JOURNAL OF ALGEBRAIC STATISTICS
Volume 13, No. 2, 2022, p. 3173-3181
https://publishoa.com
ISSN: 1309-3452

Multilinear-Regression Models Developed by Four Novel Degree-Based Topological Indices in Qspr Analysis

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Received 2022 March 25; **Revised** 2022 April 28; **Accepted** 2022 May 15.

Abstract This research article aims to propose four novel degree-based topological indices ABI_1index, ABI_2 index, ABI_3 index & ABI_4 index. Further, the values of molecular structures of eighteen structural octane isomers are calculated using these indices. The correlation coefficients of these indices with twelve physical properties are evaluated and employed for QSPR study through multiple linear regression analysis. These properties include entropy(S), acentric factor(*A.F*), enthalpy of vaporization(*HVAP*), standard heat of vaporization(*DHVAP*),boiling point(*BP*),critical temperature(*TC*),critical pressure(*PC*),critical volume(*VC*), density(*D*), quadratic mean radius(R^2_m), heat of vaporization($-\Delta H_f$),heat of formation($-\Delta H_v$) of octane isomers. This paper involves a method called multiple regression, which is a statistical technique that can be used to analyse the relationship between a single dependent variable and several independent variables. In this proposed research work, various topological indices are defined on some structural octane isomers to predict the physical and chemical properties of these compounds through Quantitative Structure-Property Relationships (QSPR).

MSC2010 codes 05C10, 05C30, 05C92, 05C90,05C09

Key words Degree-based topological index, neighborhood-degree-sum topological index, quantitative structure-property relationship(QSPR), linear regression, multiple regression.

1 Introduction Mathematics is a branch of science consisting of numerals, structures, and symbols to portray our physical world and its underlying resources. Graph theory is an essential part of this science utilizing graphs to represent pairwise relations. Graph *G* (*V*, *E*) carries two sets of objects namely the set of vertices and the set of bonds (edges) connected by vertices. Molecular graphs are employed to recreate the structure of molecules using graph theory. Chemical Graph Theory(*CGT*) holds several real-life applications that can be used in various fields of study such as chemistry, drug design, nanophysics, etc. Its applications include prediction of the Physico-chemical properties and biological activities of chemical compounds. Chemical graph theory plays a significant role in drug design due to the non-expensive and non-empirically derived experiments. Topological indices are molecular descriptors[1] to convert the massive molecular structures into numbers and possess a wide range of applications that are strongly explored. They are mainly used in quantitative structure-activity relationships(*QSAR*) and quantitative structure-property relationships (*QSPR*) in predicting Physico-chemical properties and biological activities of molecular structures.

Degree-based topological indices perform a vital role in graph theory applications. In 1975, Randic proposed the product connectivity index. Later the name was changed to Randic index. Followed by Randic, Zagreb indices are introduced by Furtula *et al*. The forgotten degree-based topological index is especially used in drug designs. Augmented Zagreb index, followed by Atom bond connectivity index is the candidate with high predicting competence of the Physico-chemical properties of chemical compounds(especially structural isomers). Inspired by the applicability of the degree-based topological indices, four novel degree-based topological indices are proposed here. These four indices work as the entrants to guesstimate twelve Physico-chemical properties of eighteen octane isomers whose chemical formula is C_nH_{2n+2}. Based

JOURNAL OF ALGEBRAIC STATISTICS
Volume 13, No. 2, 2022, p. 3173-3181
https://publishoa.com
ISSN: 1309-3452

on the structural discrimination of the octane isomers, these indices work as models to guesstimate their physical properties(QSPR analysis)[4,5,6,7,9], via multiple regression analysis[3].

2 Materials and Methods

Let *G* be a hydrogen-depicted graph whose vertices are the carbon atoms and the edges are the bonding of the carbon atoms. *V* and *E* are finite sets that contain vertices and edges of the graph *G* respectively. The degree of a vertex is, the number of edges meeting at a vertex *v*, and is denoted as d_v. The experimental values[8,12] such as entropy(S), acentric factor(*A.F*), enthalpy of vaporization(*HVAP*), standard heat of vaporization(*DHVAP*), boiling point(*BP*), critical temperature(*TC*),critical pressure(*PC*), critical volume(*VC*), density(*D*), quadratic mean radius(R^2_m), heat of vaporization($-\Delta H_f$),heat of formation($-\Delta H_v$) of octane isomers are displayed in Table 1. The values of the proposed indices[2,8,12] of octane isomers are displayed in Table 2. Table 3 shows the cross-correlation matrix of the novel indices. These indices are employed for QSPR study through multiple regression analysis to guesstimate the mentioned twelve physical properties of eighteen structural octane isomers.

