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Chromatographic Retention Times of Polychlorinated Biphenyls: from Structural Information to Property Characterization

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Abstract: The paper presents a unitary approach of the use of a Molecular Descriptors Family in structure-property/activity relationships, particularly in modelling the chromatographic retention times of polychlorinated biphenyls. Starting from molecular structure, viewed as a graph, and considering the bonds and bond types, atom types and often the 3D geometry of the molecule, a huge family of molecular descriptors called MDF was calculated. A preliminary selection of MDF members was done by simple linear regression (LR) against the measured property. The best fitted MDF subset is then submitted to multivariate linear regression (MLR) analysis in order to find the best pairs of MDF members that produce a reliable QSPR (Quantitative Structure-Property Relationship) model. The predictive capability was finally tested by randomly splitting of data into training and test sets. The best obtained models are presented and the results are discussed.

Keywords: Quantitative Structure-Property Relationship (QSPR), Molecular Descriptors Family (MDF), Polychlorinated Biphenyls (PCBs), Chromatographic Retention Time.

1. Introduction

Polychlorinated biphenyls (PCBs), organic compounds with 1 to 10 chlorine atoms attached to biphenyl, have the general chemical formula $C_{12}H_{10-x}Cl_x$. First manufactured by Monsanto in 1929, the PCBs production was banned in the 1970th due to the high toxicity of most PCBs (209) and mixtures [1]. PCBs were used as insulating fluids for industrial transformers and capacitors, and are known as persistent organic pollutants. Even if the production of the PCBs was stopped, they still have an influence on the human [2-4] and animal [5] health due to their accumulation in the environment. Moreover, the toxicity and carcinogenicity of PCBs could be related to mechanistic studies of their truncated analogue vynil chloride [6]. Ecological and toxicological aspects of polychlorinated biphenyls (PCBs) in the environment are under investigation due to their worldwide distribution [7-10].

Starting with the 20th century, several mathematical approaches, that link chemical structure and property/activity in a quantitative manner, have been introduced [11]. Nowadays, quantitative structure-property/activity relationships (QSPRs/QSARs) are currently used in pharmaceutical chemistry, toxicology and other related fields [12].

A series of properties and activities of PCBs have been investigated by QSPR/QSAR modelling: aqueous solubility [13], gas/particle partitioning in the atmosphere [14], photo degradation half-life in n-hexane solution under UV irradiation [15], n-octanol/water partition coefficients [16,17], vaporization [18,19], and sublimation enthalpy [20]. The retention time of PCB congeners has also been previously investigated and reported [21-25]. Some of the reported results are: • Hasan and Jurs [22] - five-variable regression equation with $R^2 = 0.997$ and standard deviation of 0.017; • Liu et. all [24] - five-variable regression equation with the correlation coefficient of 0.9964 ($R^2 = 0.9928$); • Ren et. all [25] - four descriptors regression model with a correlation coefficient of 0.988 ($R^2 = 0.9761$) for the test set and an average absolute relative deviation of 3.08%.

The family of molecular descriptors MDF, designed by treating the interactions among fragments of a molecular structure with the formalism of electrostatic fields and potentials, and molecular topology as well, was developed and tested in QSPR/QSAR studies [26-29].

The aim of the present study was to investigate the ability of our MDF in modelling the retention times of 209 polychlorinated biphenyls.

2. Materials and Methods

2.1 Polychlorinated Biphenyls (PCBs)

The relative response times of all PCBs obtained by using temperature-programmed, high-resolution gas chromatography on a capillary column of SE-54, reported by Mullin et al. [30] served as experimental data in this study.

Molecular structure of PCBs was drawn by using HyperChem software [31] and their 3D geometry optimised at the Extended Hückel level of theory. These calculations also provided partial charges of atoms inside the molecules. The output files *.hin files, which store the information about topology, geometry and charge distribution of the PCBs, represented the primary data for the generation of the molecular descriptors family.

2.2 Methodology of using Molecular Descriptors Family in QSPR/QSAR

Our MDF implements three criteria of fragmentation, related to pairs of atoms, in order to generate molecular fragments. Let *i* and *j* be the atoms forming a pair. The criteria are as follows:

(a) A minimal fragment is that one containing only the atom *i*, while a maximal fragment will contain all the atoms connected to *i*, excluding the atom *j*.

(b) A Szeged fragment is the set of vertices located closer to *i* than *j* (a distance-based criterion), the distance *d(i, k)* being lesser than *d(k, j)*, and

(c) A Cluj fragment is generated by excluding the path from *i* to *j* (except its terminal points) and then applying the above Szeged criterion.

Every MDF member is named with seven ordered case sensitive letters: *lMfOIpd*, every letter encoding an operator, as follows.

The 7th letter (*d*) encodes the distance metric and is either `*g*` (geometric) or `*t*` (topological). The 6th letter (*p*) encodes the atomic property and can be `*M*` (mass), `*Q*` (charge), `*C*` (cardinality), `*E*` (electronegativity), `*G*` (group electronegativity), or `*H*` (number of attached hydrogens). The 5th letter (*I*) encodes the interaction descriptor (involving two participants): `$D(d)$`, `$d(1/d)$`, `$O(p_1)$`, `$o(1/p_1)$`, `$P(p_1p_2)$`, `$p(1/p_1p_2)$`, `$Q(\sqrt{p_1p_2})$`, `$q(1/\sqrt{p_1p_2})$`, `$J(p_1d)$`, `$j(1/p_1d)$`, `$K(p_1p_2d)$`, `$k(1/p_1p_2d)$`, `$L(d\sqrt{p_1p_2})$`, `$l(1/d\sqrt{p_1p_2})$`, `$V(p_1/d)$`, `$E(p_1/d_2)$`, `$W(p_1^2/d)$`, `$w(p_1p_2/d)$`, `$F(p_1^2/d^2)$`, `$f(p_1p_2/d^2)$`, `$S(p_1^2/d^3)$`, `$s(p_1p_2/d^3)$`, `$T(p_1^2/d^4)$`, `$t(p_1p_2/d^4)$`. The 4th letter (*O*) encodes the type of overlapping interactions, which are either scalar (`*R*`, `*r*`, `*M*`, `*m*`) or vectorial (`*D*`, `*d*`). The 3rd letter (*f*) encodes the fragmentation algorithm and can be: `*m*` (minimal), `*M*` (maximal), `*D*` (Szeged, distance based), and `*P*` (Cluj, shortest paths based). The 2nd letter (*M*) encodes overlapping fragmental descriptors, which are of the type: *sized group* (`*m*`, smallest; `*M*`, largest; `*n*`, smallest absolute; `N`, largest absolute); *averaged group* (`*S*`, sum; `*A*`, average over all values; `*a*`, S divided by the number of all fragments; `*B*`, average first by atom group and then by the whole molecule; `*b*`, by bond); *geometric group* (`*P*` ,multiplication; `*G*`, geometric mean, by fragments; `*g*`, adjusted *G*; `*F*`, geometric mean by atom group and then by the whole molecule; `*f*`, by bond); *harmonic group* (`*s*`, harmonic mean, `*H*` harmonic mean, by fragments, and similarly to above `*h*`, `*I*`, and `*i*`).

MDF values enter in QSPR/QSAR modelling after a transformation (linearization procedure), one of: `*I*` (identity), `*i*` (inverse), `*A*` (absolute), `*a*` (inverse of absolute), `*L*` (logarithm of absolute), `*l*` (logarithm), which are encoded by the 1st letter.

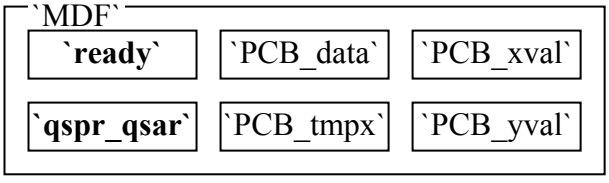
MDF use a genetic algorithm for QSPR/QSAR modelling (genetic algorithms are a particular class of evolutionary algorithms, being categorized as global search heuristics [32]). The peculiarities of the genetic algorithm used are:

- Step 1 (implies inheritance and mutation). To the solution domain (2×6×24×6×4×19 MDF members) having the genetic representation with six letters words) are applied the linearization procedure from above, when every descendent is obtained from a parent (inheritance) through a transformation (mutation). Six times more (than parents) descendants are obtained. In this step, the fitness function is defined as "have real and distinct values". A number of 490030 descendants dye due to mutation on PCB data set (remaining 297938 descendants, having genetic representation with seven letters words now).
- Step 2 (implies selection). To the solution domain (MDF descendants from Step 1) a bias procedure (selection) is applied. In this step, the fitness function is defined as "have distinct first nine digits of determination coefficient with measured property". For PCBs data set, only 99806 members pass selection. From this solution domain another selection is made: best descriptor (which correlates the best with measured property (for PCBs result being presented in Eq(1)).
- Step 3 (implies crossover). Pairs of MDF members are crossover in order to obtain models with two descriptors. Two fitness functions are used here: "have better determination coefficient" and "have better cross-validation leave-one-out score". The result for PCBs data set is given in Eq(2).

2.3 Computational Details

The MDF is calculated by a set of original programs written in PHP (Pre Hypertext Processor, [33]) and stored into a MySQL database [34] under a FreeBSD server [35]. This set of programs completes the MDF generation task. The programs create tables, insert, drop, delete, and select grants on `MDF` database (Figure 1). All programs run in a directory with the name of the set of selected compounds (actually, PCB).

Figure 1. `MDF` database for PCBs.

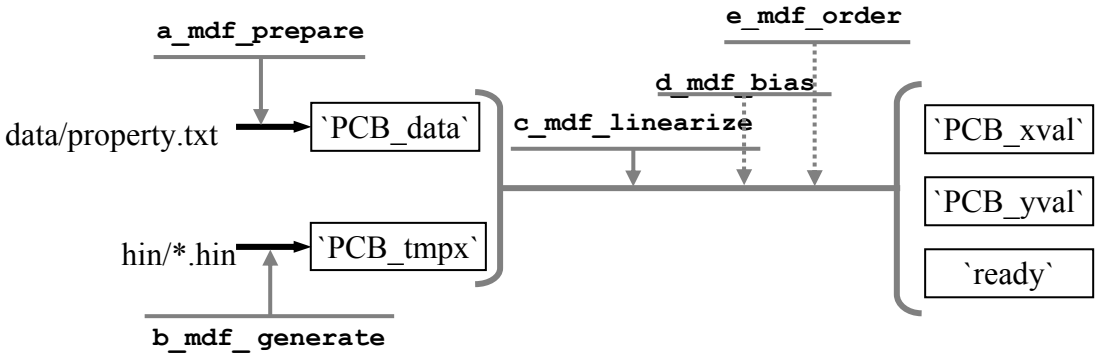


The first program, *a_mdf_prepare.php*, orders the molecules, contained as **.hin* files in a `data` subdirectory, in the same ordering as the measured property, contained in a `*property.txt*` file. The names of *.hin files and corresponding property are used to create a temporary `PCB_tmpx` table and finally the `PCB_data` table. The second program, *b_mdf_generate.php* (the most time consuming

procedure) it stores thousands records into the `PCB_tmpx` table.

