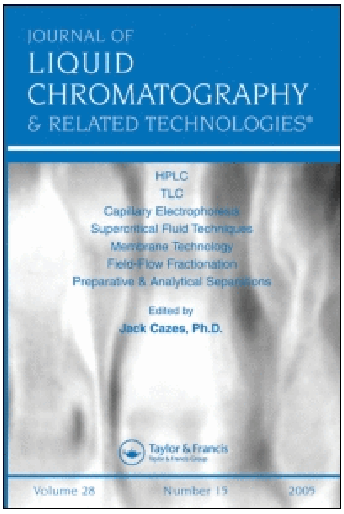

Journal of Liquid Chromatography & Related Technologies
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713597273

Using HPLC Retention Parameters to Estimate Fish Bioconcentration Factors of Organic Compounds

Rongbo Guo[a]; Xinmiao Liang[a]; Jiping Chen[a]; Qing Zhang[a]; Wenzhong Wu[a]; Antonius Kettrup[bc]
[a] Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, P.R. China [b] Institute of Ecological Chemistry, GSF-National Research Center for Environment and Health, Neuherberg, Germany [c] Lehrstuhl für Ökologische Chemie und Umweltanalytik, Technische Universität München, Freising-Weihenstephan, Germany

To cite this Article Guo, Rongbo , Liang, Xinmiao , Chen, Jiping , Zhang, Qing , Wu, Wenzhong and Kettrup, Antonius(2004) 'Using HPLC Retention Parameters to Estimate Fish Bioconcentration Factors of Organic Compounds', Journal of Liquid Chromatography & Related Technologies, 27: 12, 1861 — 1873

To link to this Article: DOI: 10.1081/JLC-120038773

URL: http://dx.doi.org/10.1081/JLC-120038773

JOURNAL OF LIQUID CHROMATOGRAPHY & RELATED TECHNOLOGIES®
Vol. 27, No. 12, pp. 1861–1873, 2004

Using HPLC Retention Parameters to Estimate Fish Bioconcentration Factors of Organic Compounds

Rongbo Guo,[1] Xinmiao Liang,[1,*] Jiping Chen,[1] Qing Zhang,[1] Wenzhong Wu,[1] and Antonius Kettrup[2,3]

[1]Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, P.R. China
[2]Institute of Ecological Chemistry, GSF-National Research Center for Environment and Health, Neuherberg, Germany
[3]Lehrstuhl für Ökologische Chemie und Umweltanalytik, Technische Universität München, Freising-Weihenstephan, Germany

ABSTRACT

Reversed-phase high performance liquid chromatography (RP-HPLC) was employed to develop predictive models for fish bioconcentration factors (BCF) of organic compounds. Estimation of BCF from RP-HPLC retention parameters on octadecyl-bonded silica gel (ODS), cyanopropyl-bonded silica gel (CN), and phenyl-bonded silica gel (Ph) columns were investigated. The results show that, for a set of compounds belonging to different chemical classes, the CN stationary phase is the best one

---

*Correspondence: Xinmiao Liang, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116011, P.R. China; E-mail: liangxm@mail.dlptt.ln.cn.

DOI: 10.1081/JLC-120038773
1082-6076 (Print); 1520-572X (Online)

www.dekker.com

among the three columns and better than *n*-octanol/water model for BCF estimation. A multi-column RP-HPLC model, using the retention parameters on the CN and Ph columns as the variables of multiple linear regression equations, was further evaluated to estimate BCF of organic compounds belonging to different chemical classes, and the results show that the multi-column RP-HPLC model is better than that of any single RP-HPLC column for BCF estimation.

Key Words: Retention parameters; Bioconcentration; HPLC; Linear regression.

INTRODUCTION

The potential uses of quantitative retention-activity relationships (QRARs) cover many areas of chemistry, biology, and environmental chemistry.[1,2] The reversed-phase high performance liquid chromatographic (RP-HPLC) method is the most popular chromatographic model used in QRARs. There are a number of advantages of the RP-HPLC method. First, it is very simple and efficient in comparison with the traditional "shake-flask" methods. Second, only a small amount of sample is needed for the measurement. Third, the method is generally insensitive to impurities or degradation products, which might either affect bulk partitioning or analysis.