The definitions of the proposed indices are as follows:

Atom Bond Interdependence index$_1$ $ABI_1(G) = \sum_{u,v\in E}\left(\sqrt{\frac{d_u}{d_v}} + \sqrt{\frac{d_v}{d_u}}\right)$

Atom Bond Interdependence index$_2$ $ABI_2(G)= \sum_{u,v\in E}\frac{d_u{}^2+d_v{}^2}{(\sqrt{d_u+d_v})}$

Atom Bond Interdependence index$_3$ $ABI_3(G)= \sum_{u,v\in E}\left(\frac{2}{(d_u+d_v)\sqrt{d_u+d_v}}\right)$ &

Atom Bond Interdependence index$_4$ $ABI_4(G)= \sum_{u,v\in E}\frac{2}{(d_u+d_v)\sqrt{d_u d_v}}$

Table 1. shows the experimental values of elemental properties of eighteen structural octane isomers.

No	*S*	*A.F*	*HVAP*	*DHVAP*	*BP*	*TC*	*PC*	*VC*	*D*	R^2_m	$-\Delta H_f$	$-\Delta H_v$
1	111.67	0.397898	73.19	9.915	125.7	296.2	24.64	0.492	0.7025	2.0449	208.6	41.49
2	109.84	0.377916	70.30	9.484	117.6	288.0	24.80	0.488	0.6980	1.8913	215.4	39.67
3	111.26	0.371002	71.3	9.521	118.9	292.0	25.60	0.464	0.7058	1.7984	212.5	39.83
4	109.32	0.371504	70.91	9.483	117.7	290.0	25.60	0.476	0.7046	1.7673	210.7	39.64
5	109.43	0.362472	71.70	9.476	118.5	292.0	25.74	0.455	0.7136	1.7673	210.7	39.64
6	103.42	0.339426	67.70	8.915	106.8	279.0	25.60	0.478	0.6953	1.6744	224.6	37.28
7	108.02	0.348247	70.20	9.272	115.6	293.0	26.60	0.468	0.7121	1.6464	213.8	38.78
8	106.98	0.344223	68.50	9.029	109.4	282.0	25.80	0.472	0.7004	1.6142	219.2	37.76
9	105.72	0.356830	68.60	9.051	109.1	279.0	25.00	0.482	0.6935	1.6449	222.5	37.85
10	104.74	0.322596	68.50	8.973	112.0	290.8	27.20	0.443	0.7100	1.7377	220.0	37.53
11	106.59	0.340345	70.20	9.316	117.7	298.0	27.40	0.466	0.7200	1.5230	212.8	38.97
12	106.06	0.332433	69.70	9.209	115.6	295.0	27.40	0.443	0.7193	1.5525	211.0	38.52
13	101.48	0.306899	69.30	9.081	118.3	305.0	28.90	0.455	0.7274	1.5212	214.8	37.99
14	101.31	0.300816	67.30	8.826	109.8	294.0	28.20	0.436	0.7161	1.4306	220.0	36.91
15	104.09	0.305370	64.87	8.402	99.24	271.1	25.50	0.468	0.6919	1.4010	224.0	35.14
16	102.06	0.293177	68.10	8.897	114.8	303.0	29.00	0.455	0.7262	1.4931	216.3	37.27
17	102.39	0.317422	68.37	9.014	113.5	295.0	27.60	0.461	0.7191	1.3698	217.3	37.75
18	93.06	0.255294	66.20	8.410	106.5	270.8	24.50	0.461	0.8242	1.4612	225.6	42.90

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https://publishoa.com
ISSN: 1309-3452

Table 2. shows the values of $ABI_1(G)$, $ABI_2(G)$, $ABI_3(G)$ & $ABI_4(G)$ with eighteen structural octane isomers.