The third program, *c_mdf_linearize.php*, completes the `PCB_data`, `PCB_xval`, and `PCB_yval` tables with linearized MDF members and statistical parameters. Note that, only real and distinct values are stored into the database. The fourth program, *d_mdf_bias.php* applied a bias procedure for data reduction. Finally, the fifth program, *e_mdf_order.php*, re-arrange the data from the `PCB_xval`, and `PCB_yval` tables in descending order of the squared correlation coefficient. When the task is complete, the fifth program writes in the `ready` table a record with the set name (Figure 2).

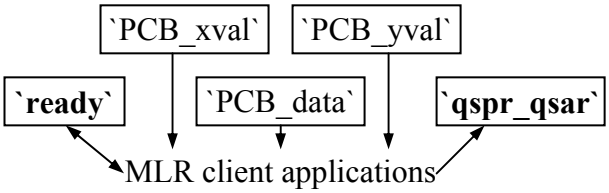
Figure 2. Preparing data for Multiple Linear Regression analysis.



The QSPR/QSAR finding procedure is made by a client programs built in Delphi programming language [36]. Bivariate correlations are performed, one with any other MDF members.

A client program (Figure 3) connects the `MDF` database, query the ready tables all together, for the ready set (now PCB set is ready), and runs for finding the best QSAR/QSPR model. Every new better QSPR/QSAR is stored into a table called `qspr_qsar`, within the same `MDF` database.

Figure 3. MLR MDF QSPR client-server.



This program, called *i_mdf_query.php*, provides complete statistical analysis of models. The user of MDF can modify, by means of this *i_mdf_query.php* program, the criteria for the best QSPR/QSAR models.

3. Results and Discussion

The above described procedure was used for finding the best QSPR model of the PCBs relative chromatographic retention times.

In monovariate correlation, the best MDF QSPR model was provided by the *iIDRwHg* MDF member, Eq(1):

$$\hat{Y}_{1d} = -0.16 + 0.09 \cdot \text{iIDRwHg}$$
$$R^2 = 0.9840;\ 95\%CI_R\ [0.9894 - 0.9939];\ \text{StErr} = 0.02;\ F = 12806;\ p < 0.0001 \quad (1)$$
$$Q^2_{cv\text{-}loo} = 0.9838$$

where $\hat{Y}_{1d}$ = estimated retention time by MDF-SAR equation with one descriptor; iIDRwHg = molecular descriptor; R^2 = square correlation coefficient; $95\%CI_R$ = 95% confidence interval for correlation coefficient; $Q^2_{cv\text{-}loo}$= cross-validation leave-one-out score.

The quality of statistics is given by R^2 (the square correlation coefficient), StErr (standard error of estimate), F (Fisher parameter) and p (type I error, or α error). The cross-validation leave-one-out score is given as Q^2. Clearly, the model shows a good predictability. The type I error of the model from Eq(1) is very small, showing a very small error of rejecting the null hypothesis when it is actually true.

About ninety-eight percents of variation in PCBs chromatographic retention time can be explained by its linear relation with a single MDF member, *iIDRwHg*, which accounts for the actual geometry (by the geometric distance operator (`*g*`)) and the number of directly bonded hydrogen atoms (`*H*`).

The best model with two descriptors was:

$$\hat{Y}_{2d} = -5.96 + 0.024 \cdot \text{ISDmsHt} - 1.02 \cdot \text{lADrtHg}$$
$$R^2 = 0.9967;\ 95\%\ CI\ [0.9977\text{-}0.9987];\ \text{StdErr} = 0.01;\ F = 30752;\ p < 0.0001 \quad (2)$$
$$Q^2_{cv\text{-}loo} = 0.9962$$

where $\hat{Y}_{2d}$ = estimated retention time by MDF-SAR equation with two descriptors.

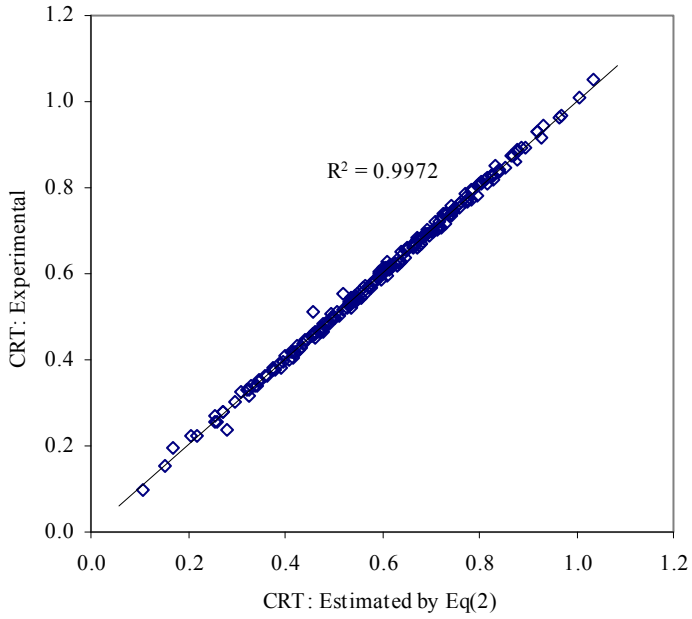
The multi-colinearity analysis shown that the two descriptors used by Eq(2) rather inter-related (R^2(ISDmsHt, lADrtHg) = 0.944) and each of them (R^2(Y, ISDmsHt) = 0.907; rank = 12614; R^2(Y, lADrtHg) = 0.973; rank = 277) are not the best descriptor in monovariate regression model (see Eq(1)). The ISDmsHt descriptor is built by a topological distance operator (`t`) while lADrtHg takes into account the genuine distance (`g`). Both of them consider the directly bonded hydrogen atom (`H`). The topological description explains more than 90% of the variance, the remaining 9.7% being completed by the information on molecular geometry.

The plot corresponding to Eq(2) is illustrated in Figure 4.

The values of the best descriptors in uni and bivariate regressions (Eq(1)&(2)), the experimental and estimated chromatographic retention time, and residuals for the PCBs set are listed in Table 1.

The accuracy of description is extremely high, even as the set of molecules is quite large. The excellent model (Eq(2)), derived for such a large set, is by itself a test of predictive ability. Indeed, if various ratios training/testing selections were considered, the quality of statistics remained very high (Table 2).

Figure 4. The plot of experimental vs chromatographic retention time (CRT) by Eq(2).



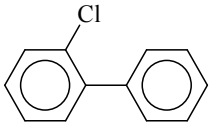
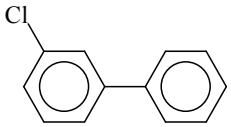
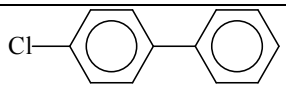
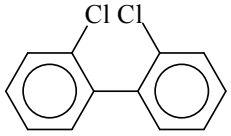
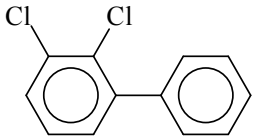
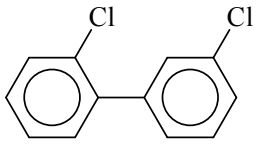
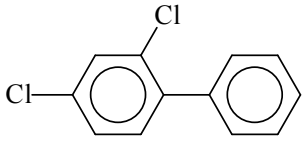
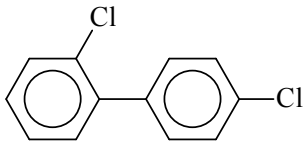
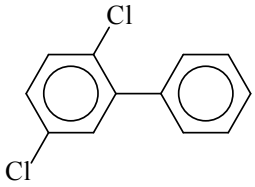
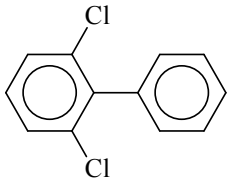
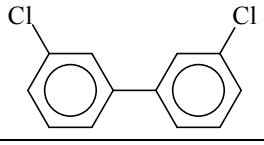
As it can be observed from Table 2, the lowest R^2 is about 0.996 in both training and test sets, which demonstrates the ability of (*ISDmsHt*, *lADrtHg*) MDF pair to described the PCBs relative retention time (Eq(2)). Note that, R^2 exceeds the upper bond of the confidence interval of Eq(2) in almost 20% of cases and is less then the lower bond in other 20% of cases. In the test set, in four cases the values of Q^2 were greater than the upper confidence boundary.

By analysing of the obtained models (Eq(1) and Eq(2)) in the light of the previously reported models, it can be observed that with a single exception ([25], $p = 0.3528$) out of three the model with one descriptor - Eq(1) - did not obtains a greater squared correlation coefficient compared with models reported in the references [22] and [24] (the differences are of -0.0064 [22], and of -0.0043 [24] respectively).

