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ORIGINAL ARTICLE

QSPR analysis of some novel neighbourhood degree-based topological descriptors

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Abstract

Topological index is a numerical value associated with a chemical constitution for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. In this work, some new indices based on neighborhood degree sum of nodes are proposed. To make the computation of the novel indices convenient, an algorithm is designed. Quantitative structure property relationship (QSPR) study is a good statistical method for investigating drug activity or binding mode for different receptors. QSPR analysis of the newly introduced indices is studied here which reveals their predicting power. A comparative study of the novel indices with some well-known and mostly used indices in structure-property modelling and isomer discrimination is performed. Some mathematical properties of these indices are also discussed here.

Keywords Chemical network · Degree · Topological descriptors · QSPR analysis

Mathematics Subject Classification 05C09 · 05C92 · 05C07 · 92E10

Introduction

The graph theory is a significant part of applied mathematics for modeling real life problems. The chemical graph theory, a fascinating branch of graph theory, provides many information on chemical compounds using an important tool called the topological index [4,43]. Theoretical molecular descriptors alias topological indices are graph invariants that play an important role in chemistry, pharmaceutical sciences, materials science, engineering and so forth. Its role on QSPR/QSAR analysis [2,22,23,37,38], to model physical and chemical properties of molecules is also remarkable. Among several types of topological indices, vertex degree based [15] topological indices are most investigated and widely used. The first vertex degree based topological index is proposed in 1975 by Randić [36] known as Connectivity index or Randic index. Connectivity index is defined by

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}},$$

where $d_G(u)$, $d_G(v)$ represent the degree of nodes u,v in the vertex set $V(G)$ of a molecular graph G. By molecular graph, we mean a simple connected graph considering atoms of chemical compound as vertices and the chemical bonds between them as edges. $E(G)$ is the edge set of G. The inverse Randic index [19] is given by

$$\mathrm{RR}(G) = \sum_{uv \in E(G)} \sqrt{d_G(u)d_G(v)}.$$

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The Zagreb indices, introduced by Gutman and Trinajestić [20], are defined as follows:

$$M_1(G) = \sum_{v \in V(G)} d_G(v)^2 = \sum_{uv \in E(G)} [d_G(u) + d_G(v)],$$

$$M_2(G) = \sum_{uv \in E(G)} [d_G(u) d_G(v)].$$

Furtula et al. [12] have introduced the forgotten topological index as follows:

$$F(G) = \sum_{v \in V(G)} d_G(v)^3 = \sum_{uv \in E(G)} [d_G(u)^2 + d_G(v)^2].$$

Zhou and Trinanjstić have designed the sum connectivity index [49] which is as follows:

$$\mathrm{SCI}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) + d_G(v)}}.$$

The symmetric division degree index [44] is defined as

$$\mathrm{SDD}(G) = \sum_{uv \in E(G)} [\frac{d_G(u)}{d_G(v)} + \frac{d_G(v)}{d_G(u)}].$$

The redefined third Zagreb index [39] is defined by

$$\mathrm{ReZG}_3(G) = \sum_{uv \in E(G)} d_G(u) d_G(v) [d_G(u) + d_G(v)].$$

For more study about degree based topological indices, readers are referred to the articles [5,10,24,25,27,32]. Recently, the present authors introduced some new indices [30,31] based on neighborhood degree sum of nodes. As a continuation, we present here some new topological indices, named as first NDe index (ND_1), second NDe index (ND_2), third NDe index (ND_3), fourth NDe index (ND_4), fifth NDe index (ND_5), and sixth NDe index (ND_6) and defined as

$$\mathrm{ND}_1(G) = \sum_{uv \in E(G)} \sqrt{\delta_G(u) \delta_G(v)},$$

$$\mathrm{ND}_2(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\delta_G(u) + \delta_G(v)}},$$

$$\mathrm{ND}_3(G) = \sum_{uv \in E(G)} \delta_G(u) \delta_G(v) [\delta_G(u) + \delta_G(v)],$$

$$\mathrm{ND}_4(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\delta_G(u) \delta_G(v)}},$$

$$\mathrm{ND}_5(G) = \sum_{uv \in E(G)} \left[\frac{\delta_G(u)}{\delta_G(v)} + \frac{\delta_G(v)}{\delta_G(u)} \right],$$