The RP-HPLC retention parameters are governed by both specific and non-specific molecular interactions between solute molecules and stationary phase. For a given compound, the retention parameters on different stationary phases, with different selectivity, involve specific molecular interactions, so they can be regarded as the solute's molecular interaction descriptors.[3] The diversity of RP-HPLC stationary phases makes it possible to select the appropriate solute's retention parameters on specific stationary phases to describe specific molecular interactions. The RP-HPLC retention factors are frequently used to estimate partition coefficients, and have, therefore, been the subject of many reviews.[4]

In practice, for scientists or engineers, a model that can be applicable to a wide range of chemicals is more promising than that only applicable to a congener set of chemicals or a narrow range of chemicals. However, the congenerity phenomenon is a common problem of the usually used RP-HPLC models.[4] To obtain a QRAR model that is valid for a wide range of chemicals, one approach is to select one HPLC system whose properties are close to the target partition system. Many scientists have been devoted to the screening of different RP-HPLC stationary phases for the estimation of soil/water organic carbon partition coefficient (K_{OC}),[5] fish bioconcentration factor

(BCF),[6] median effective concentration (EC_{50}),[7] etc. Another approach is to use a multi-parameter equation that includes different retention parameters measured on different stationary phases with different selectivity.[8]

The fish/water BCF, is a very important partition parameter for evaluating a chemical's toxicity, or fate, in an aquatic environment.[9] However, the experimental measurement of BCF is extremely difficult, costly, and time-consuming.[10] In this sense, the estimation methods of BCF are very important and necessary. Although, estimation of BCF from K_{OW},[11] molecular connectivity index (MCI),[12,13] water solubility (S_w),[14] and linear solvation energy relationship (LSER)[15] have been widely studied, the advantages of RP-HPLC encourage scientists to seek the appropriate HPLC model to estimate BCF. Hui et al.[6] used RP-HPLC retention parameters to estimate BCF and four stationary phases were tested. However, their work was only subjected to aromatic hydrocarbons. In the present study, the possibility of using RP-HPLC retention parameters to estimate fish BCF, was studied on the basis of 47 organic compounds covering a wide range of chemical classes. Correlations between BCF and the RP-HPLC retention parameters on three routinely used commercial RP-HPLC columns, e.g., octadecyl-bonded silica gel (ODS), cyano-bonded silica gel (CN), and phenyl-bonded silica gel (Ph), were investigated and compared. In addition, using a multi-column method that contains retention parameters on different stationary phases was also attempted for BCF estimation.

EXPERIMENTAL

Data

A group of 47 organic compounds including alkyl benzenes, chlorinated benzenes, alkyl hydrocarbons, polycyclic aromatic hydrocarbons (PAH), phthalates, nitroaromatics, phenols, and aniline were chosen. Their $\log K_{OW}$[16] and experimental fish/water, $\log \mathrm{BCF}$[13,15] values from the corresponding references, are listed in Table 1. Good correlations between RP-HPLC retention parameters and solvatochromic parameters has been proven by many studies,[17,18] thus, the RP-HPLC retention parameters can be accurately calculated from the solvatochromic parameters. In a previous study,[8] the LSER equations of retention parameters on ODS, CN, and Ph columns were developed using 28 test compounds covering a wide range of classes. The properties of all compounds used in the present study do not go beyond the range of classes of these 28 test compounds, of which 14 compounds were used in the present study. To avoid unnecessary additional experiments, the retention parameters of the other 33 compounds under

Table 1. The retention parameters of 47 test chemicals on ODS, CN, and Ph, and log BCF, log K_{OW}.

