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The study of the relationship between the new topological index A_m and the gas chromatographic retention indices of hydrocarbons by artificial neural networks

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Abstract

The newly developed topological indices A_{m1}–A_{m3} and the molecular connectivity indices ${}^{m}X$ were applied to multivariate analysis in structure–property correlation studies. The topological indices calculated from the chemical structures of some hydrocarbons were used to represent the molecular structures. The prediction of the retention indices of the hydrocarbons on three different kinds of stationary phase in gas chromatography can be achieved applying artificial neural networks and multiple linear regression models. The results from the artificial neural networks approach were compared with those of multiple linear regression models. It is shown that the predictive ability of artificial neural networks is superior to that of multiple linear regression method under the experimental conditions in this paper. Both the topological indices ${}^{2}X$ and A_{m1} can improve the predicted results of the retention indices of the hydrocarbons on the stationary phase studied.

Keywords: Artificial neural networks; Multiple linear regression; Topological index; Gas chromatography retention index; Prediction

1. Introduction

Retention indices are widely applied in gas chromatographic separation techniques. The study of the relationship between the structural characteristics of compounds and their retention behaviors is an important field in chromatographic separation techniques [1]. The correlation of molecular structural parameters and the corresponding chromatographic behaviors has been studied in different approaches [2–4]. However, the physicochemical parameters of many compounds have not been calculated yet [5]. Therefore, topological indices are generated to describe the structural characteristics of some molecules. Then, the topological indices can be applied as the connections between some specific properties of compounds and their chemical structures. The topological indices are the basis of the mathematical models for quantitative structure–activity relationship (QSAR) and quantitative structure–property relationship (QSPR) studies. The method of topological indexing of molecular structures has been widely used in recent years in connection with QSAR/QSPR. The key step in the development of a topological index is the selection of a graph invariant, which is a value that can be derived from the graph and is not affected by its node numbering. Over a hundred of topological indices have been described, such as the Wiener index W [6], Randic index ID [7], Hosoya index Z [8], Balaban index J [9] and the general α_N index [10]. Significant development has been found in the increasingly widespread use of topological indices, a trend that has become of growing importance in recent years. The topological indices A_{m1}–A_{m3} based on the augmented path matrices devised recently by our laboratory have been successfully employed in the studies on structure–activity relationships for alkanes, alcohols and barbiturates [11]. In another study

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[12], we further utilized these indices and the molecular connectivity indices [13] in the study of the structure–property relationship between color reagents and their color reactions with ytterbium. Some other researches about QSPR [14–16] and QSAR [17] have also been developed in the authors' laboratory.

Artificial neural networks (ANN) is often applied in non-linear modeling processes. Generally speaking, ANN is better than, or as good as multiple linear regression (MLR) in modeling non-linear process. Therefore, ANN has been applied to optimize the separation performance in capillary zone electrophoresis [18]. Moreover, ANN was also employed successfully in HPLC [19,20], ion chromatography [21,22], gas chromatography [23–25], micellar electrokinetic capillary chromatography [26,27] and capillary zone electrophoresis [28] to predict the retention (or migration) behavior in these separation performances. Recently, the applications of ANN for quantitative analysis of chiral compounds [29,30] and multicomponent determination [31] from unresolved peaks in capillary electrophoresis have also been reported.

In this paper, the newly devised topological indices A_{m1}–A_{m3} and the molecular connectivity indices ${}^{m}X$ were applied to predict the retention indices of hydrocarbons on three different kinds of stationary phase in gas chromatography by ANN and MLR. The study shows that ANN can give better predicted results than MLR.

2. Theory

There have been many papers [32–34] that describe the theory of ANN in detail. Error Back-Propagation (BP) is one of the most widely used algorithms. In this work, BP ANN is applied to calculate the retention indices of different hydrocarbons on three kinds of gas chromatography columns.