$$\mathrm{ND}_6(G) = \sum_{uv \in E(G)} [d_G(u) \delta_G(u) + d_G(v) \delta_G(v)],$$

where $\delta_G(u)$ is the sum of degrees of all neighboring vertices of $u \in V(G)$, i.e, $\delta_G(u) = \sum_{v \in N_G(u)} d_G(v)$, $N_G(u)$ being the set of adjacent vertices of u. The goal of this article is to check the chemical applicability of the above newly designed indices and discuss about some bounds of them in terms of other topological descriptors to visualize the indices mathematically.

We construct the results into two different parts. We start the first part with an algorithm for computing the indices and then some statistical regression analysis have been made to check the efficiency of the novel indices to model physical and chemical properties. Then, we would like to test their degeneracy. It follows a comparative study of these indices with other topological indices. This part ends with a discussion about the applications of the present work. The second part deals with some mathematical relation of these indices with some other well-known indices.

Computational aspects

In this section, we have designed an algorithm to make the computation of the novel indices convenient.

Algorithm 1 Computational Procedure

```
Input: Graph $G$.
Output: Calculation of $\partial$ and $degree$.
Initialization: $E \leftarrow$ no. of edges, $V \leftarrow$ no. of vertex, $conn[E][2] \leftarrow$ connection matrix, $deg[V][2] \leftarrow$ degree of each vertex, $\partial[V][2] \leftarrow n-bd$ degree of each vertex, $ver[V] \leftarrow$ Vertex array, $count \leftarrow 0$, $adj[count] \leftarrow$ adjacent element, $\partial \leftarrow 0$.
loop $i = 1$ to $V$
    For each vertex from the array $ver[V]$.
    loop $j = 1$ to $E$
        $count$ corresponding vertex from the matrix $conn[E][2]$.
    end loop
    $deg[V][2] = count$.
    loop $k = 1$ to $count$
        $adj[count]$ = store corresponding vertex.
    end loop
    loop $k = 1$ to $count$
        for each vertex from the array $adj[count]$.
        loop $j = 1$ to $E$
            Find the frequency of the vertex from the matrix $conn[E][2]$.
            Store the frequency in $\partial$ for all the vertex in $adj[count]$.
        end loop
        $\partial[V][2] = \partial$.
        $\partial = 0$.
    end loop
    $count = 0$.
end loop
For each vertex $v \in V$.
Retrieve degree and n-bd degree sum from the matrix $deg[V][2]$ and $\partial[V][2]$.
Calculate the function $f(\delta_G(u), \delta_G(v), d_G(u), d_G(u))$.
```

To make it simple and understandable, we have considered some variables and matrices. We have used conn $[E][2]$ matrix to store the connection details among vertices, whereas deg $[V][2]$ and $\delta[V][2]$ is the matrix to store degree of each vertex and neighborhood degree sum of vertex respectively. The novel indices can be considered as function of $\delta_G(u)$,$\delta_G(v)$,$d_G(u)$, and $d_G(v)$ i.e., f($\delta_G(u)$,$\delta_G(v)$,$d_G(u)$, $d_G(v)$).

Newly introduced indices in QSPR analysis

In this section, we have studied about the newly designed topological indices to model physico-chemical properties [Acentric Factor (Acent Fac.), entropy (S), enthalpy of vaporization (HVAP), standard enthalpy of vaporization (DHVAP), and heat capacity at P constant (CP)] of the octane isomers and physical properties [boiling points (bp), molar volumes (mv) at 20°C, molar refraction (mr) at 20 °C, heats of vaporization (hv) at 25 °C, critical temperature (ct), critical pressure (cp) surface tensions (st) at 20 °C and melting points (mp)] of the 67 alkanes from n-butanes to nonanes. The experimental values of physico-chemical properties of octane isomers (Table 1) are taken from http://www.moleculardescriptors.eu. The data related to 67 alkanes (Table 9) are compiled from [27]. For comparative study, different well-known existing descriptors are collected form http://www.moleculardescriptors.eu/books/books.htm. First, we have considered the octane isomers (Table 2) and then the 67 alkanes are taken into account.