Chemical	log k_{wODS}	S_{ODS}	log k_{wPh}	S_{Ph}	log k_{wCN}	S_{CN}	log K_{OW}	log BCF
Toluene[a]	2.42	2.97	1.30	1.96	0.43	1.29	2.79	0.92
Ethylbenzene[a]	2.96	3.47	1.79	2.54	0.80	1.83	3.15	1.19
1,2-Dimethylbenzene	2.91	3.45	1.67	2.36	0.85	1.90	3.12	1.15
1,3-Dimethylbenzene	2.94	3.47	1.68	2.37	0.84	1.90	3.20	1.17
1,4-Dimethylbenzene	2.93	3.47	1.68	2.37	0.84	1.89	3.15	1.17
Isopropylbenzene	3.54	4.01	2.09	2.82	1.25	2.48	3.66	1.55
Chlorobenzene[a]	2.51	3.13	1.32	1.98	0.58	1.51	2.90	1.08
1,2-Dichlorobenzene	3.12	3.63	1.81	2.52	1.01	2.10	3.43	1.95
1,3-Dichlorobenzene[a]	3.19	3.68	1.77	2.48	1.02	2.13	3.53	1.82
1,4-Dichlorobenzene	3.09	3.60	1.79	2.51	1.00	2.09	3.44	2.10
1,2,3-Trichlorobenzene	3.62	4.05	2.17	2.91	1.42	2.68	4.14	2.69
1,2,4-Trichlorobenzene	3.66	4.09	2.19	2.93	1.42	2.68	4.05	3.23
1,3,5-Trichlorobenzene	3.75	4.17	2.22	2.96	1.44	2.70	4.19	3.24
1,2,3,5-Tetrachlorobenzene	4.19	4.55	2.55	3.30	1.81	3.22	4.66	3.50
1,2,3,4-Tetrachlorobenzene	4.11	4.48	2.52	3.28	1.80	3.21	4.64	3.58
1,2,4,5-Tetrachlorobenzene	4.18	4.54	2.54	3.30	1.81	3.22	4.82	3.65
Pentachlorobenzene	4.63	4.93	2.87	3.65	2.18	3.75	5.18	3.74
Hexachlorobenzene	5.17	5.39	3.24	4.03	2.57	4.30	5.73	4.23
1,2-Dichloroethane	1.35	2.13	0.62	1.28	−0.19	0.44	1.48	0.30
Cyclohexane	3.24	3.74	1.72	2.42	0.70	1.68	3.44	2.22
Trichloroethene	2.30	2.94	1.16	1.83	0.26	1.05	2.61	1.20
Tetrachloroethene	2.96	3.49	1.60	2.29	0.70	1.66	3.40	1.70
a-Methylstyrene	3.19	3.69	1.88	2.57	1.10	2.26	3.36	1.47

Styrene	2.71	3.26	1.53	2.20	0.75	1.75	2.95	1.13
Anthracene[a]	4.20	4.56	2.68	3.40	2.15	3.60	4.45	3.13
Pyrene[a]	4.43	4.62	2.93	3.63	2.56	4.11	4.88	3.43
Biphenyl[a]	3.62	4.12	2.30	3.01	1.66	3.04	4.01	2.42
Naphthalene[a]	2.96	3.48	1.76	2.44	1.07	2.19	3.30	2.20
Fluorene[a]	3.78	4.14	2.44	3.13	1.73	3.04	4.18	3.11
Phenanthrene[a]	4.42	4.68	2.66	3.25	2.53	4.62	4.57	3.42
2-Methylnaphthalene	3.56	3.98	2.17	2.87	1.52	2.83	3.86	2.61
9-Methylanthracene	4.85	5.06	3.09	3.80	2.64	4.39	5.07	3.66
Benzo[*a*]anthracene	5.37	5.48	3.52	4.23	3.26	5.25	5.79	4.00
Benzo[*a*]pyrene	5.48	5.53	3.64	4.31	3.54	5.63	5.97	3.70
Acenaphthene	3.68	4.07	2.26	2.95	1.66	3.02	3.92	2.60
Diethylphthalate	2.33	2.98	1.82	2.52	1.43	2.88	2.47	2.58
Dimethylphthalate	1.19	1.97	1.01	1.65	0.63	1.72	1.56	1.75
Nitrobenzene[a]	1.43	2.20	0.86	1.47	0.26	1.06	1.83	1.18
2-Nitrotoluene	2.05	2.70	1.29	1.97	0.67	1.66	2.53	1.30
3-Nitrophenol	1.11	2.13	0.75	1.53	0.41	1.43	2.00	1.40
4-Nitrophenol[a]	0.98	1.99	0.73	1.56	0.31	1.37	1.91	2.10
2-Methylphenol	1.61	2.46	0.87	1.58	0.29	1.22	1.95	1.03
2,4-Dimethylphenol	1.94	2.75	1.11	1.83	0.54	1.59	2.30	2.18
4-Bromophenol	1.77	2.64	1.03	1.79	0.56	1.61	2.59	1.56
3-Chlorophenol[a]	1.82	2.72	1.04	1.80	0.43	1.40	2.50	1.25
4-Cyanophenol	0.67	1.75	0.50	1.27	0.19	1.13	1.60	0.91
Aniline[a]	0.41	1.26	0.30	0.90	−0.19	0.48	0.94	0.78

