the program to predict the environmental fate and toxicity and compare with the default values to get a more accurate site-specific model which would be more appropriate, particularly for marine compared to freshwater environments.

## II. MATERIALS AND METHODS

### A. Chemicals and Instruments

Bisphenol A (97% purity) was obtained from Sigma-Aldrich (UK). All reagents (NaOH, HCl, KCl) used were analytical grade and were supplied from Fisher Scientific (UK). Analytical grade 1-octanol was obtained from Rathburn (UK). HPLC grade acetonitrile and methanol were purchased from Fisher Scientific (UK). Nanopure water used as HPLC solvent was purified with a Barnstead Nanopure Water System (Triple Red Limited, UK). The salinity and pH of water were measured by conductivity and pH meter, SevenMulti model (METTLER TOLEDO, UK) which converts electrical conductivity (EC) to salinity. The incubator shaker used was a Stuart® orbital incubator SI500 (BIBBY SCIENTIFIC LIMITED, UK).

### B. Sample Collection

A natural seawater (2 L in a glass bottle) sample was collected from Prestwick, UK in June 2012 (55°49'40.82"N, 4°62'9.30"W).

### C. Octanol-Water Partition Coefficient ( $K_{ow}$ ) of BPA

The  $K_{ow}$  was determined using the OECD guideline 107 shake flask method at  $25 \pm 1^\circ\text{C}$  [9]. Before the determination, analytical grade 1-octanol and distilled water were saturated at the temperature of the experiment. An initial concentration of  $200 \text{ mg L}^{-1}$  of BPA was prepared in octanol, this was mixed with water to obtain the study ratios. The volume ratios between octanol and water studied were 1:20, 1:10 and 1:5. Each ratio was run in triplicate, the log  $K_{ow}$  value was obtained from the average results (n=9) from 3 ratios, where the results fell within a range of  $\pm 0.3$  units.

The major parameters that influence  $K_{ow}$  were studied in order to indicate environmental fate of BPA in the aquatic environment. This understanding leads to more efficient modeling and toxicity assessment. The parameters studied were salinity, pH and temperature. The salinities studied were 0.5, 10, 35 and 50 psu which represented the range of salinities from estuarine to seawater. Usually, freshwater salinity is less than 0.5 psu, brackish or estuarine water is between 0.5 and 17 psu, and seawater salinity is between 32 and 37 psu with the average at 35 psu. The salinity of water was adjusted by adding KCl because potassium is absorbed in water better than NaCl [27]. The effect of pH was studied

by varying pH at 6, 7, 8 and 10 which were adjusted with 0.1 M HCl or 0.1 M NaOH [28]. The temperatures studied were at 25, 35 and  $45^\circ\text{C}$  maintained in an incubator shaker. Additionally, the  $K_{ow}$  value of the natural seawater sample from Prestwick was examined.

The analysis of BPA was carried out by HPLC-UV detector. The Dionex HPLC (Dionex, UK) equipped with a LPG-3400A HPLC pump, an ACC-3000T autosampler with a 20  $\mu\text{L}$  injection loop and a VWD-3400 detector was used. The chromatographic column used was a Techsphere 5 ODS C18 column (25cm x 4.6mm) from hplc technology (UK). This was held at a constant temperature of  $25^\circ\text{C}$  within the housing unit. Mobile phases were nanopure water and HPLC grade acetonitrile (55:45 (v/v)) at a flow rate of  $1 \text{ mL min}^{-1}$ . The UV detector was set at wavelength 224 nm. The water fraction was analysed and concentration of BPA in the octanol phase was determined by subtraction from the total amount of BPA in the system ( $200 \text{ mg L}^{-1}$ ). Finally, the results were compared to the  $K_{ow}$  values from the computational program (default values).

## III. RESULTS AND DISCUSSION

### A. Octanol-Water Partition Coefficient ( $K_{ow}$ )

The dimensionless octanol-water partition coefficient ( $K_{ow}$ ) is used to predict the possible environmental fate and bioaccumulation of BPA. The  $K_{ow}$  is a measurement of the lipophilicity of a substance and is defined as the ratio of the equilibrium concentrations of a dissolved substance in octanol and water [9].