Regression model for octane isomers

We have tested the following linear regression models

$$P = m(\text{TI}) + c, \qquad (1)$$

where P is the physical property and TI is the topological index. Using the above formula, we have the following linear regression models for different neighborhood degree sum based topological indices.

1. ND_1 index:

$$\begin{aligned} S &= 141.1521 - [\text{ND}_1(G)]1.1926 \\ \text{Acent Fac.} &= 0.627 - [\text{ND}_1(G)]0.0097 \\ \text{DHVAP} &= 11.8017 - [\text{ND}_1(G)]0.0893 \end{aligned}$$

2. ND_2 index:

$$\begin{aligned} S &= 39.6776 + [\text{ND}_2(G)]27.1579 \\ \text{Acent Fac.} &= -0.2058 + [\text{ND}_2(G)]0.2238 \\ \text{DHVAP} &= 1.1069 + [\text{ND}_2(G)]2.0737 \end{aligned}$$

3. ND_3 index:

$$\begin{aligned} S &= 117.2259 - [\text{ND}_3(G)]0.0088 \\ \text{Acent Fac.} &= 0.4322 - [\text{ND}_3(G)]7.2 \times 10^{-5} \\ \text{DHVAP} &= 9.9568 - [\text{ND}_3(G)]0.0006 \end{aligned}$$

Table 1 Experimental values of physico-chemical properties for octane isomers

Octanes	Acent Fac.	S	HVAP	DHVAP	CP
n-Octane	0.397898	111.67	73.19	9.915	24.64
2-Methyl heptane	0.377916	109.84	70.3	9.484	24.8
3-Methyl heptane	0.371002	111.26	71.3	9.521	25.6
4-Methyl heptane	0.371504	109.32	70.91	9.483	25.6
3-Ethyl hexane	0.362472	109.43	71.7	9.476	25.74
2,2-Dimethyl hexane	0.339426	103.42	67.7	8.915	25.6
2,3-Dimethyl hexane	0.348247	108.02	70.2	9.272	26.6
2,4-Dimethyl hexane	0.344223	106.98	68.5	9.029	25.8
2,5-Dimethyl hexane	0.356830	105.72	68.6	9.051	25
3,3-Dimethyl hexane	0.322596	104.74	68.5	8.973	27.2
3,4-Dimethyl hexane	0.340345	106.59	70.2	9.316	27.4
2-Methyl-3-ethyl pentane	0.332433	106.06	69.7	9.209	27.4
3-Methyl-3-ethyl pentane	0.306899	101.48	69.3	9.081	28.9
2,2,3-Trimethyl pentane	0.300816	101.31	67.3	8.826	28.2
2,2,4-Trimethyl pentane	0.30537	104.09	64.87	8.402	25.5
2,3,3-Trimethyl pentane	0.293177	102.06	68.1	8.897	29
2,3,4-Trimethyl pentane	0.317422	102.39	68.37	9.014	27.6
2,2,3,3-Tetramethyl butane	0.255294	93.06	66.2	8.41	24.5

Table 2 Topological indices of octane isomers

Octanes	ND_1	ND_2	ND_3	ND_4	ND_5	ND_6
n-Octane	23.827	2.711	612	2.144	14.5	92
2-Methyl heptane	25.786	2.601	770	1.971	14.517	108
3-Methyl heptane	26.559	2.5699	892	1.956	15.117	116
4-Methyl heptane	26.518	2.588	920	1.991	15.133	116
3-Ethyl hexane	27.254	2.551	1056	1.964	15.8	124
2,2-Dimethyl hexane	29.706	2.443	1224	1.754	14.6	146
2,3-Dimethyl hexane	29.266	2.444	1212	1.784	15.533	142
2,4-Dimethyl hexane	28.478	2.469	1086	1.799	15.183	132
2,5-Dimethyl hexane	27.801	2.495	946	1.802	14.433	124
3,3-Dimethyl hexane	31.1296	2.381	1504	1.718	15.933	164
3,4-Dimethyl hexane	29.94	2.404	1332	1.753	16.333	150
2-Methyl-3-ethyl pentane	29.902	2.415	1372	1.77	16.29	150
3-Methyl-3-ethyl pentane	32.526	2.301	1778	1.645	17.364	182
2,2,3-Trimethyl pentane	33.88	2.252	1832	1.527	16.107	192
2,2,4-Trimethyl pentane	31.552	2.346	1436	1.606	14.752	162
2,3,3-Trimethyl pentane	34.627	2.214	1976	1.489	16.681	202
2,3,4-Trimethyl pentane	31.907	2.308	1530	1.589	16.057	168
2,2,3,3-Tetramethyl butane	38.749	2.076	2534	1.277	15.928	248