3. Topological indices

The newly developed topological indices A_{m1}, A_{m2} and A_{m3} [11] are generated from path matrices A, B and C, respectively. The three matrices are defined as follows:

$$A = a_{ij}, \quad \begin{cases} 1, & \text{path} = 1 \\ 0, & \text{others}(i, j = 1, 2, \ldots, n) \end{cases}$$

$$B = b_{ij}, \quad \begin{cases} 2, & \text{path} = 2 \\ 0, & \text{others}(i, j = 1, 2, \ldots, n) \end{cases}$$

$$C = c_{ij}, \quad \begin{cases} 3, & \text{path} = 3 \\ 0, & \text{others}(i, j = 1, 2, \ldots, n) \end{cases}$$

where n is the number of atoms in the corresponding molecules. By adding two columns into matrices A, B and C, respectively, augmented path matrices G_1, G_2 and G_3 are constructed. The elements in the first columns of matrices G_1, G_2 and G_3 are square roots of vertex degrees, and those in the second columns are the square roots of the Van der Waals radii of atoms. Matrices Z_1, Z_2 and Z_3 can be calculated from matrices G_1, G_2 and G_3, respectively, according to the following formula:

$$Z_1 = G_1 \times G_1'; \quad Z_2 = G_2 \times G_2'; \quad Z_3 = G_3 \times G_3'$$

where G_1', G_2' and G_3' are the transposed matrices of G_1, G_2 and G_3, respectively. The three new topological indices are defined as:

$$A_{m1} = \frac{\lambda_{max1}}{2}; \quad A_{m2} = \frac{\lambda_{max2}}{2}; \quad A_{m3} = \frac{\lambda_{max3}}{2}$$

where λ_{max1}, λ_{max2} and λ_{max3} are the largest eigenvalues of matrices Z_1, Z_2 and Z_3, respectively.

From the introductory section to the new topological index described above, it is obvious that the three path matrices can only account for the paths between the vertexes (atoms) in the molecules when the path equals to 1, 2 and 3, respectively. Therefore, the topological index generated only from the path matrices cannot describe the different kinds of atoms in the molecules or the bond properties between the corresponding atoms. In order to generate a topological index that can represent the properties of miscellaneous atoms and the chemical bonds connecting the corresponding atoms, the augmented path matrices were constructed according to the approach described above. Since the augmented path matrices include not only the "path" information but also the "property" one, the proposed topological indices based on the augmented path matrices can explain the molecular structures better. Hence, the proposed topological indices may describe some molecular properties, such as lipophilicity, branching, etc. better than other kinds of topological indices.

4. Experimental

The neural network software applied in this work includes two models: BP and quasi-Newton neural networks. The software was developed in our laboratory. All computations were performed using multivariate statistic analysis program (MSAP) package, which consists of multivariate regression analysis, pattern recognition and calculations of topological indices, etc. The retention indices of 18 hydrocarbons were acquired from the stationary phase of *n*-octadecane in GC, and those of the 16 hydrocarbons (among the 18 hydrocarbons mentioned) were from the stationary phase of 1-octadecylchloride and 1-octadecanol. All the retention indices were cited from the paper published [35]. The retention indices of the 18 compounds investigated in this work on different stationary phase, the newly devised topological indices A_m and the molecular connectivity indices ${}^{m}X$ of the different compounds are given in Table 1. The chemical structures of the corresponding hydrocarbons are shown in Fig. 1.

Table 1
Specific retention indices and two kinds of topological indices of some hydrocarbon compounds