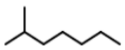
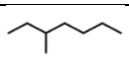
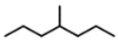
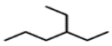
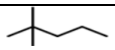
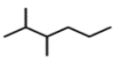
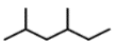
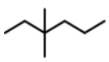
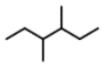
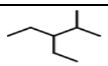
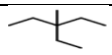
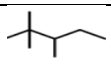
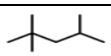
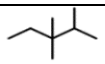
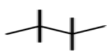
Name and Structures of octane isomers	$ABI_1(G)$	$ABI_2(G)$	$ABI_3(G)$	$ABI_4(G)$
1. n-octane	14.24264	25.77350	2.0198	2.9281
2. 2-methyl heptane 	14.78136	30.70053	1.81379	1.96206
3. 3-methyl heptane 	14.63452	30.40106	1.87758	2.05809
4. 4-methyl heptane 	14.63452	30.40106	1.87758	2.05809
5. 3-ethyl hexane 	14.48768	30.10159	1.94136	2.15411
6. 2,2-dimethyl hexane 	15.74264	41.85961	1.55764	1.68926
7. 2,3-dimethyl hexane 	15.09076	35.04900	1.69987	1.86185
8.2,4-dimethyl hexane 	15.17324	35.32809	1.67156	1.82734
9. 2,5-dimethyl hexane 	15.32008	35.62756	1.60777	1.7313
10. 3,3-dimethyl hexane 	15.48528	41.30870	1.64974	1.82851
11. 3,4-dimethyl hexane 	14.94392	34.74953	1.76365	1.95787
12. 2-methyl-3-ethyl pentane 	14.94392	34.74953	1.76365	1.95787
13. 3-methyl-3-ethyl pentane 	15.22792	40.75779	1.74184	1.96776
14. 2,2,3-trimethyl pentane 	15.99269	45.95753	1.45843	1.60586
15. 2,2,4-trimethyl pentane 	16.28136	46.78664	1.35162	1.4585
16. 2,3,3-trimethyl pentane 	15.88217	45.70609	1.48674	1.64909
17. 2,3,4-trimethyl pentane 	15.54700	39.69694	1.52217	1.6656
18.2,2,3,3-tetramethyl butane 	17.00000	56.92949	1.16169	1.2625

Table 3. shows the cross-correlation matrix of novel indices.

	$ABI_1(G)$	$ABI_2(G)$	$ABI_3(G)$	$ABI_4(G)$
$ABI_1(G)$	1.0000			
$ABI_2(G)$	0.9823	1.0000		
$ABI_3(G)$	-0.9893	-0.9537	1.0000	

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https://publishoa.com
ISSN: 1309-3452

$ABI_4(G)$	-0.8752	-0.8445	0.9005	1.0000

3 Results and discussions

Due to discrimination for structural differences, octane isomers are used as the models for the structure-property relationship. The proposed indices are having high discrimination power to use as the predicting tools of the QSPR study of isomers. The first part of this section deals with linear regression models for the mentioned properties with the proposed indices which are generated discretely and displayed in Tables 4 to 8. Followed by the linear regression models, the multiple regression model is enumerated with four proposed indices and is displayed in Table 9. The correlation coefficients of the properties of octane isomers and the novel indices in Table 4 show that entropy, *HVAP*, *DHVAP*, and acentric factors of the isomers are having a very high correlation with the indices (|r| = 0.9 approximately). Boiling point, quadratic mean radius, and heat of vaporization show a good correlation with the indices (closely |r| = 0.8). Density and critical temperature hold a moderate correlation with the indices (closely |r| = 0.5). Other properties (like critical pressure, critical volume, and heat of formation) show a very low correlation with the indices.

An extensive linear regression model is created based on the mentioned properties with the ABI_1 index, ABI_2 index, ABI_3 index, and ABI_4 index respectively.

$$ƿ = \alpha ţ + ɓ$$

Here, ƿ, α, ţ & ɓ stand for one of the physical properties of octane isomers(response variable), coefficient of the predictor variable, one of the novel indices, and constant respectively. Linear regression models are created by four proposed indices for the properties i.e., *S*, *A.F*, *HVAP*, *DHVAP*. *BP*, *TC*,*PC*,*VC*,*D*, R^2_m, $-\Delta H_f$ & $-\Delta H_v$.