4. ND_4 index:

$$\begin{aligned} S &= 69.8183 + [ND_4(G)]20.3149 \\ \text{Acent Fac.} &= 0.04656 + [ND_4(G)]0.1651 \\ \text{DHVAP} &= 6.2868 + [ND_4(G)]1.6206 \\ \text{HVAP} &= 55.1172 + [ND_4(G)]8.0164 \end{aligned}$$

5. ND_5 index:

$$\begin{aligned} S &= 144.7836 - [ND_5(G)]2.5286 \\ \text{Acent Fac.} &= 0.7245 - [ND_5(G)]0.0249 \\ \text{DHVAP} &= 10.6958 - [ND_5(G)]0.1008 \\ \text{CP} &= 3.8987 + [ND_5(G)]1.4447 \end{aligned}$$

6. ND_6 index:

$$\begin{aligned} S &= 122.3482 - [ND_6(G)]0.1122 \\ \text{Acent Fac.} &= 0.4730 - [ND_6(G)]0.0009 \\ \text{DHVAP} &= 10.3438 - [ND_6(G)]0.0081 \end{aligned}$$

The correlations of the novel descriptors with different physico-chemical properties are depicted in the Figs. 1, 2, 3, 4, 5 and 6.

Now we describe above linear models in the Tables 3, 4, 5, 6, 7 and 8. Here c, m, r, SE, F, SF stands for intercept, slope, correlation coefficient, standard error, F test, and significance F respectively. Correlation coefficient tells how strong the linear relationship is. The standard error of the regression

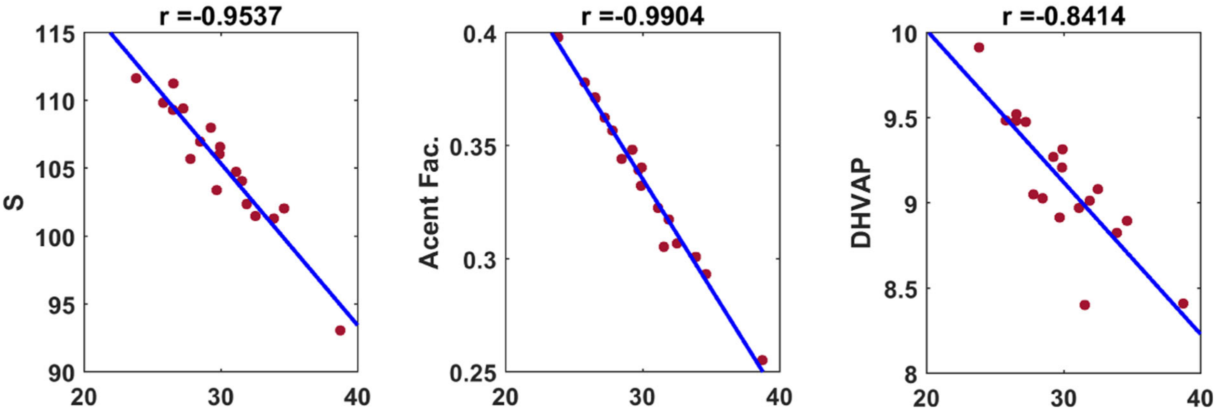


Fig. 1 Correlation of ND_1 index with S, Acent Fac., and DHVAP for octane isomers