Compounds	*n*-Octadecane	1-Octadecylchloride	1-Octadecanol	A_{m1}	A_{m2}	A_{m3}	${}^0X$	${}^1X$	${}^2X$
n-Pentane	500	500	500	9.897	11.661	12.250	4.121	2.414	1.354
2,2-Dimethylbutane	538	521	521	12.265	25.316	20.659	5.207	2.501	2.914
Cyclopentane	561	547	565	11.500	17.500	27.500	3.536	2.500	1.768
3-Methypentane	583	576	575	12.053	16.650	21.840	4.992	2.808	1.922
n-Hexane	600	600	600	11.896	14.329	14.840	4.823	2.914	1.707
2,4-Dimethylpentane	629	624	625	14.041	22.645	20.265	5.862	3.126	3.023
Benzene	636	697	676	16.400	22.400	18.900	4.243	3.000	2.121
Cyclohexane	656	–	–	14.000	19.400	15.400	4.243	3.000	2.121
2,3-Dimethylpentane	670	667	668	14.107	20.772	30.774	5.862	3.181	2.630
3-Methylhexane	675	–	–	13.991	19.513	23.409	5.699	3.308	2.302
n-Heptane	700	700	700	13.863	16.885	18.860	5.536	3.414	2.061
2,2-Dimethylhexane	719	716	718	16.047	28.768	23.761	6.621	3.561	3.554
2,5-Dimethylhexane	728	724	725	15.944	22.871	21.779	6.569	3.628	3.365
2,2,3-Trimethylpentane	735	734	728	16.200	29.463	40.499	6.784	3.481	3.675
2,3,4-Trimethylpentane	750	749	753	16.105	25.215	38.462	6.732	3.558	3.347
2-Methylheptane	764	763	764	15.877	21.468	23.826	6.406	3.770	2.890
2,2,5-Trimethylhexane	776	770	771	17.985	30.603	25.912	7.492	3.917	4.493
n-Octane	800	800	800	15.811	19.238	22.150	6.242	3.914	2.414

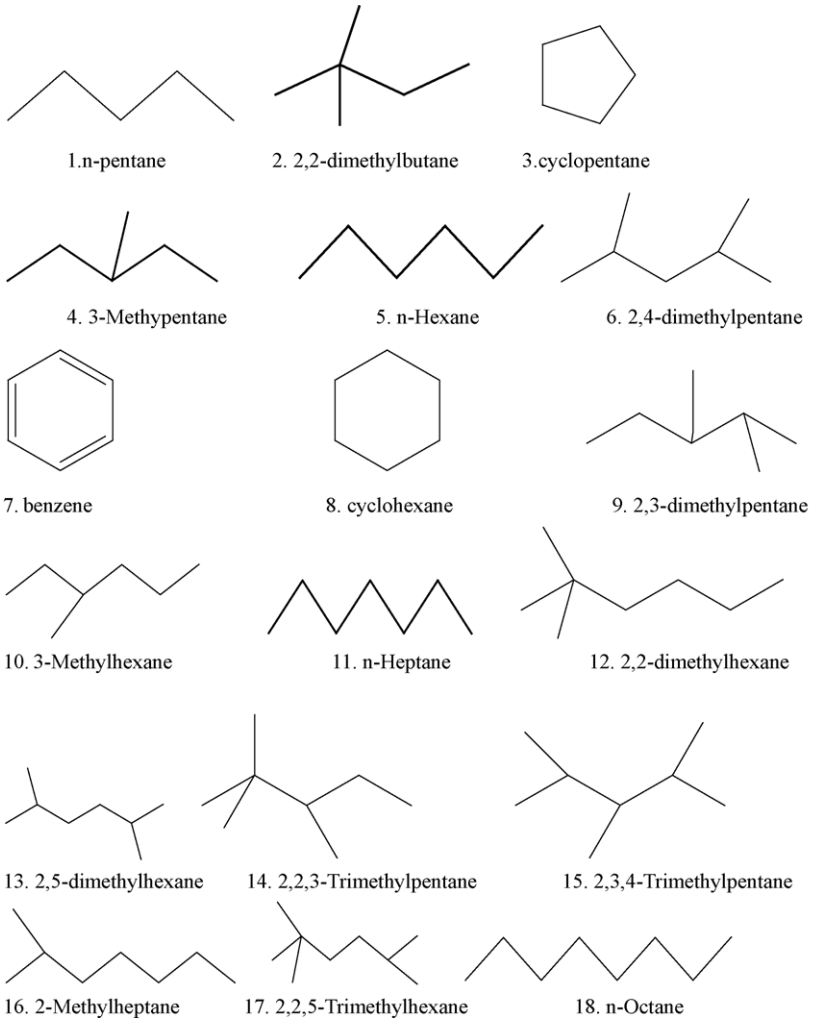

Fig. 1. The structures of the corresponding hydrocarbons.

5. Results and discussion

5.1. Calculation of topological index

The topological indices A_{m1}–A_{m3} and the molecular connectivity indices ${}^0X$–${}^2X$ were calculated using the MSAP package. A total of six topological indices were guaranteed for each hydrocarbon.