Analyzing the model with two molecular descriptors it was identified a statistical significant differences between correlation coefficient of this model and of the model reported by [24] ($p < 0.0001$) or by [25] ($p < 0.0001$). There was not identified a statistical difference between the Eq(2) and the model reported by [22] ($p = 0.7263$). The following remarks can be revealed by summarizing the above results:

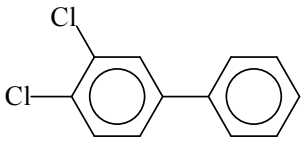
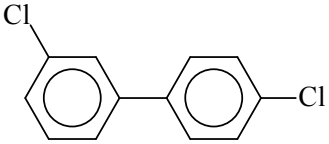
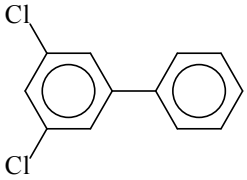
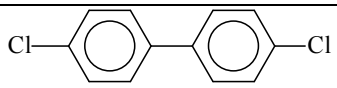
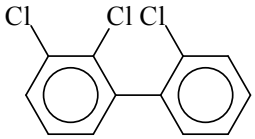
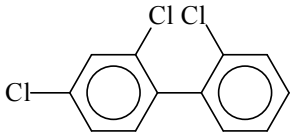
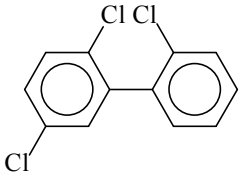
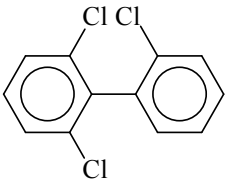
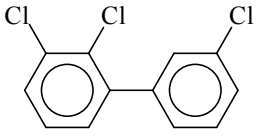
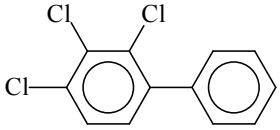
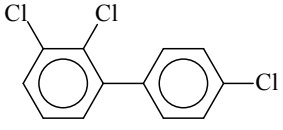
- The MDF model obtained by Eq(1) is a better model comparing with previously reported ones [22, 24,25] in terms of number of variables used (one descriptor for the model from Eq(1), five descriptors for the model reported in [22] and [24], four descriptors for the model reported in [25]).
- The MDF model obtained by Eq(2) is significantly better models comparing with models reported in [24] and [25] in terms of correlation coefficients. Moreover, it is a better model comparing with model reported in [22] in terms of number of variables used (two descriptors used by the Eq(2), and five descriptors used by the model reported in [22]).

Table 1. PCBs MDF descriptors, estimated and residuals obtained by Eq(1)&Eq(2).

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB001		0.0997	10.02	-0.0122	-0.5363	133.20	-3.42	0.1119	-0.0122
PCB002		0.1544	10.60	0.0041	0.1800	134.27	-3.47	0.1503	0.0041
PCB003		0.1937	9.96	0.0376	1.6541	135.23	-3.40	0.1561	0.0376
PCB004		0.2245	10.14	0.0054	0.2377	134.89	-3.42	0.2191	0.0054
PCB005		0.2785	9.75	0.0251	1.1035	133.36	-3.41	0.2534	0.0251
PCB006		0.2709	10.15	-0.0193	-0.8496	136.72	-3.38	0.2902	-0.0193
PCB007		0.2566	10.72	0.0028	0.1234	134.60	-3.48	0.2538	0.0028
PCB008		0.2783	10.27	-0.0048	-0.2094	133.35	-3.43	0.2831	-0.0048
PCB009		0.2570	11.12	0.0348	1.5315	134.95	-3.55	0.2222	0.0348
PCB010		0.2243	11.75	0.0333	1.4623	133.57	-3.57	0.1910	0.0333
PCB011		0.3238	11.26	0.0168	0.7378	133.12	-3.52	0.3070	0.0168

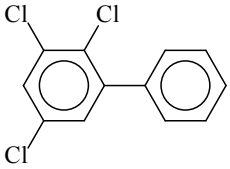
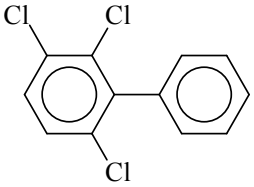
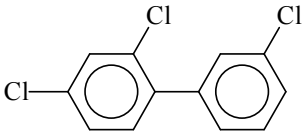
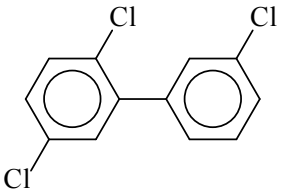
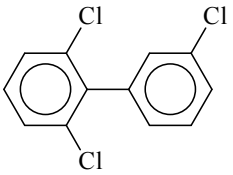
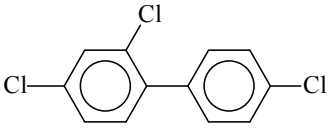
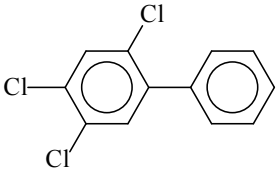
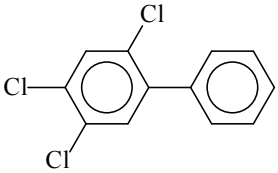
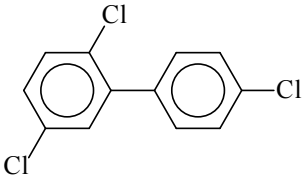
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d, 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d, 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB012		0.3298	11.52	0.0442	1.9425	132.24	-3.57	0.2856	0.0442
PCB013		0.3315	11.09	0.0065	0.2857	134.24	-3.49	0.3250	0.0065
PCB014		0.2373	10.98	-0.0393	-1.7268	133.10	-3.50	0.2766	-0.0393
PCB015		0.3387	10.98	0.0036	0.1567	131.58	-3.51	0.3351	0.0036
PCB016		0.3625	10.45	0.0193	0.8481	132.74	-3.45	0.3432	0.0193
PCB017		0.3398	10.97	-0.0184	-0.8086	133.06	-3.51	0.3582	-0.0184
PCB018		0.3378	10.72	-0.0125	-0.5510	131.64	-3.50	0.3503	-0.0125
PCB019		0.3045	10.16	0.0042	0.1849	132.62	-3.44	0.3003	0.0042
PCB020		0.4170	11.56	0.0015	0.0644	132.66	-3.57	0.4155	0.0015
PCB021		0.4135	11.09	-0.0179	-0.7855	133.32	-3.50	0.4314	-0.0179
PCB022		0.4267	11.05	0.0005	0.0212	131.66	-3.52	0.4262	0.0005

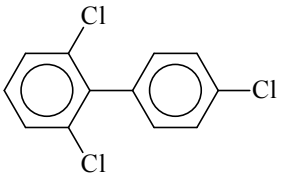
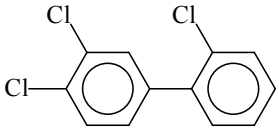
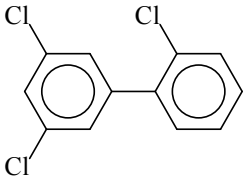
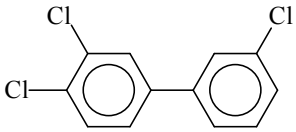
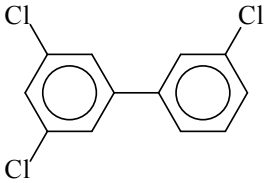
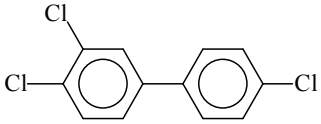
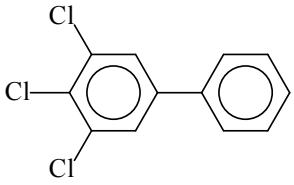
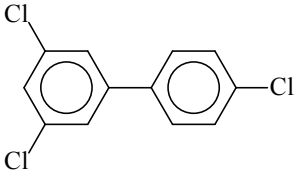
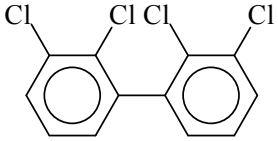
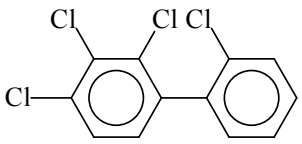
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d,\ 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d,\ 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB023		0.3770	11.05	-0.0239	-1.0517	132.19	-3.51	0.4009	-0.0239
PCB024		0.3508	10.52	0.0042	0.1838	131.49	-3.46	0.3466	0.0042
PCB025		0.3937	10.80	-0.0283	-1.2445	133.28	-3.48	0.4220	-0.0283
PCB026		0.3911	10.24	-0.0015	-0.0653	133.94	-3.42	0.3926	-0.0015
PCB027		0.3521	10.75	0.0056	0.2482	132.13	-3.50	0.3465	0.0056
PCB028		0.4031	10.23	-0.0294	-1.2916	131.25	-3.45	0.4325	-0.0294
PCB029		0.3820	12.03	-0.0161	-0.7060	132.78	-3.65	0.3981	-0.0161
PCB030		0.3165	11.48	-0.0323	-1.4195	133.66	-3.57	0.3488	-0.0323
PCB031		0.4094	11.55	0.0086	0.3793	132.00	-3.60	0.4008	0.0086

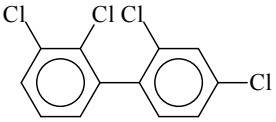
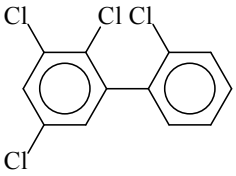
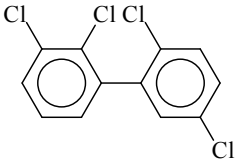
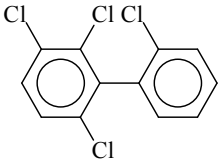
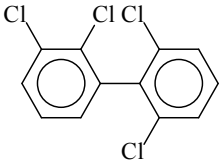
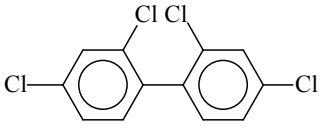
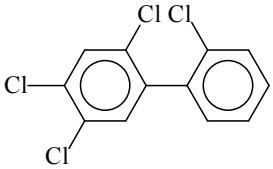
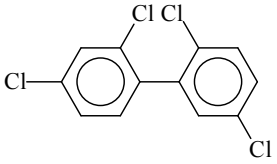
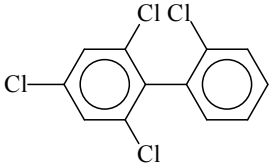
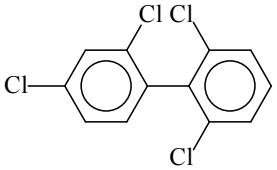
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d,\ 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d,\ 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB032		0.3636	11.22	0.0089	0.3932	131.75	-3.57	0.3547	0.0089
PCB033		0.4163	11.25	0.0057	0.2490	132.12	-3.58	0.4106	0.0057
PCB034		0.3782	12.89	-0.0103	-0.4521	130.80	-3.73	0.3885	-0.0103
PCB035		0.4738	12.32	0.0138	0.6063	131.52	-3.67	0.4600	0.0138
PCB036		0.4375	12.42	0.0027	0.1167	130.24	-3.68	0.4348	0.0027
PCB037		0.4858	11.87	0.0184	0.8096	129.97	-3.61	0.4674	0.0184
PCB038		0.5102	12.09	0.0635	2.7897	130.07	-3.66	0.4467	0.0635
PCB039		0.4488	11.53	0.0041	0.1782	131.14	-3.59	0.4447	0.0041
PCB040		0.5102	11.58	0.0012	0.0545	129.81	-3.60	0.5090	0.0012
PCB041		0.4990	12.15	-0.0127	-0.5568	130.26	-3.67	0.5117	-0.0127