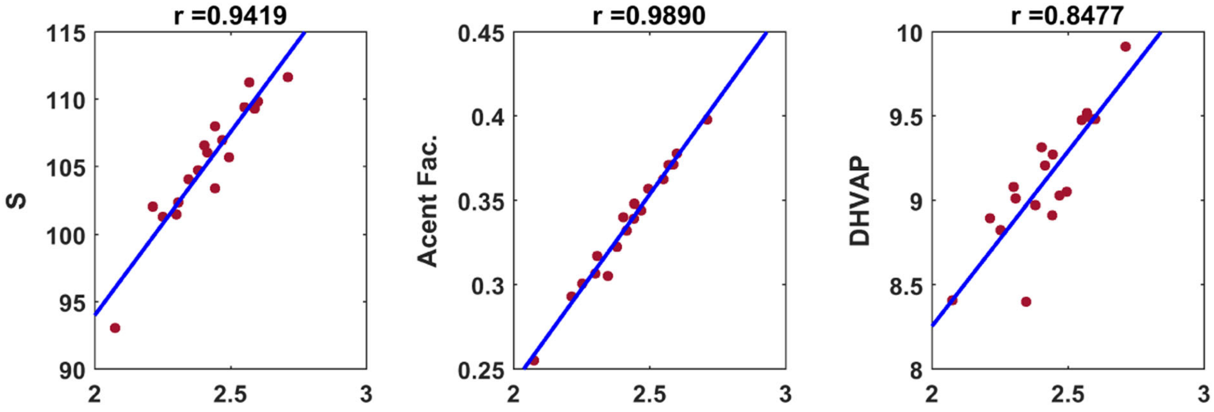


Fig. 2 Correlation of ND_2 index with *S*, Acent Fac., and DHVAP for octane isomers

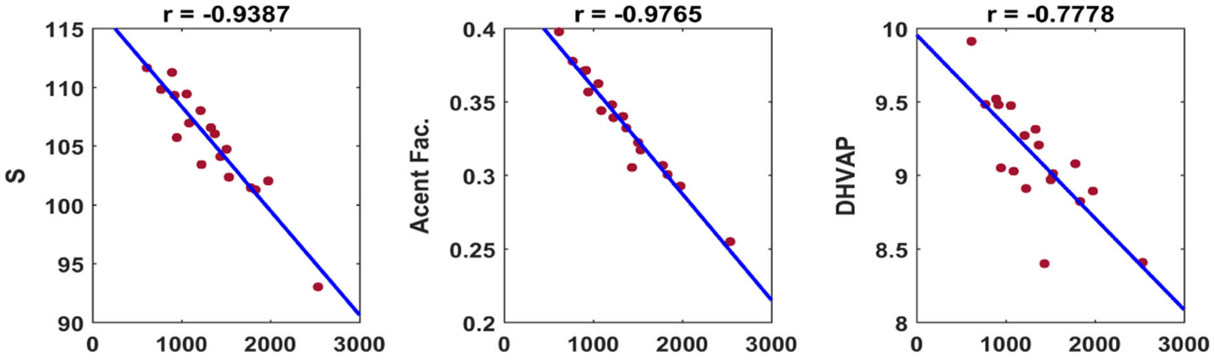
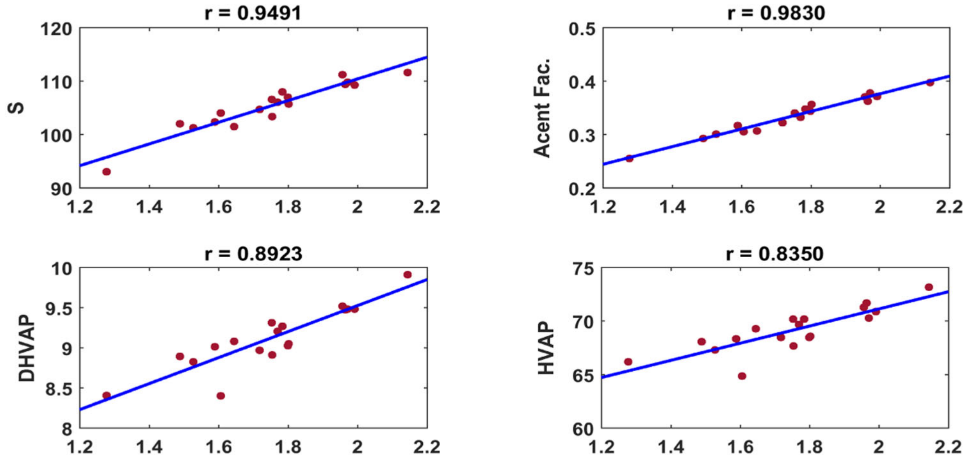