5.2. Input variable selection

According to the calculated results through MLR, it is shown that the topological indices A_{m1} and ${}^1X$ have good correlation to the retention indices. Furthermore, the combination of A_{m1}, ${}^1X$ and ${}^2X$ can also give better-predicted results through MLR. So both the combination of A_{m1} and ${}^1X$ and that of A_{m1}, ${}^1X$ and ${}^2X$ were used as the input variables of ANN, respectively. All the calculated results of MLR are shown in Tables 2–4, respectively.

Table 2
Calculated results of MLR using A_m

Topological index	Stationary phase		
	n-Octadecane	1-Octadecylchloride	1-Octadecanol
A_{m1}			
n	18	16	16
s	41.7298	38.2497	40.4755
R	0.8844	0.9208	0.9113
A_{m2}			
n	18	16	16
s	74.2697	82.2550	86.1633
R	0.5586	0.5442	0.5492
A_{m3}			
n	18	16	16
s	78.4931	87.8277	87.0063
R	0.4788	0.4944	0.4682
$A_{m1}A_{m2}$			
n	18	16	16
s	38.1667	27.7666	32.6496
R	0.9106	0.9620	0.9474
$A_{m2}A_{m3}$			
n	18	16	16
s	74.9579	84.5335	83.5937
R	0.5827	0.5623	0.5733
$A_{m1}A_{m3}$			
n	18	16	16
s	42.8311	39.6925	41.8907
R	0.8859	0.9208	0.9118
$A_{m1}A_{m2}A_{m3}$			
n	18	16	16
s	36.5448	25.2547	26.6787
R	0.9240	0.9711	0.9602

n is the number of experimental samples; *s* is standard deviation; *R* is correlation coefficient.

Table 3
Calculated results of MLR using ${}^mX$

Topological index	Stationary phase		
	n-Octadecane	1-Octadecylchloride	1-Octadecanol
${}^0X$			
n	18	16	16
s	210.8607	146.6521	139.6329
R	0.7784	0.7141	0.7455
${}^1X$			
n	18	16	16
s	42.7935	60.5458	56.3637
R	0.8788	0.7867	0.8169
${}^2X$			
n	18	16	16
s	69.3215	82.0716	80.2848
R	0.6316	0.5417	0.5772
${}^0X{}^1X$			
n	18	16	16
s	44.1197	62.4705	58.2166
R	0.8755	0.7893	0.8212
${}^0X{}^2X$			
n	18	16	16
s	56.1728	66.6626	63.2142
R	0.7917	0.7564	0.7849
${}^0X{}^1X{}^2X$			
n	18	16	16
s	45.6481	64.7715	60.3940
R	0.8786	0.7911	0.8225

n is the number of experimental samples; *s* is standard deviation; *R* is correlation coefficient.

5.3. n-Octadecane stationary phase

The relationship between the topological indices and the retention indices of the 18 kinds of hydrocarbons was investigated.

5.3.1. Case I

A_{m1} and ${}^1X$ were the input variables of the ANN, and the output of the ANN was the retention index of the corresponding compound. The process of optimizing the number of logic units in the hidden layer in Case I is shown in Fig. 2. The logic

Table 4
Calculated results of MLR using ${}^1X$, ${}^2X$ and A_{m1}

	Stationary phase		
	n-Octadecane	1-Octadecylchloride	1-Octadecanol
A	24.2834	−13.0523	−6.6093
B	26.3369	35.2631	32.4803
C	110.9453	93.4988	100.2300
D	−22.9744	−46.5818	−42.1076
n	15[a]	13[a]	13[a]
s	11.3961	9.6486	11.0013
R	0.9930	0.9960	0.9948

A, *B*, *C* and *D* are the coefficients of the regression equation, which can be described as retention index = $A + B\,A_{m1} + C\,{}^1X + D\,{}^2X$. *n* is the number of experimental samples; *s* is standard deviation; *R* is correlation coefficient.

[a] For the hydrocarbons studied on each stationary phase, three of the compounds were used as verification set, and the others were training set.