The log  $K_{ow}$  obtained from this experiment at  $25 \pm 1^\circ\text{C}$  was  $3.42 \pm 0.03$ . The result was supported by log  $K_{ow}$  value for BPA measured by Bayer at ambient pH values which was 3.4 [1].

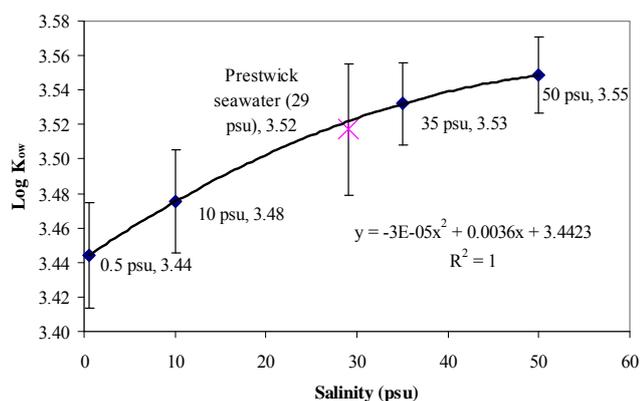
The  $K_{ow}$  of natural seawater (NSW) from Prestwick was determined. In this study, the log  $K_{ow}$  of NSW at  $25 \pm 1^\circ\text{C}$  was  $3.52 \pm 0.04$ . The higher log  $K_{ow}$  in the NSW is possibly due to the salinity and pH [14]. The NSW had a salinity of 29 psu and a pH of 8 whereas distilled water had zero salinity and a pH between 6 and 7. Therefore, the effects of these parameters on partitioning behavior were studied.

### B. Effect of Salinity

The effect of salinity on  $K_{ow}$  value was studied. Previous studies indicated that salt content in aqueous phase affects water solubility and the partitioning of organic chemicals into other phases. This effect is referred to as the salting-out effect which can change the  $K_{ow}$  value [29], [30]. Artificial water was adjusted by adding KCl to give a salinity range from 0.5 to 50 psu [27]. Then the  $K_{ow}$  values at various salinities of water were investigated again using OECD 107 but using water of known salinity to make up the ratios as previously described. The results are presented in Fig. 1.

From the results, the correlation equation obtained from artificial water (salinity range 0.5 – 50 psu) as in (4).

$$\text{Log } K_{ow} = [-0.00003 \text{ Salinity}^2 (\text{psu})] + [0.0036 \text{ Salinity}] + 3.4423, \quad R^2 = 1 \quad (4)$$

Fig. 1. Log K<sub>ow</sub> of BPA at various salinity

Therefore, the relationship between salinity of water and log K<sub>ow</sub> is that an increase in the salinity increases the log K<sub>ow</sub>. Consequently, greater salinity seems to lead to higher bioaccumulation of BPA in the lipid of aquatic organisms and it also means that it will also persist for longer in marine environment as greater adsorption to soil/sediments will also occur. This study supports previous work [25] in that the bioaccumulation of BPA in marine organisms is possibly higher than that in freshwater organisms. This curve clearly fitted a polynomial curve as the R<sup>2</sup> value was 1. The log K<sub>ow</sub> value of the natural seawater from Prestwick coast (salinity 29 psu) almost fell within the range of log K<sub>ow</sub> values of the synthetic waters that were tested. From this correlation equation (Log K<sub>ow</sub> = [-0.00003 Salinity<sup>2</sup> (psu)] + [0.0036 Salinity (psu)] + 3.4423, R<sup>2</sup> = 1), the log K<sub>ow</sub> of the natural seawater from Prestwick was calculated at 3.52. This concurs with the measured value of 3.52.