Fig. 3 Correlation of ND_3 index with *S*, Acent Fac., and DHVAP for octane isomers

Fig. 4 Correlation of ND_4 index with *S*, Acent Fac., and DHVAP for octane isomers

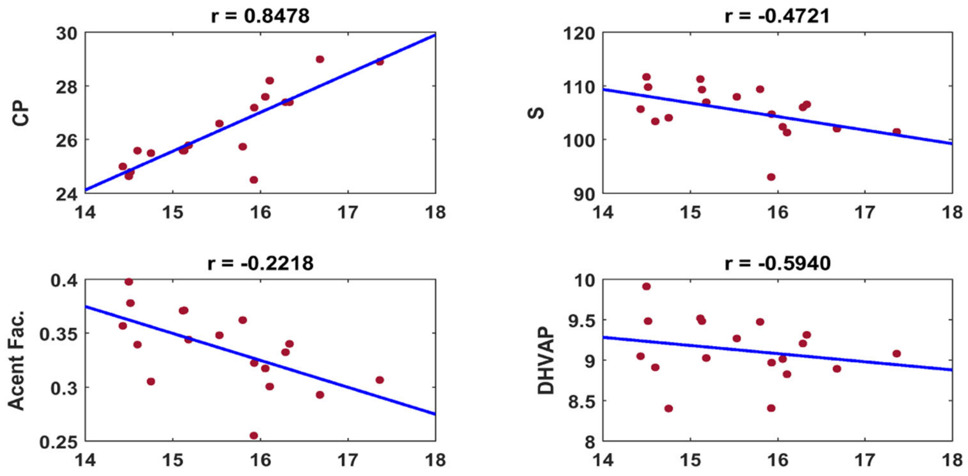


is the precision that the regression coefficient is measured. To check whether the results are reliable, Significance *F* can be useful. If this value is less than 0.05, then the model is statistically significant. If significance *F* is greater than 0.05, it is probably better to stop using that set of independent variable.

Regression model for 67 alkanes

We have tested here the model described in (1) for 67 alkanes from n-butanes to nonanes. we have the following linear regression models for different neighborhood degree sum-based topological indices.

Fig. 5 Correlation of ND_5 index with S, Acent Fac., and DHVAP for octane isomers



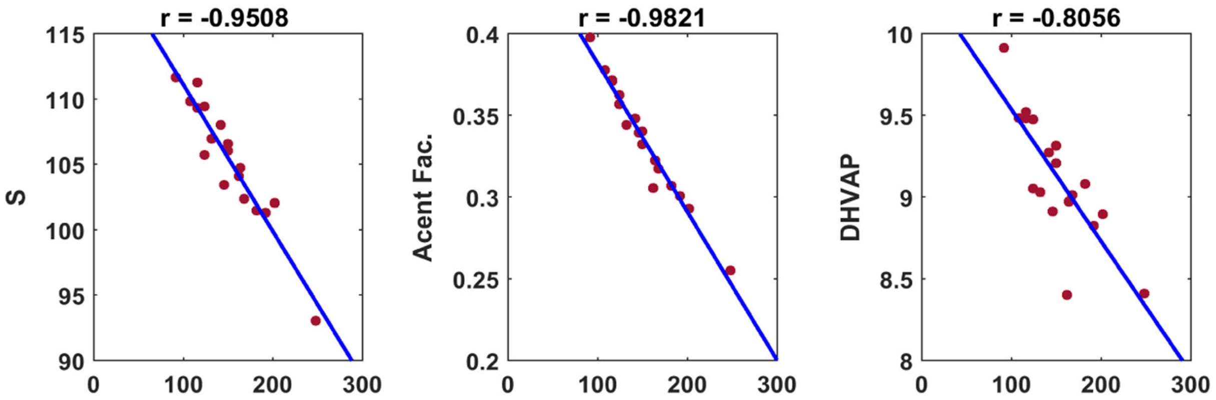


Fig. 6 Correlation of ND_6 index with S, Acent Fac., and DHVAP for octane isomers