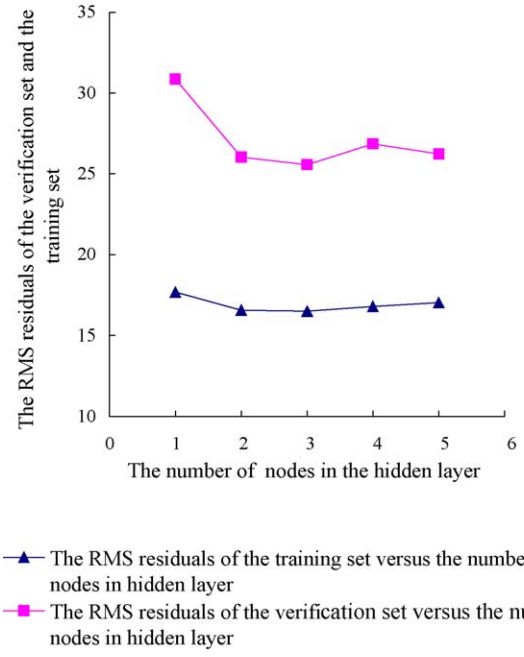

Fig. 2. The optimization of the number of the nodes in the hidden layer of ANN applied on the *n*-octadecane stationary phase in Case I.

units in the hidden layer were optimized to be three, so a 2:3:1 architecture of ANN can be acquired. The samples composed by the 18 compounds were divided into two sets at random. One is a training set, including 14 compounds; the other is a verification set, including four compounds. The MSAP for calculation can search the optimized training times automatically, so "over training" can be avoided conveniently. The predicted residual of the ANN and that of the MLR were calculated by formula (1):

$$E_{\text{pred}} = \frac{\sqrt{\sum_{p=1}^{P}(i_{\text{ptrue}} - i_{\text{ppred}})^2}}{\sqrt{\sum_{p=1}^{P}(i_{\text{ptrue}})^2}} \quad (1)$$

In the formula, E_{pred} is the predicted residual, i_{ptrue} is the target retention index and i_{ppred} is the predicted one. P is the number of all the samples in the training and the verification sets.

5.3.2. Case II

The input values of the ANN were the combination of ${}^1X$, ${}^2X$ and A_{m1}. The output values of the ANN were the retention indices of the corresponding compounds. The process of optimizing the number of logic units in the hidden layer in Case II is shown in Fig. 3. The optimized number of the logic units in the hidden layer was two. So ANN of 3:2:1 architecture can be constructed. The sample has 18 compounds, among which four were chosen to be used as a verification set at random, and the others were used as a training set.

The predicted residuals of the ANN were also calculated by formula (1). The predicted values, the target values and the ANN predicted residuals of the two cases and those of the MLR models are shown in Table 5.

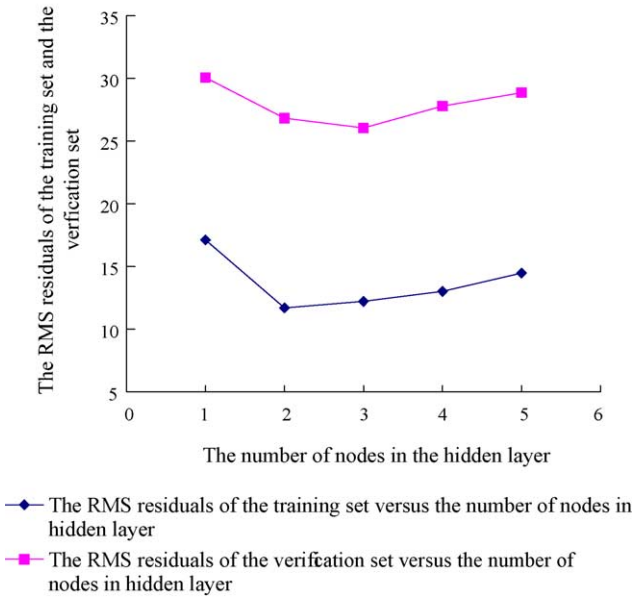

Fig. 3. The optimization of the number of the nodes in the hidden layer of ANN applied on the *n*-octadecane stationary phase in Case II.

From Table 5, it is shown that ANN has better-predicted results than MLR models. In the case of the stationary phase, ${}^1X$, ${}^2X$ and A_{m1} networks has a better predictive ability than A_{m1} and ${}^1X$ networks.