Linear regression model 1

Atom Bond Interdependence index$_1$ $ABI_1(G)$

Table 4. shows the statistical specifications of linear model 1

Properties	|r|	*S.E*	*F*
S	0.91066	1.92391	77.73233
A.F	0.90492	0.01555	72.34068
HVAP	0.93270	0.75328	107.0078
DHVAP	0.95738	0.114124	175.7763
BP	0.81576	3.65007	31.82773
TC	0.50677	8.65811	5.52884
PC	0.12618	1.46976	0.25886
VC	0.33497	0.01498	2.02218
D	0.56629	0.02484	7.55324
R^2_m	0.73426	0.12669	18.71794

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$-\Delta H_f$	0.85708	2.80327	44.28327
$-\Delta H_v$	0.23784	1.77918	0.959376

S = -5.9182($ABI_1(G)$) +195.9656

$A.F$ = -0.04615($ABI_1(G)$) + 1.04187

$HVAP$ = -2.71873($ABI_1(G)$) + 110.7617

$DHVAP$ = -0.52791($ABI_1(G)$) + 17.20376

BP = -7.1847($ABI_1(G)$) + 223.6384

TC = -0.710304($ABI_1(G)$) + 398.3423

PC = 0.260906($ABI_1(G)$) + 22.4013

VC = -0.00743($ABI_1(G)$) + 0.57833

D = 0.023817($ABI_1(G)$) + 0.35114

R^2_m = -0.19124($ABI_1(G)$) + 4.55601

$-\Delta H_f$ = 6.508617($ABI_1(G)$) + 117.0695

$-\Delta H_v$ = -0.60802($ABI_1(G)$) + 47.90979

Linear Regression model 2

Properties	|r|	*S.E*	*F*
S	0.94762	1.48737	140.8264
A.F	0.95826	0.01045	179.7558
HVAP	0.89226	0.94306	62.48156
DHVAP	0.93863	0.13628	118.4903
BP	0.73418	4.28471	18.70883
TC	0.37770	9.29931	2.66228
PC	0.25054	1.43435	1.07157
VC	0.44840	0.014211	4.02652
D	0.62785	0.02346	10.41113
R^2_m	0.75141	0.12314	20.74864
$-\Delta H_f$	0.78588	3.36480	25.84169
$-\Delta H_v$	0.21610	1.78847	0.78375

Atom Bond Interdependence index$_2$ $ABI_2(G)$

S = -0.55332($ABI_2(G)$) +126.3746

$A.F$ = -0.00439($ABI_2(G)$) + 0.50210

$HVAP$ = -0.23369($ABI_2(G)$) + 78.01591

$DHVAP$ = -0.0465($ABI_2(G)$) + 10.88802

BP = -0.58098($ABI_2(G)$) + 135.7168

TC = -0.47566($ABI_2(G)$) + 307.6803

PC = 0.046546($ABI_2(G)$) + 24.63005

VC = -0.0089($ABI_2(G)$) + 0.49848

D = 0.002373($ABI_2(G)$) + 0.62568

R^2_m = -0.01758($ABI_2(G)$) + 2.29607

$-\Delta H_f$ = 0.53621($ABI_2(G)$) + 196.3425

$-\Delta H_v$ = -0.04963($ABI_2(G)$) + 40.48696

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https://publishoa.com
ISSN: 1309-3452

Linear Regression model 3

Table 5. shows the statistical specifications of linear model 2

Properties	|r|	*S.E*	*F*
S	0.88422	2.17498	57.34142
A.F	0.87996	0.01736	54.90051
HVAP	0.94127	0.70523	124.3391
DHVAP	0.95550	0.11656	167.8533
BP	0.83638	3.45920	37.25150
TC	0.52488	8.54856	6.08413
PC	0.11435	1.47189	0.21197
VC	0.29936	0.01517	1.57501
D	0.52731	0.02561	6.16247
R^2_m	0.77020	0.119026	23.33192
$-\Delta H_f$	0.85969	2.7795	45.31862
$-\Delta H_v$	0.26896	1.76425	1.24767