Table 3 Statical parameters linear QSPR model for $ND_1(G)$

Physical properties	c	m	r	SE	F	SF
S	141.1521	− 1.1926	− 0.9537	1.4010	160.7549	9.2E−10
Acent Fac.	0.627	− 0.0097	− 0.9904	0.0050	824.2198	3.42E−15
DHVAP	11.8017	− 0.0893	− 0.8414	0.2135	38.7783	1.21E−05

Table 4 Statical parameters of linear QSPR model for $ND_2(G)$

Physical properties	c	m	r	SE	F	SF
S	39.6776	27.1579	0.9419	1.5629	126.0258	5.37E−09
Acent Fac.	− 0.2058	0.2238	0.9890	0.0054	717.1224	1.02E−14
DHVAP	1.1069	2.0737	0.8477	0.2096	40.8614	8.92E−06

Table 5 Statical parameters of linear QSPR model for $ND_3(G)$

Physical properties	c	m	r	SE	F	SF
S	117.2259	− 0.0088	−0.9387	1.6052	118.6526	8.25E−09
Acent Fac.	0.4322	− 7.2E−05	−0.9765	0.0079	328.2359	4.37E−12
DHVAP	9.9568	− 0.0006	−0.7778	0.2483	24.5074	0.000145

Table 6 Statical parameters of linear QSPR model for $ND_4(G)$

Physical properties	c	m	r	SE	F	SF
S	69.8183	20.3149	0.9491	1.4667	145.2802	1.93E−09
Acent Fac.	0.0465	0.1651	0.9830	0.0067	458.9889	3.31E−13
DHVAP	6.2868	1.6206	0.8923	0.1784	62.5202	6.45E−07
HVAP	55.1172	8.0164	0.8350	1.1493	36.8449	1.62E−05

Table 7 Statical parameters of linear QSPR model for $ND_5(G)$

Physical properties	c	m	r	SE	F	SF
CP	3.8987	1.4447	0.8478	0.7856	40.9017	8.87E−06
S	144.7836	−2.5286	−0.4721	4.1049	4.5895	0.047895
Acent Fac.	0.7245	−0.0249	−0.2218	0.0294	8.7253	0.009335
DHVAP	10.6958	−0.1008	−0.5940	0.3853	0.8280	0.376344

Table 8 Statical parameters of linear QSPR model for $ND_6(G)$

Physical properties	c	m	r	SE	F	SF
S	122.3482	−0.1122	−0.9508	1.4420	150.8369	1.47E−09
Acent Fac.	0.4730	−0.0009	−0.9821	0.0069	434.0329	5.09E−13
DHVAP	10.3438	−0.0081	−0.8056	0.2341	29.5844	5.46E−05

1. ND_1 index:

$$\begin{aligned}
\mathrm{bp} &= -8.8069 + [ND_1(G)]4.0114\\
\mathrm{ct} &= 135.4475 + [ND_1(G)]5.1317\\
\mathrm{cp} &= 34.6560 - [ND_1(G)]0.2721\\
\mathrm{mv} &= 100.8619 + [ND_1(G)]2.0398\\
\mathrm{mr} &= 20.1480 + [ND_1(G)]0.6398\\
\mathrm{hv} &= 21.8703 + [ND_1(G)]0.5616\\
\mathrm{st} &= 14.3557 + [ND_1(G)]0.2177\\
\mathrm{mp} &= -131.654 + [ND_1(G)]0.7933
\end{aligned}$$

2. ND_2 index:

$$\begin{aligned}
\mathrm{bp} &= -95.9303 + [ND_2(G)]84.2834\\
\mathrm{ct} &= 47.6081 + [ND_2(G)]98.1177\\
\mathrm{cp} &= 43.8159 - [ND_2(G)]7.0529\\
\mathrm{mv} &= 50.7515 + [ND_2(G)]45.1187\\
\mathrm{mr} &= 6.7917 + [ND_2(G)]13.1956\\
\mathrm{hv} &= 3.9821 + [ND_2(G)]14.0794\\
\mathrm{st} &= 9.6530 + [ND_2(G)]4.5432\\
\mathrm{mp} &= -150.6221 + [ND_2(G)]17.6077
\end{aligned}$$