[a] The experimental retention parameters measured in Ref. [8].

study were calculated from their solvatochromic parameters by LSER equations developed in the previous study,[8] and the solvatochromic parameters of chemicals were obtained from the Refs.[16–19]. The retention parameters of 47 chemicals on ODS, CN, and Ph columns are presented in Table 1.

Methods

For binary mobile phase RP-HPLC system the retention factor (k) of solute can be expressed as follows.[20]

$$\log k = \log k_{\mathrm{w}} - S\varphi \tag{1}$$

where $\log k_{\mathrm{w}}$ and S are the regression constants, φ is the content of organic solvent in solvent/water mixture. The $\log k_{\mathrm{w}}$ can be regarded as the retention factor with pure water as the mobile phase. The S reflects the effect of binary mobile phase on retention. $\log k_{\mathrm{w}}$ is the most commonly used parameter in QRARs. BCF estimation from $\log k_{\mathrm{w}}$ can be calculated from the following equation:

$$\log \mathrm{BCF} = a \log k_{\mathrm{w}} + b \tag{2}$$

where a and b are the regression coefficients. The S parameter has proven to be a useful molecular descriptor, and it describes the molecular interactions different from those described by $\log k_{\mathrm{w}}$.[8] BCF estimation from the combination of $\log k_{\mathrm{w}}$ and S can be calculated according to Eq. (3):

$$\log \mathrm{BCF} = a_1 \log k_{\mathrm{w}} + a_2 S + b_1 \tag{3}$$

where the ratio of a_2 and a_1 shows the optimum eluent composition to achieve the best correlation between BCF and RP-HPLC retention parameters. Thus, Eq. (3) has the best potential of a single binary mobile phase RP-HPLC system for the estimation of BCF by optimizing the solvent/water binary mobile phase.

The combination of RP-HPLC retention parameters containing different molecular interactions, can possibly describe the whole molecular interactions involved in environmental media/water partition. The RP-HPLC multi-column method has proven to be a promising model of K_{OC} estimation for a wide range of chemicals. The normal form of the multi-column HPLC method for the estimation of partition coefficients is:[8]

$$\log K = \sum_{i=1}^{j} a_i \log k_i + c \tag{4}$$

where K is the partition coefficient, k is the RP-HPLC retention factor. For the binary mobile phase system, k can be substituted by $\log k_w$ and S. In this study, K is BCF, therefore, Eq. (4) can be rewritten as:

$$\log \mathrm{BCF} = \sum_{i=1}^{j} (a_i \log k_{wi} + b_i S_i) + c \tag{5}$$

where a_i, b_i, and c are the regression constants, j is the number of the chromatographic systems, which have different selectivity.