5.4. 1-Octadecylchloride stationary phase

On the stationary phase, the relationship between the topological indices and the retention indices of the 16 hydrocarbons was also studied.

Table 5
Comparison between the target and the predicted retention indices of the compounds on the n-octadecane stationary phase

	Predicted results of Case I	Predicted results of case II	Predicted results by MLR	Target indices
	540.6	539.1	521.7	500
	549.5	540.3	557.8	538
	545.9	558.6	563.9	561
	587.9	584.9	609.1	583
	604.7	596.8	621.7	600
	650.9	640.5	671.4	629
	645.0	643.6	740.3	636
	634.7	645.4	677.1	656
	658.7	660.0	688.3	670
	677.0	678.3	706.9	675
	694.3	695.8	720.8	700
	737.2	735.6	760.3	719
	748.6	748.1	769.4	728
	722.6	719.1	752.7	735
	736.9	732.6	766.3	750
	769.4	769.5	794.3	764
	787.6	790.2	829.3	776
	782.7	784.3	819.5	800
Residuals	2.42%	2.13%	5.54%	

5.4.1. Case I

A_{m1} and ^1X were also used as the input variables of the ANN. The output values of the ANN were also the retention indices of the compounds. The optimized number of logic units in the hidden layer was three, so a 2:3:1 architecture ANN was acquired. The 16 compounds were divided into two parts, one was a verification set, including four compounds, and the other was a training set, including 12 compounds. The predicted residual of the ANN was also calculated by formula (1).

5.4.2. Case II

In this case, the input values of ANN were ^1X, ^2X and A_{m1}. The output values of ANN were the retention indices of the corresponding compounds. The optimized number of the logic units in the hidden layer was three, so a 3:3:1 architecture of ANN was formed. There were 16 compounds in the sample, among which four compounds were selected at random to be a verification set; and the others were used as a training set. The predicted residual of the ANN was calculated by formula (1).

The predicted values, the target values and the ANN predicted residuals of case I, case II and those of the MLR models are shown in Table 6.

From Table 6, it is shown that the predicted results of ANN are better than those of the MLR models. On the other hand, ANN using ^1X, ^2X and A_{m1} as the input variables can give better-predicted results than ANN using ^1X and A_{m1} can.

5.5. 1-Octadecanol stationary phase

The correlation relationship between the retention indices of the 16 compounds and the corresponding topological indices was studied on the stationary phase.

Table 6
Comparison between the target and the predicted retention indices of the compounds on the 1-octadecylchloride stationary phase

	Predicted results of Case I	Predicted results of case II	Predicted results by MLR	Target indices
	525.0	518.2	498.6	500
	531.8	521.4	517.5	521
	530.2	529.6	543.9	547
	577.4	567.4	585.0	576
	597.7	588.2	599.4	600
	657.7	628.4	633.5	624
	695.6	697.7	747.0	697
	664.7	657.3	659.3	667
	694.9	714.5	699.0	700
	723.5	731.7	720.2	716
	731.6	743.0	731.6	724
	719.4	719.8	712.5	734
	723.7	737.8	731.6	749
	760.7	764.0	764.7	763
	770.5	769.5	778.1	770
	787.8	777.1	798.0	800
Residuals	2.14%	1.90%	2.24%	

Table 7
Comparison between the target and the predicted retention indices of the compounds on the 1-octadecanol stationary phase

	Predicted results of Case I	Predicted results of case II	Predicted results by MLR	Target indices
	530.5	538.2	499.8	500
	547.9	524.0	519.7	521
	541.9	564.6	543.0	565
	576.7	584.1	585.4	575
	589.2	598.7	600.0	600
	656.4	611.6	635.5	625
	666.0	680.8	737.4	676
	666.3	664.8	659.7	668
	704.0	707.2	699.1	700
	738.1	733.6	721.9	718
	747.2	741.8	733.2	725
	727.5	726.2	713.7	728
	737.9	741.1	732.2	753
	765.0	754.7	765.3	764
	779.5	759.9	780.9	771
	779.0	760.0	797.6	800
Residuals	2.63%	2.43%	2.72%	

5.5.1. Case I

We use ^1X and A_{m1} as the input values of ANN again. The output values of the ANN were still the retention indices of the corresponding compounds. The optimized number of the logic units in the hidden layer was three, then ANN of 2:3:1 architecture was created. Among the 16 compounds of the sample, four of them were selected at random as the verification set, and the others were used as the training set. The predicted residual of the ANN was calculated by formula (1), too.