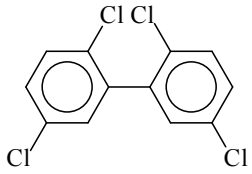
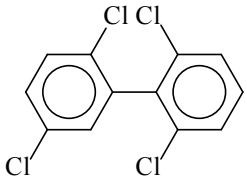
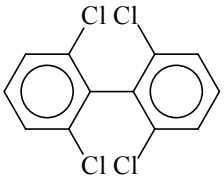
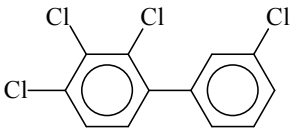
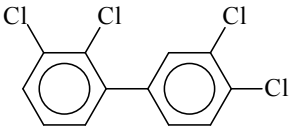
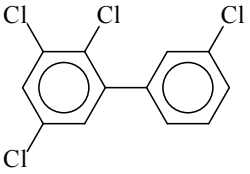
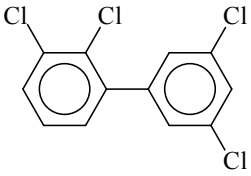
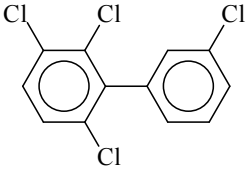
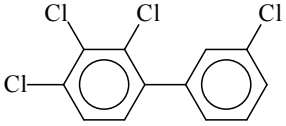
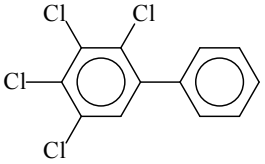
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d,\ 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d,\ 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB042		0.4870	11.30	-0.0324	-1.4222	129.77	-3.59	0.5194	-0.0324
PCB043		0.4587	12.11	-0.0267	-1.1744	130.59	-3.66	0.4854	-0.0267
PCB044		0.4832	11.60	-0.0088	-0.3869	129.80	-3.61	0.4920	-0.0088
PCB045		0.4334	12.57	0.0004	0.0168	130.50	-3.74	0.4330	0.0004
PCB046		0.4450	13.43	0.0088	0.3881	128.67	-3.82	0.4362	0.0088
PCB047		0.4639	12.87	-0.0562	-2.4723	128.32	-3.76	0.5201	-0.0562
PCB048		0.4651	12.62	-0.0098	-0.4320	128.24	-3.75	0.4749	-0.0098
PCB049		0.4610	14.04	-0.0314	-1.3821	126.70	-3.90	0.4924	-0.0314
PCB050		0.4007	10.02	-0.0122	-0.5363	133.20	-3.42	0.1119	-0.0122
PCB051		0.4242	10.60	0.0041	0.1800	134.27	-3.47	0.1503	0.0041

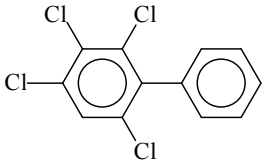
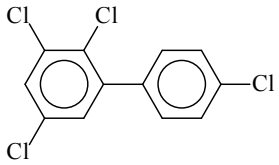
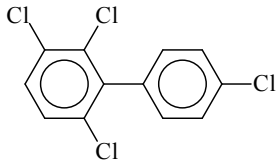
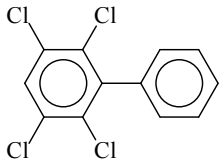
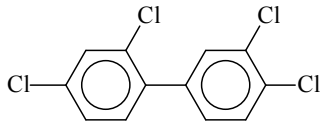
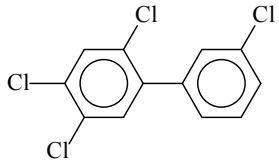
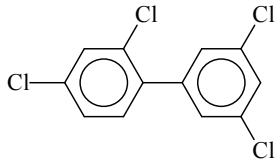
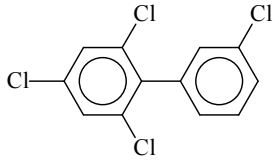
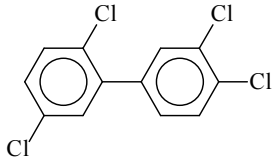
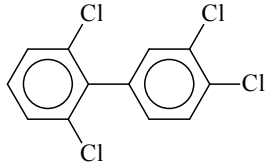
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d,\ 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d,\ 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB052		0.4557	9.96	0.0376	1.6541	135.23	-3.40	0.1561	0.0376
PCB053		0.4187	10.14	0.0054	0.2377	134.89	-3.42	0.2191	0.0054
PCB054		0.3800	9.75	0.0251	1.1035	133.36	-3.41	0.2534	0.0251
PCB055		0.5562	10.15	-0.0193	-0.8496	136.72	-3.38	0.2902	-0.0193
PCB056		0.5676	10.72	0.0028	0.1234	134.60	-3.48	0.2538	0.0028
PCB057		0.5515	10.27	-0.0048	-0.2094	133.35	-3.43	0.2831	-0.0048
PCB058		0.5267	11.12	0.0348	1.5315	134.95	-3.55	0.2222	0.0348
PCB059		0.4860	11.75	0.0333	1.4623	133.57	-3.57	0.1910	0.0333
PCB060		0.5676	11.26	0.0168	0.7378	133.12	-3.52	0.3070	0.0168
PCB061		0.5331	11.52	0.0442	1.9425	132.24	-3.57	0.2856	0.0442

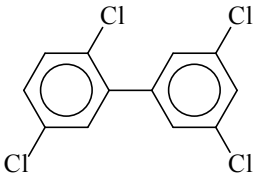
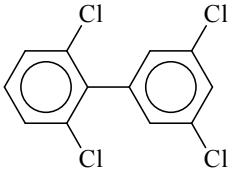
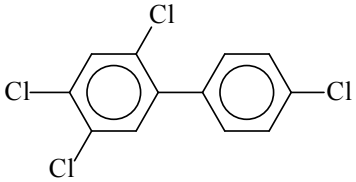
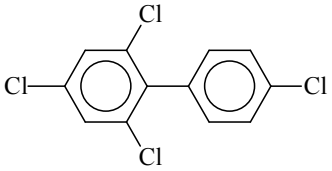
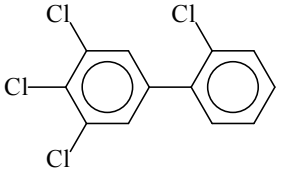
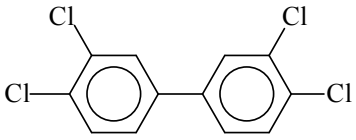
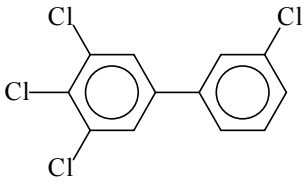
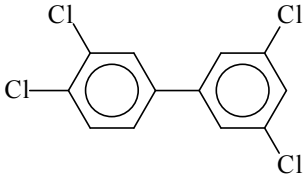
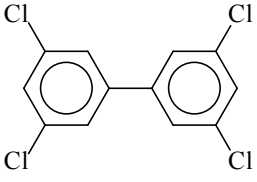
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d, 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d, 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB062		0.4685	11.09	0.0065	0.2857	134.24	-3.49	0.3250	0.0065
PCB063		0.5290	10.98	-0.0393	-1.7268	133.10	-3.50	0.2766	-0.0393
PCB064		0.4999	10.98	0.0036	0.1567	131.58	-3.51	0.3351	0.0036
PCB065		0.4671	10.45	0.0193	0.8481	132.74	-3.45	0.3432	0.0193
PCB066		0.5447	10.97	-0.0184	-0.8086	133.06	-3.51	0.3582	-0.0184
PCB067		0.5214	10.72	-0.0125	-0.5510	131.64	-3.50	0.3503	-0.0125
PCB068		0.5040	10.16	0.0042	0.1849	132.62	-3.44	0.3003	0.0042
PCB069		0.4510	11.56	0.0015	0.0644	132.66	-3.57	0.4155	0.0015
PCB070		0.5407	11.09	-0.0179	-0.7855	133.32	-3.50	0.4314	-0.0179
PCB071		0.4989	11.05	0.0005	0.0212	131.66	-3.52	0.4262	0.0005

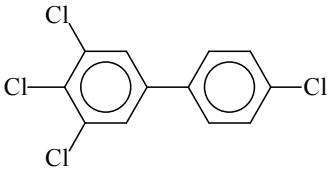
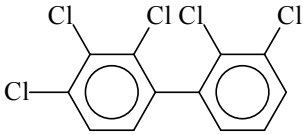
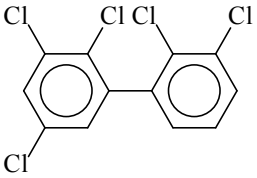
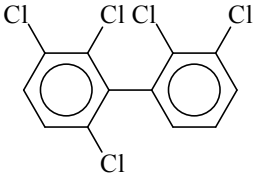
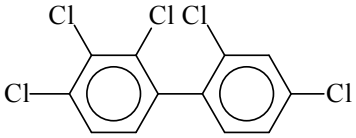
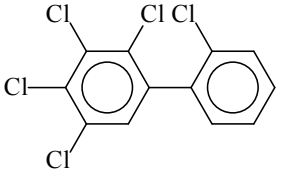
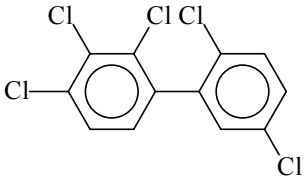
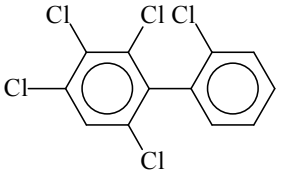
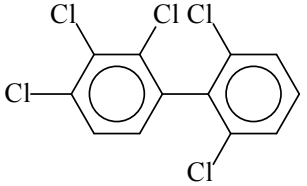
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d, 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d, 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB072		0.4984	11.05	-0.0239	-1.0517	132.19	-3.51	0.4009	-0.0239
PCB073		0.4554	10.52	0.0042	0.1838	131.49	-3.46	0.3466	0.0042
PCB074		0.5341	10.80	-0.0283	-1.2445	133.28	-3.48	0.4220	-0.0283
PCB075		0.4643	10.24	-0.0015	-0.0653	133.94	-3.42	0.3926	-0.0015
PCB076		0.5408	10.75	0.0056	0.2482	132.13	-3.50	0.3465	0.0056
PCB077		0.6295	10.23	-0.0294	-1.2916	131.25	-3.45	0.4325	-0.0294
PCB078		0.6024	12.03	-0.0161	-0.7060	132.78	-3.65	0.3981	-0.0161
PCB079		0.5894	11.48	-0.0323	-1.4195	133.66	-3.57	0.3488	-0.0323
PCB080		0.5464	11.55	0.0086	0.3793	132.00	-3.60	0.4008	0.0086