RESULTS AND DISCUSSION

Estimation of BCF from $\log K_{OW}$

As a standard hydrophobic parameter of a compound, $\log K_{OW}$ is the most frequently used parameter for the estimation of BCF.[11] For the purpose of comparison, in the present study, the correlations between BCF and $\log K_{OW}$ were studied for the congener chemicals and the entire chemical set separately. Good linear correlations were obtained for two classes of the congener chemicals. The correlation coefficients (r^2) are 0.99 for six alkylbenzenes and 0.91 for 12 chlorobenzenes, respectively, and the experimental log BCF against the predicted log BCF from $\log K_{OW}$ for 12 chlorobenzenes is shown in Fig. 1. But for the group of 47 tested chemicals with various functional

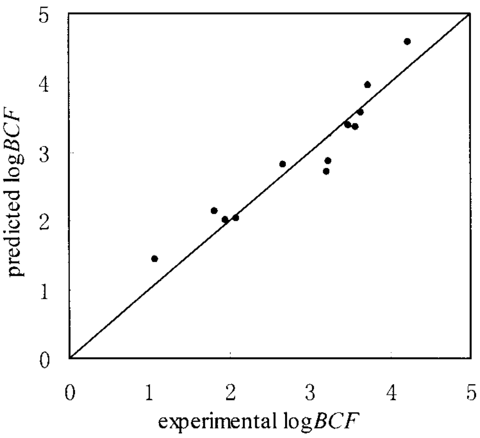

Figure 1. Plot of experimental log BCF vs. predicted log BCF from $\log K_{ow}$ for 12 chlorobenzenes.

Marcel Dekker, Inc.
270 Madison Avenue, New York, New York 10016

groups, the r^2 is only 0.75, which was much lower in comparing with those for congener chemicals. The linear regression correlation between log BCF and log K_{OW} for the entire 47 chemicals is:

$$\begin{aligned}&\log \mathrm{BCF} = 0.75 \log K_{OW} - 0.40\\ &r^2 = 0.75, \quad \mathrm{SE} = 0.52, \quad F = 140, \quad n = 47\end{aligned} \tag{6}$$

where r^2 is the correlation coefficients; SE is the standard error; F is the significance factor; n is the number of test chemicals. The plot of the experimental log BCF against the predicted log BCF from log K_{OW} for all the 47 chemicals is shown in Fig. 2. Apparently, a congenerity phenomenon exists in the correlation between log K_{OW} and log BCF.

Estimation of BCF from log k_w and S on a Single Column

As a common practice, log k_w has been usually used to estimate partition coefficients in QRARs.[2] By using the form of Eq. (2), the correlations between log k_w and BCF were studied for the ODS, CN, and Ph columns. Similar to the results of log K_{OW} for BCF estimation, the congenerity phenomenon apparently existed in the estimation of log BCF from log k_w. For all of the three columns, the good correlations between log k_w and log BCF were found for congeneric chemicals. For the six alkylbenzenes, the r^2 values are 0.99 for the ODS, 0.96 for the CN, and 0.95 for the Ph, and for the 12 chlorobenzenes,

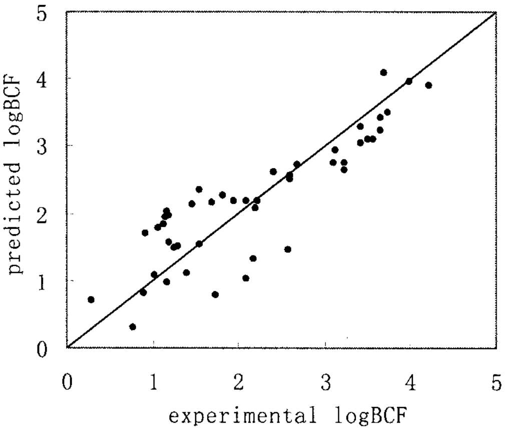

Figure 2. Plot of experimental log BCF vs. predicted log BCF from log K_{ow} for all 47 compounds.

they are 0.91, 0.92, and 0.92, respectively. However, for all the 47 chemicals belonging to several chemical classes, the r^2 decreases largely. The regression results for the three columns are shown as follows:

$$\text{ODS: } \log \text{BCF} = 0.07 + 0.69 \log k_w, \quad \text{SE} = 0.59, \quad F = 98.72, \quad r^2 = 0.69 \tag{7}$$

$$\text{CN: } \log \text{BCF} = 0.88 + 1.08 \log k_w, \quad \text{SE} = 0.48, \quad F = 178.83, \quad r^2 = 0.80 \tag{8}$$

$$\text{Ph: } \log \text{BCF} = 0.08 + 1.14 \log k_w, \quad \text{SE} = 0.51, \quad F = 146.32, \quad r^2 = 0.76 \tag{9}$$