### C. Effect of pH

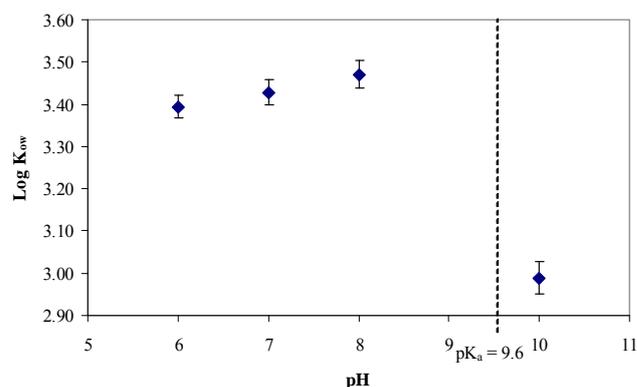
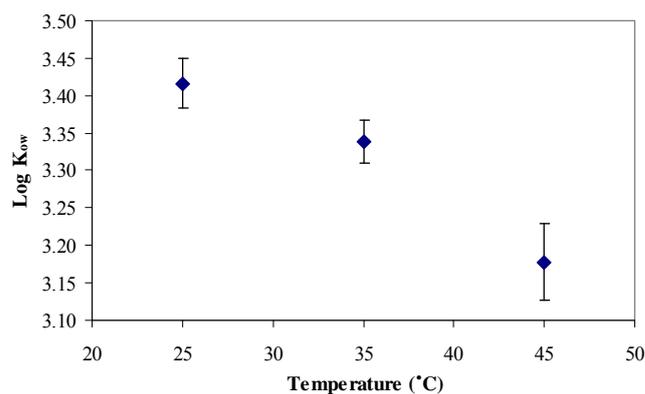
The pH is an important factor in controlling the partitioning of BPA. Varying the pH of the water was achieved by adding 0.1 M HCl or 0.1 M NaOH [28]. The effect of pH on K<sub>ow</sub> was studied at different pH (6, 7, 8 and 10). The results are shown in Fig. 2.

The results show the highest log K<sub>ow</sub> occurred at approximately pH 8. The log K<sub>ow</sub> of BPA increased slightly at pH from 6 – 8 but decreased significantly at pH 10. A possible reason is the dissociation of BPA in the system, as pH 10 is within its pK<sub>a</sub> range (9.6 - 10.2) [1]; in fact, BPA is a weak organic acid and can be deprotonated to exist in the system as an anionic form and/or neutral form of BPA. If pH > pK<sub>a</sub>, the ionized form is predominant and it has been suggested that the K<sub>ow</sub> value is largest if the chemical is in the neutral form due to (5) [14].

$$K_{ow} = \frac{\text{Concentration in octanol, (mg L}^{-1}\text{)}}{\text{Concentration in water, (mg L}^{-1}\text{)}} \quad (5)$$

### D. Effect of Temperature

The effect of temperature on K<sub>ow</sub> value was studied at temperatures between 25 and 45°C using an incubator shaker. The results are shown in Fig. 3.

Fig. 2. Log K<sub>ow</sub> of BPA at various pHFig. 3. Log K<sub>ow</sub> of BPA at various temperatures

The results indicate that the log K<sub>ow</sub> values of BPA decreased with increasing temperature. The partitioning of BPA between octanol and water is a function of the Gibbs free energy which relates to temperature and can be shown in (6) [11].

$$\Delta_{tr}G = -RT \ln K \quad (6)$$

Where  $\Delta_{tr}G$  is change of transfer reaction in Gibbs free energy, R is the ideal gas constant (J mol<sup>-1</sup> K<sup>-1</sup>), T is temperature (in Kelvin) and K is the equilibrium constant. Thus, the increased solubility leads to reduced K<sub>ow</sub> values with concomitant decreases in bioaccumulation and sorption to sediments.

### E. Prediction of Environmental Fate and Toxicity

The experimental values of log K<sub>ow</sub> were compared to estimated and experimental values from EPI Suite™ as shown in Table I.

Table I shows the difference between experimental log K<sub>ow</sub> values obtained and the values given from the estimation program, the default values are presented in bold font. Compared to the experimental values as shown above, the predicted log K<sub>ow</sub> value from KOWWIN™ in EPI Suite™ which is estimated by using an atom/fragment contribution method without accounting for environmental conditions is overestimated, whereas the experimental value from the database in the program appeared underestimated. Furthermore, there is no K<sub>ow</sub> value for seawater in EPI Suite™. These lead to disparity predictions of environmental fate and toxicity, especially in the marine environment. Subsequently,

the experimental  $K_{ow}$  was input into EPI suite™ to get a more accurate prediction of environmental fate.

EPI Suite™ used  $K_{ow}$  to estimate many physico-chemical properties related to the environmental fate and the toxicity of a molecule such as bioconcentration factor (BCF), soil/sediment sorption coefficient ( $K_{oc}$ ), water solubility (S), acute toxicity ( $LC_{50}$ ) and chronic toxicity (chronic value). The  $K_{ow}$  was also used to assess toxicity in the aquatic environment.