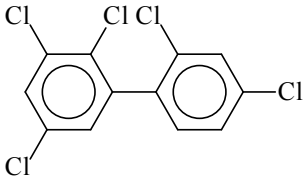
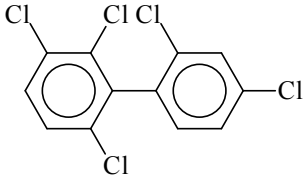
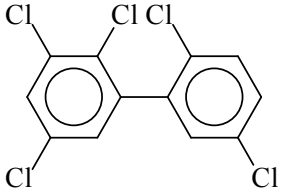
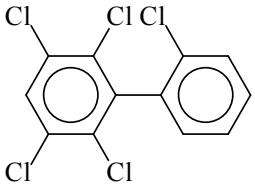
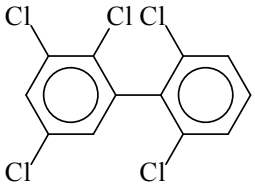
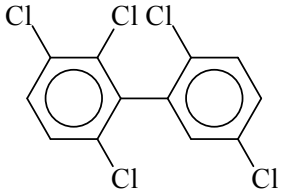
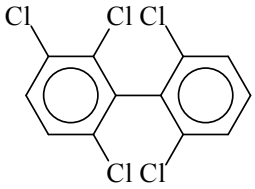
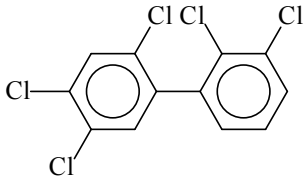
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d, 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d, 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB081		0.6149	11.22	0.0089	0.3932	131.75	-3.57	0.3547	0.0089
PCB082		0.6453	11.25	0.0057	0.2490	132.12	-3.58	0.4106	0.0057
PCB083		0.6029	12.89	-0.0103	-0.4521	130.80	-3.73	0.3885	-0.0103
PCB084		0.5744	12.32	0.0138	0.6063	131.52	-3.67	0.4600	0.0138
PCB085		0.6224	12.42	0.0027	0.1167	130.24	-3.68	0.4348	0.0027
PCB086		0.6105	11.87	0.0184	0.8096	129.97	-3.61	0.4674	0.0184
PCB087		0.6175	12.09	0.0635	2.7897	130.07	-3.66	0.4467	0.0635
PCB088		0.5486	11.53	0.0041	0.1782	131.14	-3.59	0.4447	0.0041
PCB089		0.5779	11.58	0.0012	0.0545	129.81	-3.60	0.5090	0.0012

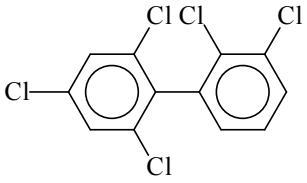
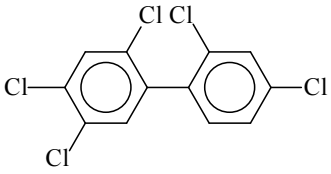
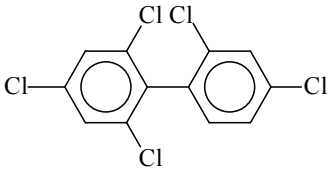
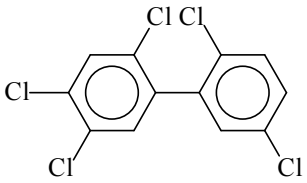
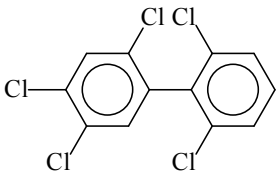
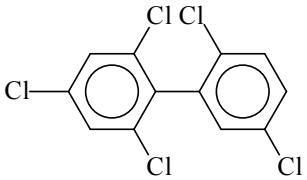
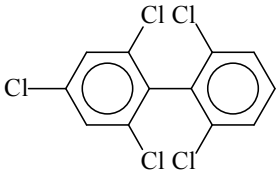
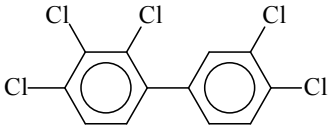
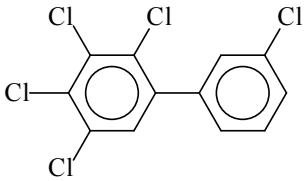
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d, 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d, 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB090		0.5814	12.15	-0.0127	-0.5568	130.26	-3.67	0.5117	-0.0127
PCB091		0.5549	11.30	-0.0324	-1.4222	129.77	-3.59	0.5194	-0.0324
PCB092		0.5742	12.11	-0.0267	-1.1744	130.59	-3.66	0.4854	-0.0267
PCB093		0.5437	11.60	-0.0088	-0.3869	129.80	-3.61	0.4920	-0.0088
PCB094		0.5331	12.57	0.0004	0.0168	130.50	-3.74	0.4330	0.0004
PCB095		0.5464	13.43	0.0088	0.3881	128.67	-3.82	0.4362	0.0088
PCB096		0.5057	12.87	-0.0562	-2.4723	128.32	-3.76	0.5201	-0.0562
PCB097		0.6100	12.62	-0.0098	-0.4320	128.24	-3.75	0.4749	-0.0098

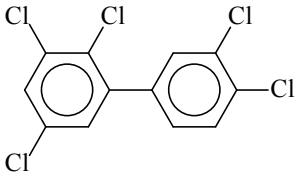
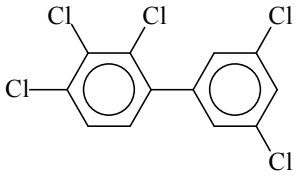
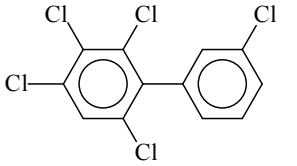
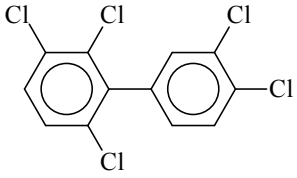
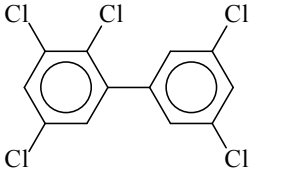
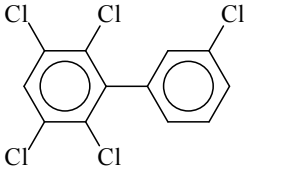
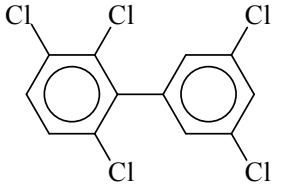
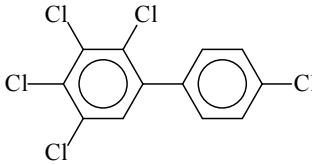
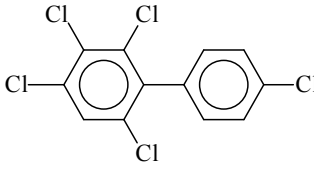
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d, 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d, 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB098		0.5415	14.04	-0.0314	-1.3821	126.70	-3.90	0.4924	-0.0314
PCB099		0.5880	10.02	-0.0122	-0.5363	133.20	-3.42	0.1119	-0.0122
PCB100		0.5212	10.60	0.0041	0.1800	134.27	-3.47	0.1503	0.0041
PCB101		0.5816	9.96	0.0376	1.6541	135.23	-3.40	0.1561	0.0376
PCB102		0.5431	10.14	0.0054	0.2377	134.89	-3.42	0.2191	0.0054
PCB103		0.5142	9.75	0.0251	1.1035	133.36	-3.41	0.2534	0.0251
PCB104		0.4757	10.15	-0.0193	-0.8496	136.72	-3.38	0.2902	-0.0193
PCB105		0.7049	10.72	0.0028	0.1234	134.60	-3.48	0.2538	0.0028
PCB106		0.6680	10.27	-0.0048	-0.2094	133.35	-3.43	0.2831	-0.0048

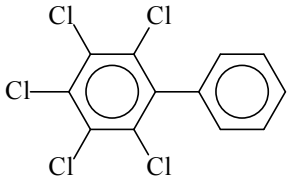
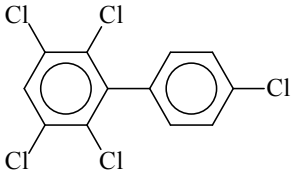
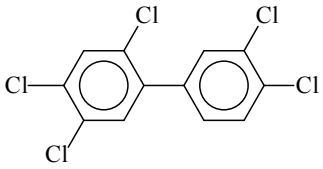
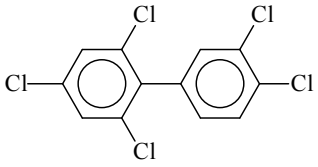
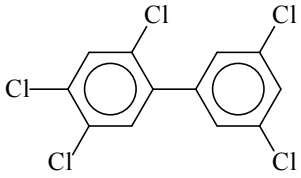
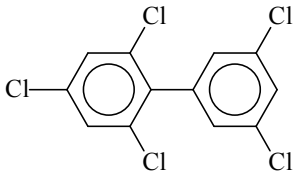
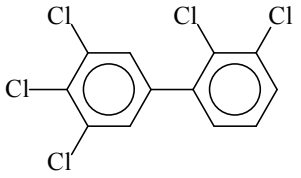
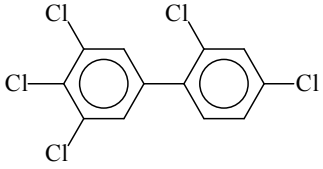
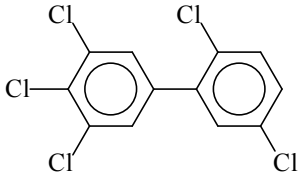
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d,\ 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d,\ 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB107		0.6628	11.12	0.0348	1.5315	134.95	-3.55	0.2222	0.0348
PCB108		0.6626	11.75	0.0333	1.4623	133.57	-3.57	0.1910	0.0333
PCB109		0.6016	11.26	0.0168	0.7378	133.12	-3.52	0.3070	0.0168
PCB110		0.6314	11.52	0.0442	1.9425	132.24	-3.57	0.2856	0.0442
PCB111		0.6183	11.09	0.0065	0.2857	134.24	-3.49	0.3250	0.0065
PCB112		0.5986	10.98	-0.0393	-1.7268	133.10	-3.50	0.2766	-0.0393
PCB113		0.5862	10.98	0.0036	0.1567	131.58	-3.51	0.3351	0.0036
PCB114		0.6828	10.45	0.0193	0.8481	132.74	-3.45	0.3432	0.0193
PCB115		0.6171	10.97	-0.0184	-0.8086	133.06	-3.51	0.3582	-0.0184