Compared with ODS and Ph columns, the CN column has the lowest standard error, and the highest F value and r^2, which show that the CN column is the best one for the estimation of log BCF from $\log k_w$. Comparing the results of Eq. (8) with those of Eq. (6), it is shown that the CN column is also a better model than the *n*-octanol model for BCF estimation on the basis of the 47 chemicals. In previous studies,[8] a similar result was found in the estimation of $\log K_{OC}$ from $\log k_w$ on RP-HPLC columns, and the CN column was also the best model for K_{OC} estimation compared with the *n*-octanol model and other RP-HPLC columns. This may be a result of the structures of the bonded CN phase and the complex composition of natural organic matter. In contrast to the ODS and Ph stationary phases, the CN stationary phase contains lipophilic ($-CH_2-CH_2-CH_2-$) and polar ($-CN$) moieties, which are based on a silica matrix. The binary-composition of the CN stationary phase, consisting of polar and non-polar sites, enables polar and non-polar groups of a molecule to interact in a more similar manner such as in organisms.

On the basis of Eq. (3), the contribution of S parameter to $\log k_w$ for log BCF estimation can be evaluated. The r^2 between log BCF and the combination of $\log k_w$ and S by Eq. (3) is 0.72 for the ODS column and 0.80 for the Ph column. It is clear, that the values of the correlation coefficients of the combinations are increased in comparison with those of corresponding single $\log k_w$. But for the case of the CN column, almost no improvement of the r^2 was found for the combination of $\log k_w$ and S compared with single $\log k_w$. This shows that S parameter on the ODS or Ph column has a contribution; however, that on the CN column has no contribution to $\log k_w$ for improving the efficiency of log BCF estimation.

Multi-column RP-HPLC Method for Estimation of BCF

On the basis of Eq. (5), using the different retention parameters on the ODS, CN, and Ph columns as the variables of the multiple linear regression equation, a systematic examination of various combinations of retention parameters for the estimation of BCF was performed. The statistical results of the best three combinations are listed in Table 2, and r^2 values of any other combinations are lower than 0.83. The valuable multi-column HPLC model that has a high correlation coefficient and contains the simplest variables is the combination of $\log k_{\mathrm{wCN}}$, $\log k_{\mathrm{wPh}}$ and S_{Ph}. Its regression equation is:

$$\log \mathrm{BCF} = -2.21 - 4.35 \log k_{\mathrm{wPh}} + 4.38 S_{\mathrm{Ph}} + 1.02 \log k_{\mathrm{wCN}}$$
$$\mathrm{SE} = 0.43, \quad F = 75, \quad r^2 = 0.84, \quad n = 47 \tag{10}$$

The linear correlation of the predicted log BCF by Eq. (10) vs. experimental log BCF is shown in Fig. 3.

Although, as a single chromatographic system, the CN column is the best one for estimation of BCF among the three columns. The results of Eq. (10) show that its accuracy can be improved by including $\log k_{\mathrm{wPh}}$ and S_{Ph} parameters on a Ph column. This implies, that the molecular interactions involved in $\log k_{\mathrm{wPh}}$ and S_{Ph} are complementary to those involved in $\log k_{\mathrm{wCN}}$ for modeling fish/water partition.

The multi-column method involves several retention parameters that describe different specific molecular interactions, therefore, the correlation was improved compared with that based on a single chromatographic parameter, or a single chromatographic system. This result indicates that it is possible to use the multi-column RP-HPLC method to estimate BCF values for a wide range of chemical classes, but more work to verify the RP-HPLC multi-column method in detail is needed.