5.5.2. Case II

^1X, ^2X and A_{m1} were used as the input variables of the ANN, and the output values of the ANN were the retention indices of the corresponding compounds. The best number of the logic units in the hidden layer was three, so a 3:3:1 ANN was applied in this case. Of all the 16 compounds, four were composed of the verification set, and the others were used as the training set. The predicted residual of the ANN was calculated by formula (1), too.

The predicted values, the target values, and the ANN predicted residuals of the two cases and those of the MLR models are shown in Table 7.

From the calculated results, a conclusion can be drawn that ANN using ^1X, ^2X and A_{m1} as input variables can give the best-predicted results in this case. On the other hand, we found that the MLR model gave worse predicted results than those of ANN using ^1X and A_{m1} as the input values.

6. Testing the established models

In order to test the predictive ability of the established ANN models, a test data set was constructed in the exper-

Table 8
The predicted residuals of all the experimental samples used as test specimens in established ANN models

	n-Octadecane stationary phase (%)	1-Octadecyl-chloride stationary phase (%)	1-Octadecanol stationary phase (%)
Case I	3.72	4.11	4.39
Case II	3.41	3.97	3.96

imental samples acquired from each kind of GC stationary phase. In each experimental data set, every experimental sample was applied as test sample once while the other samples were used as training or verification data set. All the corresponding established ANN models were based on the optimized structures of neural networks. The predicted residuals between the target and the predicted retention indices were also calculated by formula (1). All the calculated results of this section are listed in Table 8. It is shown that for all the experimental samples on each kind of GC stationary phase, ANN using ^1X, ^2X and A_{m1} as input variables can predict the retention indices of the corresponding hydrocarbons better than ANN applying ^1X and A_{m1} as the input values can.

7. Conclusions

From the research results above, it can be concluded that ANN have more powerful predictive ability than MLR. That is to say, ANN can give better-predicted results than MLR in non-linear problems in general. On the other hand, for the retention indices of the hydrocarbons on the three kinds of stationary phase, the introduction of the input variable ^2X to ANN leads to better-predicted results. It is shown that the molecular connectivity index ^2X has more correlation to the retention indices of the hydrocarbons on the stationary phase studied in this paper. According to the calculated results of MLR, to all the three kinds of the stationary phase, only by introducing the new topological index A_{m1} can better-predicted results be acquired. Probably the new topological index A_{m1} can represent the retention behavior of the compounds on the stationary phase better than the molecular connectivity indices ^mX. The predicted retention indices on the *n*-octadecane stationary phase in Case I versus the experimental retention indices is shown in Fig. 4.

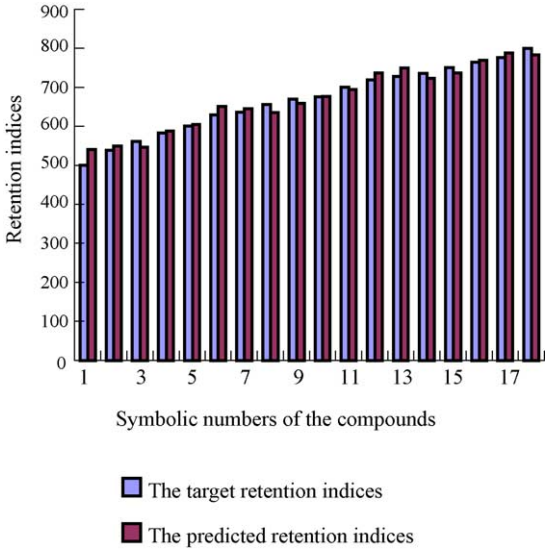

Fig. 4. The predicted retention indices on *n*-octadecane stationary phase in Case I vs. the target retention indices.

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