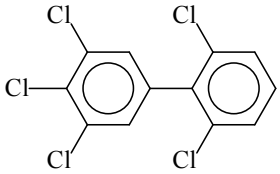
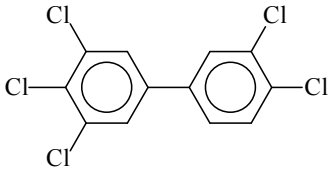
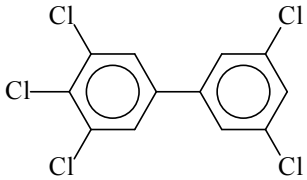
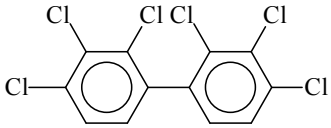
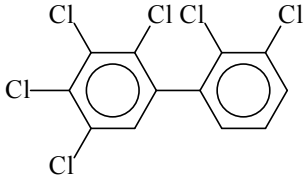
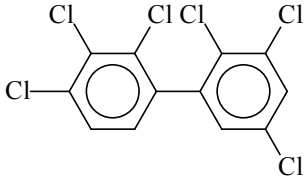
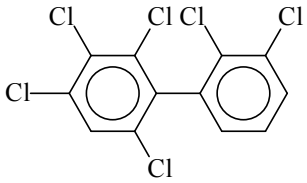
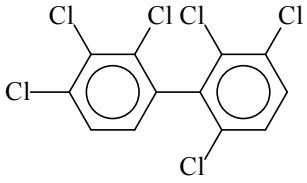
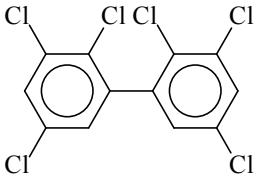
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d, 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d, 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB116		0.6132	10.72	-0.0125	-0.5510	131.64	-3.50	0.3503	-0.0125
PCB117		0.6150	10.16	0.0042	0.1849	132.62	-3.44	0.3003	0.0042
PCB118		0.6693	11.56	0.0015	0.0644	132.66	-3.57	0.4155	0.0015
PCB119		0.5968	11.09	-0.0179	-0.7855	133.32	-3.50	0.4314	-0.0179
PCB120		0.6256	11.05	0.0005	0.0212	131.66	-3.52	0.4262	0.0005
PCB121		0.5518	11.05	-0.0239	-1.0517	132.19	-3.51	0.4009	-0.0239
PCB122		0.6871	10.52	0.0042	0.1838	131.49	-3.46	0.3466	0.0042
PCB123		0.6658	10.80	-0.0283	-1.2445	133.28	-3.48	0.4220	-0.0283
PCB124		0.6584	10.24	-0.0015	-0.0653	133.94	-3.42	0.3926	-0.0015

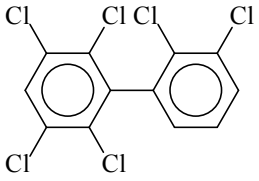
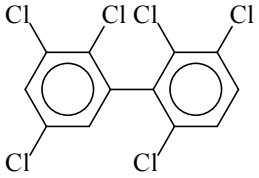
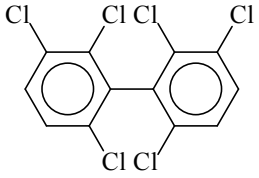
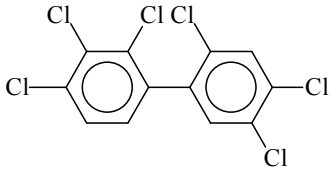
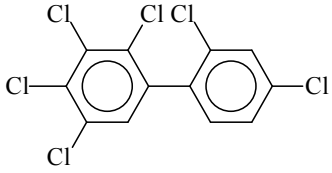
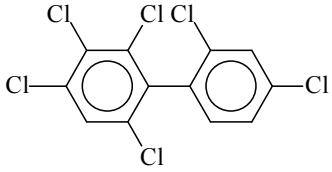
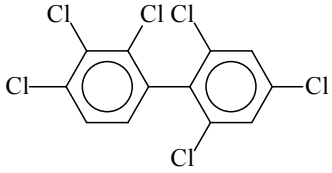
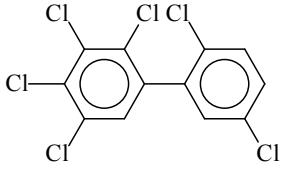
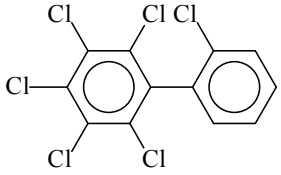
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d, 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d, 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB125		0.6142	10.75	0.0056	0.2482	132.13	-3.50	0.3465	0.0056
PCB126		0.7512	10.23	-0.0294	-1.2916	131.25	-3.45	0.4325	-0.0294
PCB127		0.7078	12.03	-0.0161	-0.7060	132.78	-3.65	0.3981	-0.0161
PCB128		0.7761	11.48	-0.0323	-1.4195	133.66	-3.57	0.3488	-0.0323
PCB129		0.7501	11.55	0.0086	0.3793	132.00	-3.60	0.4008	0.0086
PCB130		0.7184	11.22	0.0089	0.3932	131.75	-3.57	0.3547	0.0089
PCB131		0.6853	11.25	0.0057	0.2490	132.12	-3.58	0.4106	0.0057
PCB132		0.7035	12.89	-0.0103	-0.4521	130.80	-3.73	0.3885	-0.0103
PCB133		0.6871	12.32	0.0138	0.6063	131.52	-3.67	0.4600	0.0138

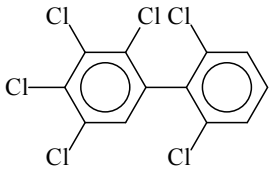
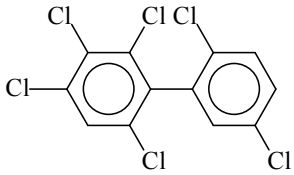
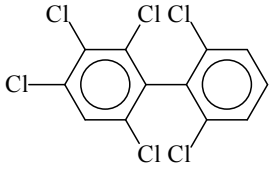
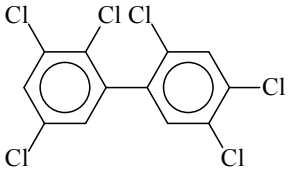
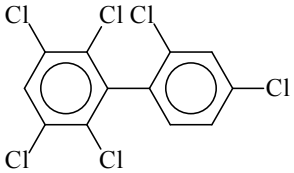
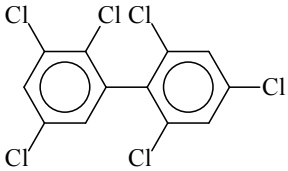
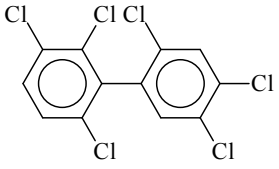
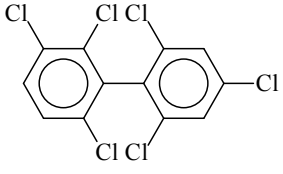
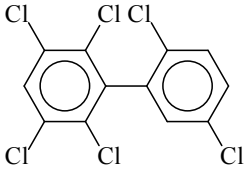
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d,\ 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d,\ 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB134		0.6796	12.42	0.0027	0.1167	130.24	-3.68	0.4348	0.0027
PCB135		0.6563	11.87	0.0184	0.8096	129.97	-3.61	0.4674	0.0184
PCB136		0.6257	12.09	0.0635	2.7897	130.07	-3.66	0.4467	0.0635
PCB137		0.7329	11.53	0.0041	0.1782	131.14	-3.59	0.4447	0.0041
PCB138		0.7403	11.58	0.0012	0.0545	129.81	-3.60	0.5090	0.0012
PCB139		0.6707	12.15	-0.0127	-0.5568	130.26	-3.67	0.5117	-0.0127
PCB140		0.6707	11.30	-0.0324	-1.4222	129.77	-3.59	0.5194	-0.0324
PCB141		0.7200	12.11	-0.0267	-1.1744	130.59	-3.66	0.4854	-0.0267
PCB142		0.6848	11.60	-0.0088	-0.3869	129.80	-3.61	0.4920	-0.0088

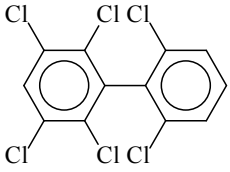
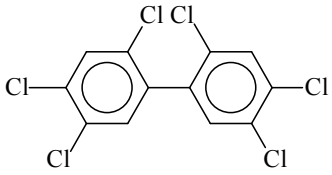
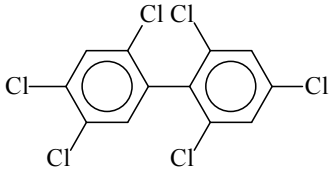
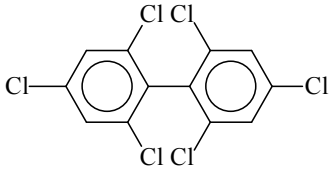
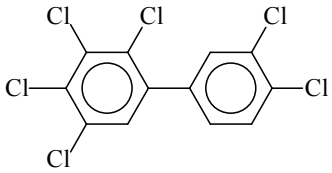
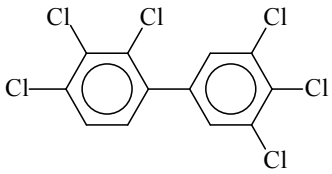
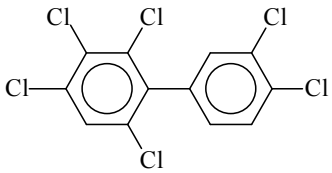
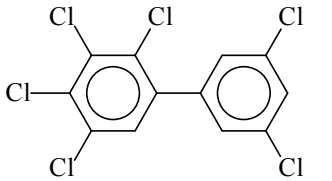
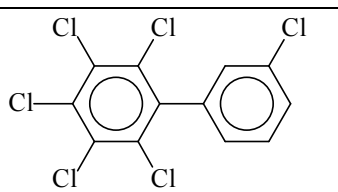
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d, 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d, 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB143		0.6789	12.57	0.0004	0.0168	130.50	-3.74	0.4330	0.0004
PCB144		0.6563	13.43	0.0088	0.3881	128.67	-3.82	0.4362	0.0088
PCB145		0.6149	12.87	-0.0562	-2.4723	128.32	-3.76	0.5201	-0.0562
PCB146		0.6955	12.62	-0.0098	-0.4320	128.24	-3.75	0.4749	-0.0098
PCB147		0.6608	14.04	-0.0314	-1.3821	126.70	-3.90	0.4924	-0.0314
PCB148		0.6243	10.02	-0.0122	-0.5363	133.20	-3.42	0.1119	-0.0122
PCB149		0.6672	10.60	0.0041	0.1800	134.27	-3.47	0.1503	0.0041
PCB150		0.5969	9.96	0.0376	1.6541	135.23	-3.40	0.1561	0.0376
PCB151		0.6499	10.14	0.0054	0.2377	134.89	-3.42	0.2191	0.0054