Table I presents a comparison of these prediction data, using both experimental values from this study and default values from EPI Suite™. The differences between these predicted data of BPA depended on the input values. The experimental prediction for Prestwick coast showed lower toxicity but higher adsorption capacity to sediment and higher bioaccumulation than the default model. As a result, organisms might have greater opportunity to accumulate BPA than the program predicates.

The default values from the computational program are useful as a screening-level tool. However, to get more accurate prediction and assessment for site-specific investigations it is necessary to take environmental conditions into account. Salinity, pH and temperature all affect  $\log K_{ow}$  with subsequent influence on toxicity, bioaccumulation and sorption. Even small changes in these parameters can have an impact on behavior. Therefore, the experimental values are necessary to predict accurately the environmental impact. Experimental values assist and aid the understanding of real environmental behavior of BPA in specific sites which can lead to more appropriate prevention and remediation technology and more effective exposure assessment.

TABLE I: THE  $K_{ow}$  AND COMPARISON OF THE PREDICTIONS OBTAINED FROM THE EPI SUITE PROGRAM™

Parameters	Log $K_{ow}$	BCF <sup>a</sup> (L kg <sup>-1</sup> wet-wt)	$K_{oc}$ <sup>a</sup> (L kg <sup>-1</sup> )	Water solubility <sup>a</sup> (mg L <sup>-1</sup> )	Toxicity in fish <sup>a</sup> (mg L <sup>-1</sup> )	
					LC <sub>50</sub> <sup>b</sup> (96 h)	ChV <sup>c</sup> (30 d)
Distilled water	3.42 <sup>d</sup>	83.85	1414	146.9	3.173	0.773
Prestwick seawater	3.52 <sup>d</sup>	97.61	1606	116.5	2.773	0.664
Salinity 50 psu	3.55 <sup>d</sup>	102.2	1669	109.9	2.663	0.634
pH 10	2.99 <sup>d</sup>	43.63	817.8	330.4	5.663	1.489
45°C	3.18	58.23	1042	227.4	4.384	1.114
EPI Suite™ KOWWIN™	3.64 <sup>e</sup>	117.1	1871	92.04	<b>2.350</b> <sup>g</sup>	<b>0.550</b> <sup>g</sup>
EPI Suite™ expkow database	3.32 <sup>f</sup>	<b>72.03</b> <sup>g</sup>	<b>1245</b> <sup>g</sup>	<b>172.7</b> <sup>g</sup>	3.631	0.900

<sup>a</sup> The prediction data using  $K_{ow}$  as the input values

<sup>b</sup> Lethal concentration 50 is the concentration of a chemical that will kill 50% of the test subjects, indicating acute toxicity

<sup>c</sup> Chronic value is the geometric mean of the no observed effect concentration (NOEC) and the lowest observed effect concentration LOEC [31]

<sup>d</sup> The experimental values from this study at 25°C

<sup>e</sup> The estimated value obtained from KOWWIN™ version 1.68 in EPI Suite™, default value for toxicity prediction (ECOSAR™ version 1.00).

<sup>f</sup> The experimental value from [32] in database in EPI Suite™, default value in physico-chemical properties and fate prediction.

<sup>g</sup> The default values from EPI Suite™ version 4.1 [18]

#### IV. CONCLUSION

The computation program, EPI Suite™, is useful as a screening-level tool for environmental and risk assessment when acceptable measured data are unavailable. It provides partition coefficients by calculation from the inherent chemical and physical properties of the compound, without taking environmental conditions into account. According to this study, the bioaccumulation, sorption capacity and toxicity of BPA in aquatic environments vary with changes of environmental conditions such as salinity, pH and temperature. Furthermore, the interpretation of results implies that BPA in seawater potentially may inflict greater adverse effects than those from a freshwater environment. Thus, it is necessary to take the environmental conditions into consideration, normally by determining the partition coefficients experimentally in order to get more accurate data to assess environmental fate and ecological risk of the chemicals. However, by measuring salinity researchers can now more accurately and easily evaluate the EPI Suite™ model to suit saltwater rather than just freshwater environments. This is clearly shown by the agreement of the  $K_{ow}$  values from the correlation to salinity and the measured value.