CONCLUSION

This study shows that, for estimation of BCF of a set of organic chemicals covering a wide range of classes, the predictability of the CN column model is

Table 2. The statistic results of the best three different combinations of RP-HPLC retention parameters.

Combination of retention parameters	r^2	SE	F	n
$\log k_{\mathrm{wODS}}$, S_{ODS}, $\log k_{\mathrm{wCN}}$, S_{CN}, $\log k_{\mathrm{wPh}}$, S_{Ph}	0.84	0.44	36	47
$\log k_{\mathrm{wCN}}$, S_{CN}, $\log k_{\mathrm{wPh}}$, S_{Ph}	0.84	0.44	56	47
$\log k_{\mathrm{wCN}}$, $\log k_{\mathrm{wPh}}$, S_{Ph}	0.84	0.43	75	47

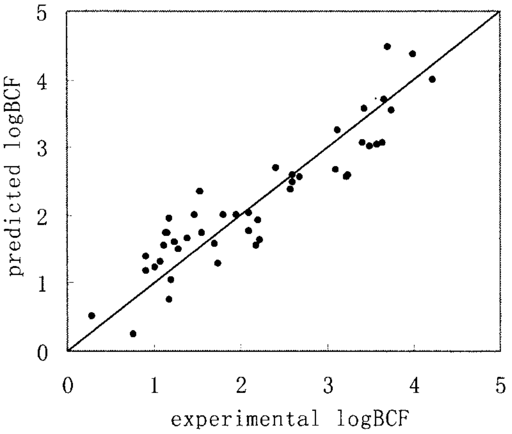

Figure 3. Plot of experimental log BCF vs. predicted log BCF from the combination of log k_{wCN}, log k_{wPh}, and S_{Ph} for all 47 compounds.

superior to the ODS and Ph column models, and also better than that of the *n*-octanol model. In addition, the estimation correlation can be improved by using the multi-column method including different retention parameters, which describe more molecular interactions than that involved in single column system.

ACKNOWLEDGMENTS

Financial support from the Science and Technology Foundation of Liaoning Province is gratefully acknowledged. The authors thank Dr. Karl-Werner Schramm, Prof. Jingwen Chen, and Prof. Lefeng Zhang for many helpful and valuable comments on the manuscript.

REFERENCES

1. William, J.L. Modeling of oil–water partitioning and membrane permeation using reversed-phase chromatography. J. Chromatogr. A **1993**, *656*, 469–484.
2. Braumann, T. Determination of hydrophobic parameters by reversed-phase liquid chromatography: theory, experimental techniques, and application in studies on quantitative structure–activity relationships. J. Chromatogr. A **1986**, *373*, 191–225.