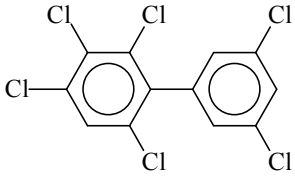
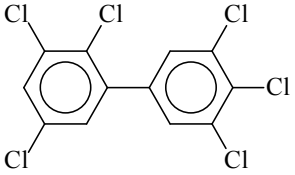
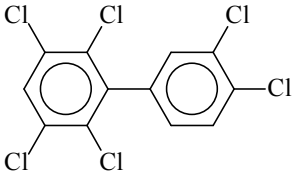
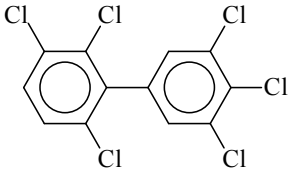
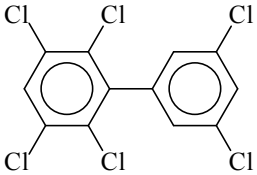
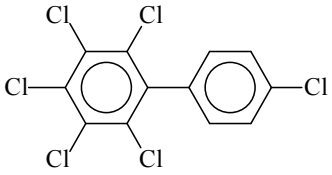
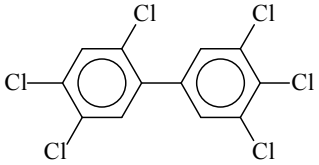
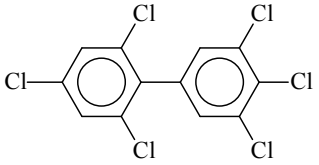
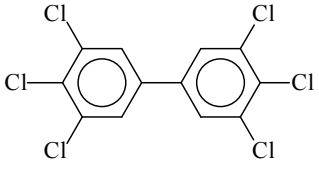
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d,\ 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d,\ 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB152		0.6062	9.75	0.0251	1.1035	133.36	-3.41	0.2534	0.0251
PCB153		0.7036	10.15	-0.0193	-0.8496	136.72	-3.38	0.2902	-0.0193
PCB154		0.6349	10.72	0.0028	0.1234	134.60	-3.48	0.2538	0.0028
PCB155		0.5666	10.27	-0.0048	-0.2094	133.35	-3.43	0.2831	-0.0048
PCB156		0.8105	11.12	0.0348	1.5315	134.95	-3.55	0.2222	0.0348
PCB157		0.8184	11.75	0.0333	1.4623	133.57	-3.57	0.1910	0.0333
PCB158		0.7429	11.26	0.0168	0.7378	133.12	-3.52	0.3070	0.0168
PCB159		0.7655	11.52	0.0442	1.9425	132.24	-3.57	0.2856	0.0442
PCB160		0.7396	11.09	0.0065	0.2857	134.24	-3.49	0.3250	0.0065

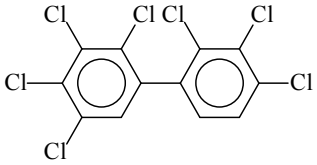
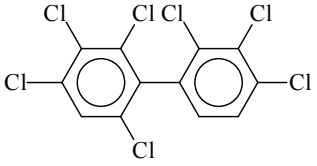
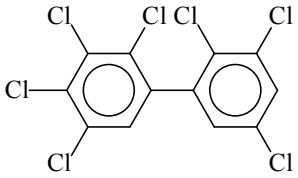
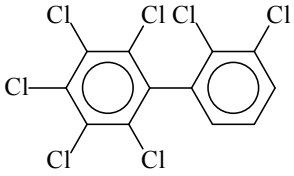
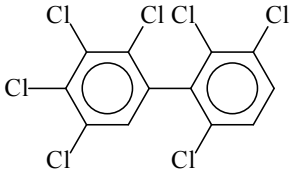
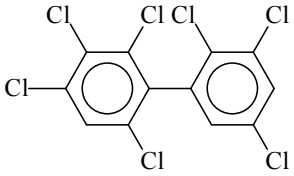
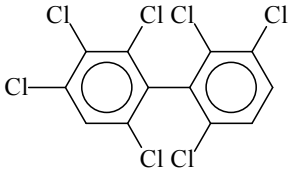
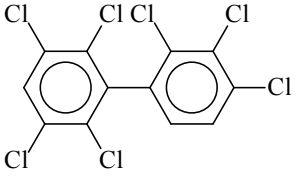
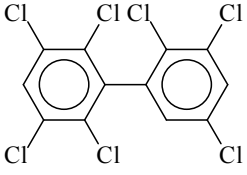
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d, 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d, 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB161		0.6968	10.98	-0.0393	-1.7268	133.10	-3.50	0.2766	-0.0393
PCB162		0.7737	10.98	0.0036	0.1567	131.58	-3.51	0.3351	0.0036
PCB163		0.7396	10.45	0.0193	0.8481	132.74	-3.45	0.3432	0.0193
PCB164		0.7399	10.97	-0.0184	-0.8086	133.06	-3.51	0.3582	-0.0184
PCB165		0.6920	10.72	-0.0125	-0.5510	131.64	-3.50	0.3503	-0.0125
PCB166		0.7572	10.16	0.0042	0.1849	132.62	-3.44	0.3003	0.0042
PCB167		0.7814	11.56	0.0015	0.0644	132.66	-3.57	0.4155	0.0015
PCB168		0.7068	11.09	-0.0179	-0.7855	133.32	-3.50	0.4314	-0.0179
PCB169		0.8625	11.05	0.0005	0.0212	131.66	-3.52	0.4262	0.0005

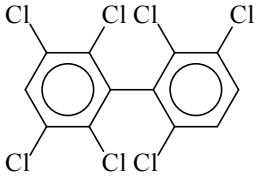
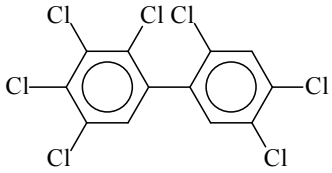
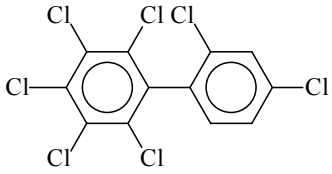
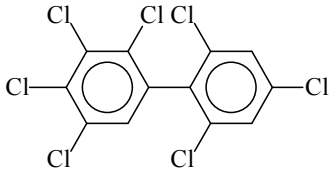
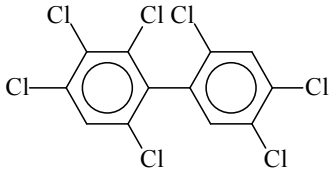
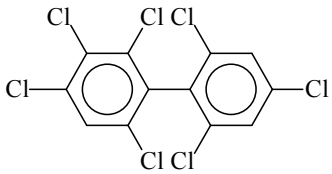
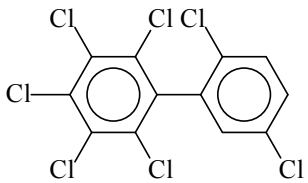
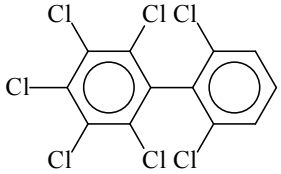
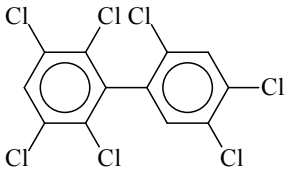
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d, 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d, 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB170		0.8740	11.05	-0.0239	-1.0517	132.19	-3.51	0.4009	-0.0239
PCB171		0.8089	10.52	0.0042	0.1838	131.49	-3.46	0.3466	0.0042
PCB172		0.8278	10.80	-0.0283	-1.2445	133.28	-3.48	0.4220	-0.0283
PCB173		0.8152	10.24	-0.0015	-0.0653	133.94	-3.42	0.3926	-0.0015
PCB174		0.7965	10.75	0.0056	0.2482	132.13	-3.50	0.3465	0.0056
PCB175		0.7611	10.23	-0.0294	-1.2916	131.25	-3.45	0.4325	-0.0294
PCB176		0.7305	12.03	-0.0161	-0.7060	132.78	-3.65	0.3981	-0.0161
PCB177		0.8031	11.48	-0.0323	-1.4195	133.66	-3.57	0.3488	-0.0323
PCB178		0.7537	11.55	0.0086	0.3793	132.00	-3.60	0.4008	0.0086