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#### REFERENCES

- [1] C. A. Staples, P. B. Dorn, G. M. Klecka, S. T. O'Block, and L. R. Harris, "A Review of the Environmental Fate, Effects, and Exposures of Bisphenol A," *Chemosphere*, vol. 36, no. 10, pp. 2149-2173, 1998.
- [2] Environment Canada, *Screening Assessment for the Challenge Phenol, 4,4'-(1-methylethylidene)bis- (Bisphenol A) Chemical Abstracts Service Registry Number 80-05-7*, Canada: Environment Canada, 2008.
- [3] J. D. Meeker, S. Sathyanarayana, and S. H. Swan, "Phthalates and other additives in plastics: human exposure and associated health outcomes," *Phil. Trans. R. Soc. B.*, vol. 364, pp. 2097-2113, 2009.
- [4] C. E. Talsness, A. J. M. Andrade, S. N. Kuriyama, J. A. Taylor, and F. S. vom Saal, "Components of plastic: experimental studies in animals and relevance for human health," *Phil. Trans. R. Soc. B.*, vol. 364, pp. 2079-2096, 2009.
- [5] EPA. *Bisphenol A Action Plan*, Washington, DC, U.S.A.: United States Environmental Protection Agency, 2010.
- [6] EPA. *Bisphenol A (CASRN 80-05-7)*, Washington, DC, U.S.A.: United States Environmental Protection Agency, 1993.
- [7] NTP. *NTP-CERHR Monograph on the Potential Human Reproductive and Developmental Effects of Bisphenol A*, U.S.A.: National Toxicology Program, 2008.
- [8] C. P. Groshart, P. C. Okkerman, and A. M. C. M. Pijnenburg, *Chemical study on Bisphenol A*, the Netherlands: Ministerie van Verkeer en Waterstaat, 2001.
- [9] OECD. *Organization for Economic Co-operation and Development (OECD) Guideline for Testing of Chemicals: Partition Coefficient (n-octanol/water): Shake Flask Method (107)*, Paris, France: OECD publisher, 1995.
- [10] R. W. Gossett, D. A. Brown, and D. R. Young, "Predicting the Bioaccumulation of Organic Compounds in Marine Organisms using Octanol/Water Partition Coefficients," *Marine Pollution Bulletin*, vol. 14, no. 10, pp. 387-392, 1983.
- [11] J. Sangster, "Octanol-Water Partition Coefficients of Simple Organic Compounds," *J. Phys. Chem. Ref. Data*, vol. 18, no. 3, 1989.
- [12] A. T. Fisk, R. J. Norstrom, C. D. Cymbalisty, and D. C. G. Muir, "Dietary Accumulation and Depuration of Hydrophobic Organochlorines: Bioaccumulation Parameters and Their Relationship with the Octanol/Water Partition Coefficient," *Environ. Toxicol. Chem.*, vol. 17, no. 5, pp. 951-961, 1998.