Atom Bond Interdependence index$_3$ $ABI_3(G)$

Table 6. shows the statistical specifications of linear model 3

S = 18.38151($ABI_3(G)$) +74.8117

$A.F$ = -0.14355($ABI_3(G)$) + 0.09679

$HVAP$ = 8.77664($ABI_3(G)$) + 54.55195

$DHVAP$ = 1.68538($ABI_3(G)$) + 6.32051

BP = 23.56351($ABI_3(G)$) + 74.47914

TC = 23.53342($ABI_3(G)$) + 250.4826

PC = -0.75633($ABI_3(G)$) + 27.6525

VC = 0.021247($ABI_3(G)$) + 0.42924

D = 0.07094($ABI_3(G)$) + 0.83366

R^2_m = 0.641668($ABI_3(G)$) + 0.561703

$-\Delta H_f$ = -20.8832($ABI_3(G)$) + 251.4221

$-\Delta H_v$ = 2.19939($ABI_3(G)$) + 34.94512

Linear Regression model 4

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Table 7. shows the statistical specifications of linear model 4

Properties	|r|	S.E	F
S	0.76812	2.98163	23.02566
A.F	0.80171	0.02184	28.78429
HVAP	0.90214	0.90112	69.95547
DHVAP	0.91361	0.16065	80.78544
BP	0.83919	3.43204	38.09771
TC	0.48933	8.758687	5.03723
PC	0.17864	1.45777	0.52744
VC	0.37978	0.01471	2.69662
D	0.40395	0.02757	3.11993
R^2_m	0.79508	0.11319	27.49628
$-\Delta H_f$	0.80416	3.23437	29.28415
$-\Delta H_v$	0.37971	1.69456	2.69543

Atom Bond Interdependence index$_4$ $ABI_4(G)$

$S = 9.97156(ABI_4(G)) + 86.78659$

$A.F = 0.08167(ABI_4(G)) + 0.18321$

$HVAP = 5.25289(ABI_4(G)) + 59.35101$

$DHVAP = 1.00633(ABI_4(G)) + 7.24652$

$BP = 14.76402(ABI_4(G)) + 86.12878$

$TC = 13.70055(ABI_4(G)) + 264.0687$

$PC = -0.73787(ABI_4(G)) + 27.77167$

$VC = 0.01683(ABI_4(G)) + 0.43317$

$D = -0.03394(ABI_4(G)) + 0.77895$

$R^2_m = 0.41365(ABI_4(G)) + 0.85727$

$-\Delta H_f = -12.1986(ABI_4(G)) + 239.4423$

$-\Delta H_v = 1.93899(ABI_4(G)) + 34.98467$

The second part of this section deals with the multiple regression model which contains the four novel indices $ABI_1(G)$, $ABI_2(G)$, $ABI_3(G)$ & $ABI_4(G)$ and is defined as

JOURNAL OF ALGEBRAIC STATISTICS
Volume 13, No. 2, 2022, p. 3173-3181
https://publishoa.com
ISSN: 1309-3452

$$p = \sum_{i=1}^{4} \alpha_i \, ABI_i(G) + \delta$$

Multiple Regression models as per $ABI_i(G)$

S = 14.79761$ABI_1(G)$ + [-1.22817 $ABI_2(G)$] + 26.83173 $ABI_3(G)$ + [-2.30504 $ABI_4(G)$] + [-114.83680]

$A.F$ = 0.18744$ABI_1(G)$ + [-0.01324 $ABI_2(G)$] + 0.29245 $ABI_3(G)$ + [-0.00363 $ABI_4(G)$] + [-2.51077]

$HVAP$ = [-4.59733$ABI_1(G)$] + 0.17791 $ABI_2(G)$ + [-2.8137 $ABI_3(G)$] + 2.13778 $ABI_4(G)$ + 133.4567

$DHVAP$ = [-0.4338$ABI_1(G)$] + [-0.00098 $ABI_2(G)$] + [-0.2729 $ABI_3(G)$] + 0.38300 $ABI_4(G)$ +15.53971

BP = [-41.1337$ABI_1(G)$] + 2.06231 $ABI_2(G)$ + [-52.9033 $ABI_3(G)$] + 11.31843 $ABI_4(G)$ + 731.8851

TC = [-135.052$ABI_1(G)$] + 6.82920 $ABI_2(G)$ + [-191.075 $ABI_3(G)$] + 13.25397 $ABI_4(G)$ + 2390.677

PC = [-21.208$ABI_1(G)$] + 1.10937 $ABI_2(G)$ + [-30.1711 $ABI_3(G)$] + [-0.02161 $ABI_4(G)$] + 359.1336

VC = 0.12921$ABI_1(G)$ + [-0.00871 $ABI_2(G)$] + 0.10662 $ABI_3(G)$ + 0.01919 $ABI_4(G)$ + [-1.39568]