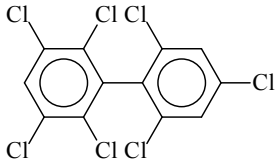
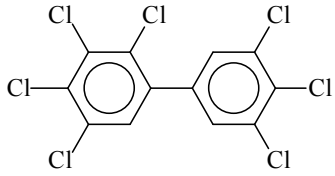
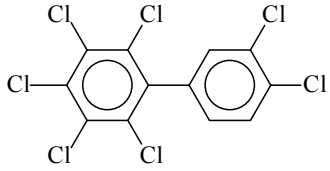
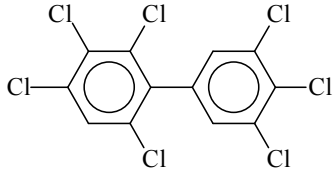
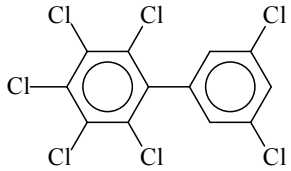
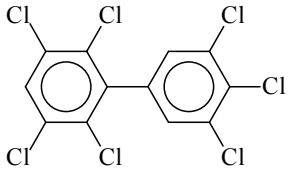
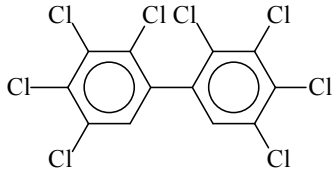
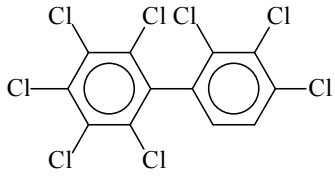
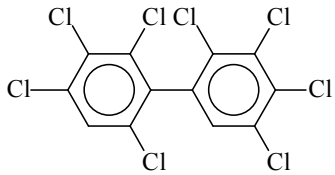
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d, 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d, 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB179		0.7205	11.22	0.0089	0.3932	131.75	-3.57	0.3547	0.0089
PCB180		0.8362	11.25	0.0057	0.2490	132.12	-3.58	0.4106	0.0057
PCB181		0.7968	12.89	-0.0103	-0.4521	130.80	-3.73	0.3885	-0.0103
PCB182		0.7653	12.32	0.0138	0.6063	131.52	-3.67	0.4600	0.0138
PCB183		0.7720	12.42	0.0027	0.1167	130.24	-3.68	0.4348	0.0027
PCB184		0.7016	11.87	0.0184	0.8096	129.97	-3.61	0.4674	0.0184
PCB185		0.7848	12.09	0.0635	2.7897	130.07	-3.66	0.4467	0.0635
PCB186		0.7416	11.53	0.0041	0.1782	131.14	-3.59	0.4447	0.0041
PCB187		0.7654	11.58	0.0012	0.0545	129.81	-3.60	0.5090	0.0012

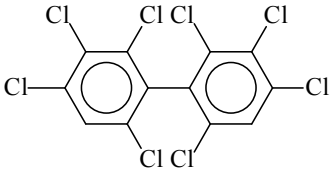
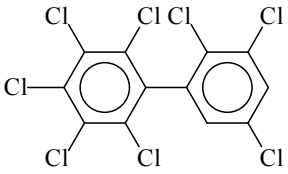
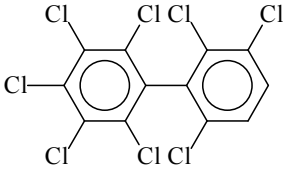
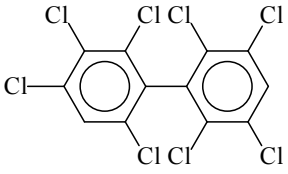
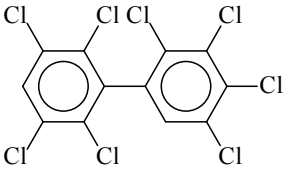
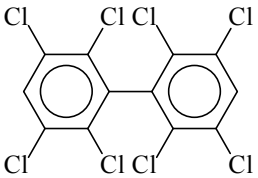
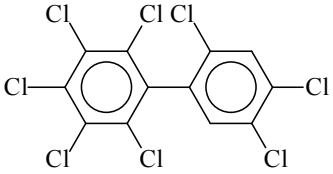
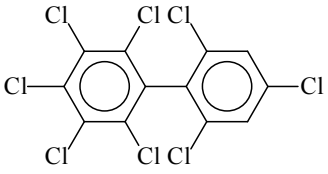
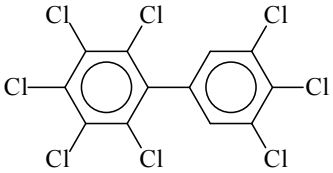
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d, 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d, 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB188		0.6920	12.15	-0.0127	-0.5568	130.26	-3.67	0.5117	-0.0127
PCB189		0.9142	11.30	-0.0324	-1.4222	129.77	-3.59	0.5194	-0.0324
PCB190		0.8740	12.11	-0.0267	-1.1744	130.59	-3.66	0.4854	-0.0267
PCB191		0.8447	11.60	-0.0088	-0.3869	129.80	-3.61	0.4920	-0.0088
PCB192		0.8269	12.57	0.0004	0.0168	130.50	-3.74	0.4330	0.0004
PCB193		0.8397	13.43	0.0088	0.3881	128.67	-3.82	0.4362	0.0088
PCB194		0.9620	12.87	-0.0562	-2.4723	128.32	-3.76	0.5201	-0.0562
PCB195		0.9321	12.62	-0.0098	-0.4320	128.24	-3.75	0.4749	-0.0098
PCB196		0.8938	14.04	-0.0314	-1.3821	126.70	-3.90	0.4924	-0.0314

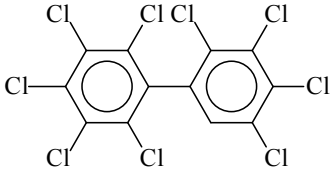
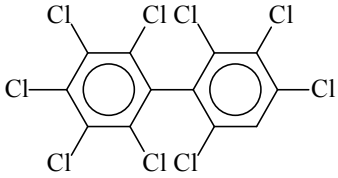
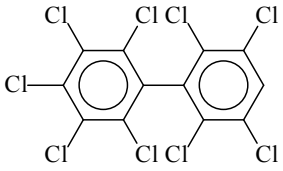
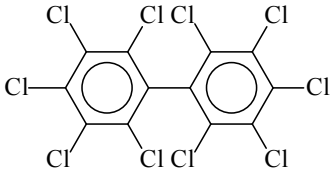
iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d, 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d, 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB197		0.8293	10.02	-0.0122	-0.5363	133.20	-3.42	0.1119	-0.0122
PCB198		0.8845	10.60	0.0041	0.1800	134.27	-3.47	0.1503	0.0041
PCB199		0.8494	9.96	0.0376	1.6541	135.23	-3.40	0.1561	0.0376
PCB200		0.8197	10.14	0.0054	0.2377	134.89	-3.42	0.2191	0.0054
PCB201		0.8875	9.75	0.0251	1.1035	133.36	-3.41	0.2534	0.0251
PCB202		0.8089	10.15	-0.0193	-0.8496	136.72	-3.38	0.2902	-0.0193
PCB203		0.8938	10.72	0.0028	0.1234	134.60	-3.48	0.2538	0.0028
PCB204		0.8217	10.27	-0.0048	-0.2094	133.35	-3.43	0.2831	-0.0048
PCB205		0.9678	11.12	0.0348	1.5315	134.95	-3.55	0.2222	0.0348

iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d, 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d, 2d}$ = residuals.

Table 1. (Continued)

Mol	PCB structure	Y	iIDRwHg	$\hat{Y}_{1d}$	Y- $\hat{Y}_{1d}$	ISDmsHt	lADrtHg	$\hat{Y}_{2d}$	Y- $\hat{Y}_{2d}$
PCB206		1.0103	11.75	0.0333	1.4623	133.57	-3.57	0.1910	0.0333
PCB207		0.9423	11.26	0.0168	0.7378	133.12	-3.52	0.3070	0.0168
PCB208		0.9320	11.52	0.0442	1.9425	132.24	-3.57	0.2856	0.0442
PCB209		1.0496	11.09	0.0065	0.2857	134.24	-3.49	0.3250	0.0065

iIDRwHg, ISDmsHt, and lADrtHg = the value of the descriptor - Eq(1)& Eq(2); $\hat{Y}_{1d, 2d}$ = relative retention time: estimated by Eq(1) and Eq(2), respectively; Y = relative retention time: experimental [30]; Y- $\hat{Y}_{1d, 2d}$ = residuals.

Table 2. Training vs Test Experiments: Results.

Training set						Test set		
No	Coefficients			Statistics		No	Statistics	
PCBs	Intercept	ISDmsHt	lADrtHg	R^2	F	PCBs	Q^2	F
9	-6.06	0.0243	-1.0294	0.999	2640†	200	0.997	32807†
19	-6.18	0.0248	-1.0442	0.998	4827†	190	0.997	28567†
29	-5.94	0.0237	-1.0195	0.996	3342†	180	0.997	32047†
39	-5.80	0.0230	-1.0040	0.998	8406†	170	0.997	27678†
49	-5.89	0.0234	-1.0172	0.998	9608†	160	0.997	25667†
59	-6.30	0.0257	-1.0448	0.996	6924†	150	0.998	27578†
69	-6.21	0.0251	-1.0440	0.996	7641†	140	0.998	29667†
79	-5.95	0.0238	-1.0170	0.996	9186†	130	0.998	29915†
89	-6.12	0.0246	-1.0348	0.997	16315†	120	0.997	19049†
99	-6.06	0.0244	-1.0278	0.997	15763†	110	0.997	20314†
109	-6.07	0.0244	-1.0304	0.996	13489†	100	0.998	26764†
119	-6.10	0.0245	-1.0361	0.997	19333†	90	0.997	14990†
129	-6.07	0.0245	-1.0284	0.997	19823†	80	0.998	17306†
139	-5.98	0.0240	-1.0219	0.997	21316†	70	0.997	11610†
149	-6.07	0.0244	-1.0297	0.997	25972†	60	0.997	10077†
159	-6.03	0.0241	-1.0287	0.997	31071†	50	0.997	5692†
169	-6.03	0.0242	-1.0258	0.997	25723†	40	0.998	12671†
179	-5.97	0.0239	-1.0203	0.997	30942†	30	0.997	4938†
189	-6.02	0.0242	-1.0247	0.997	31570†	20	0.998	3383†
199	-6.01	0.0241	-1.0243	0.997	34566†	10	0.998	1450†

† $p < 0.0001$

4. Conclusions

The MDF methodology provides excellent QSPR models, with good stability and predictive ability. It has the disadvantage to be time consuming (it calculates a huge pool of molecular descriptors and provides exhaustive mono- and bivariate regressions) but this is compensated by the high quality of the QSPR models.

Thus, the variance of chromatographic retention time of PCBs is 99.7% explained by two molecular descriptors, showing us that the property is related with geometry and topology, as well as with directly bounded hydrogen's of PCBs.

The selection of the MDF members from a huge family offers not only a QSPR model, but also a strong instrument to investigate the structural causality of a measured property. Thus, the chromatographic property of PCBs is determined by the molecular topology, geometry and the non-chlorinated (i.e., the remained hydrogenated) positions on the PCB structure.

Acknowledgements

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Notes

Virtual library of QSPR/QSAR models:

- http://l.academicdirect.org/Chemistry/SARs/MDF_SARs/sar/

Training and test analysis:

- http://l.academicdirect.org/Chemistry/SARs/MDF_SARs/qsar_qspr_s/

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