3. Roman, K. Quantitative structure-retention relationships. Anal. Chem. **1992**, *64*, 619A–631A.
4. Dorsey, J.G.; Khaledi, M.G. Hydrophobicity estimation by reversed-phase liquid chromatography—implications for biological partitioning processes. J. Chromatogr. A **1993**, *656*, 485–499.
5. Szabo, G.; Guczi, J.; Kördel, W.; Zsolnay, A.; Major, V.; Keresztes, P. Comparison of different HPLC stationary phases for determination of soil/water distribution coefficient, KOC, values of organic chemicals in RP-HPLC system. Chemosphere **1999**, *39* (1), 431–442.
6. Hong, H.; Wang, L.S.; Han, S.K.; Zou, G.W. The estimation of bioconcentration factors of aromatic hydrocarbons by high-performance liquid chromatography. Toxicol. Environ. Chem. **1996**, *56* (1–4), 185–191.
7. Warne, M.St.J.D.; Connel, W.; Hawker, D.W. Development of QSAR's based on high performance liquid chromatography capacity factors to describe non-specific toxicity. Chemosphere **1989**, *19* (8/9), 1113–1128.
8. Guo, R.; Liang, X.; Chen, J.; Zhang, Q.; Kettrup, A. Prediction of soil adsorption coefficients from retention parameters on three reversed phase high performance liquid chromatographic columns. Anal. Chem. **2002**, *74*, 655–660.
9. Blum, D.J.W.; Speece, R.E. Determining chemical toxicity to aquatic species. Environ. Sci. Technol. **1990**, *24* (3), 284–293.
10. Eaton, J.G.; Parrish, P.R.; Hendricks, A.C. *ASTM STP 707*; American Society for Testing and Materials: Philadelphia, 1980; 116–129.
11. Devillers, J.; Bintein, S.; Domine, D. Comparison of BCF models based on log P. Chemosphere **1996**, *33* (6), 1047–1065.
12. Lu, X.; Tao, S.; Cao, J.; Dawson, R.W. Prediction of fish bioconcentration factors of nonpolar organic pollutants based on molecular connectivity indices. Chemosphere **1999**, *39* (6), 987–999.
13. Sabljic, A. The prediction of fish bioconcentration factors of organic pollutants from the molecular connectivity model. Z. Gesamte Hyg. **1987**, *33*, 493–496.
14. Lyman, W.J.; Reehl, W.F.; Ronsenblat, D.H. *Handbook of Chemical Property Estimation Methods*; McGraw-Hill: New York, 1982.
15. Park, J.H.; Lee, H.J. Estimation of bioconcentration factors in fish, adsorption coefficient for soil and sediments and interfacial tension with water for organic nonelectrolytes based on the linear solvation energy relationships. Chemosphere **1993**, *26* (10), 1905–1916.
16. Poole, S.K.; Poole, F.C. Chromatographic models for the sorption of neutral organic compounds by soil from water and air. J. Chromatogr. A **1999**, *845*, 381–400.

17. Abraham, M.H. Scales of solute hydrogen-bonding: their construction and application to physical and biochemical processes. Chem. Soc. Rev. **1993**, *22*, 73–83.
18. Wang, A.; Lay, C.T.; Carr, P.W. Global linear solvation energy relationships for retention prediction in reversed-phase liquid chromatography. J. Chromatogr. A **1999**, *848*, 21–37.
19. Abraham, M.H.; Ahdonian-Haftvan, J.; Whiting, G.S.; Leo, A. Hydrogen bonding part 34. The factors that influence the solubility of gases and vapours in water at 298 K, and a new method for its determination. J. Chem. Soc. Perkin Trans. 2 **1994**, 1777–1791.
20. Syder, L.R.; Dolan, J.W.; Gant, J.R. Gradient elution in high-performance liquid chromatography. J. Chromatogr. **1979**, *165*, 3–7.

Received July 14, 2003
Accepted February 20, 2004
Manuscript 6193

Marcel Dekker, Inc.
270 Madison Avenue, New York, New York 10016

Downloaded At: 19:26 23 January 2011

Request Permission or Order Reprints Instantly!

Interested in copying and sharing this article? In most cases, U.S. Copyright Law requires that you get permission from the article's rightsholder before using copyrighted content.

All information and materials found in this article, including but not limited to text, trademarks, patents, logos, graphics and images (the "Materials"), are the copyrighted works and other forms of intellectual property of Marcel Dekker, Inc., or its licensors. All rights not expressly granted are reserved.

Get permission to lawfully reproduce and distribute the Materials or order reprints quickly and painlessly. Simply click on the "Request Permission/ Order Reprints" link below and follow the instructions. Visit the U.S. Copyright Office for information on Fair Use limitations of U.S. copyright law. Please refer to The Association of American Publishers' (AAP) website for guidelines on Fair Use in the Classroom.

The Materials are for your personal use only and cannot be reformatted, reposted, resold or distributed by electronic means or otherwise without permission from Marcel Dekker, Inc. Marcel Dekker, Inc. grants you the limited right to display the Materials only on your personal computer or personal wireless device, and to copy and download single copies of such Materials provided that any copyright, trademark or other notice appearing on such Materials is also retained by, displayed, copied or downloaded as part of the Materials and is not removed or obscured, and provided you do not edit, modify, alter or enhance the Materials. Please refer to our Website User Agreement for more details.

Request Permission/Order Reprints

Reprints of this article can also be ordered at

http://www.dekker.com/servlet/product/DOI/101081JLC120038773