D = [-0.11744$ABI_1(G)$ + 0.00950 $ABI_2(G)$ + [-0.17021 $ABI_3(G)$] + 0.03488 $ABI_4(G)$ + 2.370651

R^2_m = 1.85160$ABI_1(G)$ + [-0.07658 $ABI_2(G)$] + 3.75279 $ABI_3(G)$ + 0.10171 $ABI_4(G)$ + [-30.2392]

$-\Delta H_f$ = 40.9270$ABI_1(G)$ + [-1.79253 $ABI_2(G)$] + 56.62328 $ABI_3(G)$ + [-6.14174 $ABI_4(G)$] + [-424.43815]

$-\Delta H_v$ = 2.58921$ABI_1(G)$ + [-0.02106 $ABI_2(G)$] + 4.88705 $ABI_3(G)$ + 3.32205$ABI_4(G)$ + [-14.5534].

Table 8. shows, the statistical specifications of multiple regression model.

Properties	|r|	S.E	F
S	0.96152	1.41932	39.8063
A.F	0.99576	0.00373	380.7134
HVAP	0.955037	0.68700	33.72164
DHVAP	0.97034	0.10600	52.35452
BP	0.93052	2.56405	20.98091
TC	0.91073	4.60168	15.80343
PC	0.85110	0.86294	8.54141
VC	0.78945	0.01083	5.37613
D	0.70506	0.49711	3.21266
R^2_m	0.93015	0.07602	20.85669
$-\Delta H_f$	0.93604	2.12418	22.99729
$-\Delta H_v$	0.43206	1.83267	0.74594

Tables 4 to 8 show the results of |r|, S.E & F for the twelve physical properties of eighteen octane isomers with novel indices. Linear regression models from 1 to 4 show the QSPR studies(linear regression analysis) of the novel indices

$ABI_1(G)$, $ABI_2(G)$, $ABI_3(G)$ & $ABI_4(G)$ with physical properties of octane isomers independently. In the end, the multiple linear regression model containing the four novel indices gives significant results and will be discussed below.

The correlation coefficients of $ABI_1(G)$, $ABI_2(G)$, $ABI_3(G)$ & $ABI_4(G)$ with entropy(S) are 0.91,0.948, 0.88 & 0.77 respectively whereas the combination of four indices gives 0.962. The range of |r| from 0.80 to 0.958 in linear regression models is based on the novel indices with acentric factor($A.F$) whereas in the multiple regression model, it gives 0.99576. This shows that the multiple regression model is more predictable than the linear regression models based on these indices with acentric factors.

Similarly, for *HVAP* and *DHVAP*, the multiple regression model gives significant results compared with linear regression models. The correlation coefficients of the boiling point of octane isomers with the novel indices are ranging from 0.73 to 0.84 whereas a combination of these indices gives 0.93052. This is the highest value by comparing the correlation coefficients of the boiling point of octane isomers with a well-established degree-based topological index.

The correlation coefficients of novel indices with *TC, PC, VC* are ranging from 0.13 to 0.53 whereas in combination, it gives 0.91073, 0.85110,0.78945 respectively. Especially, by considering the critical pressure, it correlates with the indices is very poor but in combination, it is remarkably high(0.85110). Density, one of the physical properties of octane isomers, is moderately correlated with the indices separately and together. R^2_m, $-\Delta H_f$ are highly correlated with the indices in both cases. $-\Delta H_v$ is poorly correlated with the novel indices while done separately and in combination.

From the overall observation of these regression models, we conclude that multiple regression model with the four novel indices is a wonderful model in the QSPR study of structure-physical property relationships of octane isomers.

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