- [13] W. M. Meylan, P. H. Howard, R. S. Boethring, D. Aronson, H. Printup, and S. Gouchie, "Improved Method for Estimating Bioconcentration/Bioaccumulation Factor from Octanol/Water Partition Coefficient," *Environ. Toxicol. Chem.*, vol. 18, no. 4, pp. 664-672, 1999.
- [14] H. J. Geyer, G. G. Rimkus, I. Scheunert, A. Kauna, K.-W. Schramm, A. Kettrup, M. Zeeman, D. C. G. Muir, L. G. Hansen, and D. Mackay, "Bioaccumulation and Occurrence of Endocrine-Disruption Chemicals (EDCs), Persistent Organic Pollutants (POPs), and Other Organic Compounds in Fish and Other Organisms Including Humans," in *The Handbook of Environmental Chemistry*, vol. 2, J. B. Beek, Ed. Berlin/Heidelberg, Germany: Springer, 2000.
- [15] M. Müller and M. Nendza, *Literature Study: Effects of Molecular Size and Lipid Solubility on Bioaccumulation Potential*, Germany: Fraunhofer Institute for Molecular biology and Applied Ecology, 2007.
- [16] G. G. Briggs, "Theoretical and Experimental Relationships between Soil Adsorption, Octanol-Water Partition Coefficients, Water Solubilities, Bioconcentration Factors, and the Parachor," *J. Agric. Food Chem.*, vol. 29, pp. 1050-1059, 1981.
- [17] W. J. Lyman, W. F. Reehl, and D. H. Rosenblatte. *Handbook of chemical property estimation methods—Environmental behavior of organic compounds*, Washington, DC, U.S.A.: American Chemical Society, 1990, 960 p.
- [18] EPA. *Estimation Programs Interface (EPI) Suite™ for Microsoft® Windows, v4.10*, Washington, DC, U.S.A.: United States Environmental Protection Agency, 2011.
- [19] M. A. Major, K. A. Bostian, and D. H. Rosenblatt, *The Effect of Changes in Acidity and Salinity on the Octanol Water Partition Coefficient of Methylmercuric Species Present in Aquatic Environments at High pE*, U.S.A.: U. S. Army Biomedical Research & Development Laboratory, 1991.
- [20] K. Inaba, H. Shiraishi, and Y. Soma, "Research Note: Effects of Salinity, pH and Temperature on Aqueous Solubility of Four Organotin Compounds," *Wat. Res.*, vol. 29, no. 5, pp. 1415-1417, 1995.
- [21] B. I. Escher and R. P. Schwarzenbach, "Partitioning of Substituted Phenols in Liposome-Water, Biomembrane-Water, and Octanol-Water Systems," *Environ. Sci. Technol.*, vol. 30, no. 1, pp. 260-270, 1996.
- [22] J. Heinonen, J. Honkanen, J. V. K. Kukkonen, and I. J. Holopainen, "Bisphenol A Accumulation in the Freshwater Clam *Pisidium amnicum* at Low Temperatures," *Arch. Environ. Contam. Toxicol.*, vol. 43, pp. 50-55, 2002.
- [23] J. Eggleton and K. V. Thomas, "A review of factors affecting the release and bioavailability of contaminants during sediment disturbance events: a review," *Environment International*, vol. 30, pp. 973-980, April 2004.
- [24] S. Bangedphol, H. E. Keenan, C. Davidson, A. Sakultantimetha, and A. Songsasen, "The Partition Behavior of Tributyltin and Prediction of Environmental Fate, Persistence and Toxicity in Aquatic Environments," *Chemosphere*, vol. 77, pp. 1326-1332, 2009.
- [25] J.-H. Kang and F. Kondo, "Bisphenol A degradation in seawater is different from that in river water," *Chemosphere*, vol. 60, pp. 1288-1292, March 2005.
- [26] S. Chakka, V. M. Boddu, S. W. Maloney, and R. Damavarapu, "Prediction of Physicochemical Properties of Energetic Materials via EPI Suite," in *Energetic Materials: Thermophysical Properties, Predictions, and Experimental Measurements*, V. Bodda and P. Redner, Ed. U.S.A.: CRC Press, 2010, pp. 77-92.
- [27] APHA, Standard methods for the examination of water and wastewater (APHA: 2520B), Washington, DC, U.S.A.: American Public Health Association, Water Environment Federation, 1999.
- [28] E. D. Burton, I. R. Phillips, and D. W. Hawker, "Sorption and desorption behavior of tributyltin with natural sediments," *Environ. Sci. Technol.*, vol. 38, pp. 6694-6700, 2004.
- [29] H. Rydberg, *Solvent Extraction Principles and Practice*, 2nd ed., New York, U.S.A.: Marcel Dekker, Inc., 2004.
- [30] S. Endo, A. Pfennigsdorff, and K.-U. Goss, "Salting-Out Effect in Aqueous NaCl Solutions: Trends with Size and Polarity of Solute Molecules," *Environ. Sci. Technol.*, vol. 46, pp. 1496-1503, 2012.
- [31] K. Mayo-Bean, K. Moran, B. Meylan, and P. Ranlow, *Methodology Document for the ECOSAR Class Program*, Washington, D.C., U.S.A.: United States Environmental Protection Agency, May 2012.
- [32] C. Hansch, A. Leo, and D. Hoekman, *Exploring QSAR: Hydrophobic, electronic, and steric constants*, Washington, DC, U.S.A.: American Chemical Society, 1995.



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