3. ND_3 index:

$$\begin{aligned}
\mathrm{bp} &= 60.7738 + [ND_3(G)]0.0372\\
\mathrm{ct} &= 220.3722 + [ND_3(G)]0.0508\\
\mathrm{cp} &= 29.0689 - [ND_3(G)]0.0019\\
\mathrm{mv} &= 140.8691 + [ND_3(G)]0.0159\\
\mathrm{mr} &= 32.2248 + [ND_3(G)]0.0054\\
\mathrm{hv} &= 32.9914 + [ND_3(G)]0.0043\\
\mathrm{st} &= 18.2408 + [ND_3(G)]0.0020\\
\mathrm{mp} &= -118.9098 + [ND_3(G)]0.0078
\end{aligned}$$

4. ND_4 index:

$$\begin{aligned}
\mathrm{bp} &= -69.6148 + [ND_4(G)]100.5729\\
\mathrm{ct} &= 86.3449 + [ND_4(G)]112.5233\\
\mathrm{cp} &= 42.1443 - [ND_4(G)]8.7145\\
\mathrm{mv} &= 75.6867 + [ND_4(G)]48.0647\\
\mathrm{mr} &= 14.6003 + [ND_4(G)]13.7704\\
\mathrm{hv} &= 9.3610 + [ND_4(G)]16.3338\\
\mathrm{st} &= 12.1161 + [ND_4(G)]4.8742\\
\mathrm{mp} &= -146.0101 + [ND_4(G)]21.4463
\end{aligned}$$

5. ND_5 index:

$$\begin{aligned}
\mathrm{bp} &= -62.0831 + [ND_5(G)]11.0891\\
\mathrm{ct} &= 73.9689 + [ND_5(G)]13.7538\\
\mathrm{cp} &= 38.1279 - [ND_5(G)]0.7430\\
\mathrm{mv} &= 74.7263 + [ND_5(G)]5.5594\\
\mathrm{mr} &= 12.0902 + [ND_5(G)]1.7348\\
\mathrm{hv} &= 11.8876 + [ND_5(G)]1.7079\\
\mathrm{st} &= 10.2382 + [ND_5(G)]0.6757
\end{aligned}$$

Table 9 Experimental values of physical properties for 67 alkanes

Alkanes	bp (°C)	mv (cm^3)	mr (cm^3)	hv (kJ)	ct (°C)	cp (atm)	st (dyne/cm)	mp (°C)
Butane	– 0.05				152.01	37.47		– 138.35
2-Methyl propane	– 11.73				134.98	36		– 159.6
Pentane	36.074	115.205	25.2656	26.42	196.62	33.31	16	– 129.72
2-Methyl butane	27.852	116.426	25.2923	24.59	187.7	32.9	15	– 159.9
2,2-Dimethyl propane	9.503	112.074	25.7243	21.78	160.6	31.57		– 16.55
Hexane	68.74	130.688	29.9066	31.55	234.7	29.92	18.42	– 95.35
2-Methyl pentane	60.271	131.933	29.945	29.86	224.9	29.95	17.38	– 153.67
3-Methyl pentane	63.282	129.717	29.8016	30.27	231.2	30.83	18.12	– 118
2,2-Methyl butane	4.741	132.744	29.9347	27.69	216.2	30.67	16.3	– 99.87
2,3-Dimethyl butane	57.988	130.24	29.8104	29.12	227.1	30.99	17.37	– 128.54
Heptane	98.427	146.54	34.5504	36.55	267.55	27.01	20.26	– 90.61
2-Methyl hexane	90.052	147.656	34.5908	34.8	257.9	27.2	19.29	– 118.28
3-Methyl hexane	91.85	145.821	34.4597	35.08	262.4	28.1	19.79	– 119.4
3-Ethyl pentane	93.475	143.517	34.2827	35.22	267.6	28.6	20.44	– 118.6
2,2-Dimethyl pentane	79.197	148.695	34.6166	32.43	247.7	28.4	18.02	– 123.81
2,3-Dimethyl pentane	89.784	144.153	34.3237	34.24	264.6	29.2	19.96	– 119.1
2,4-dimethyl pentane	80.5	148.949	34.6192	32.88	247.1	27.4	18.15	– 119.24
3,3-Dimethyl pentane	86.064	144.53	34.3323	33.02	263	30	19.59	– 134.46
Octane	125.665	162.592	39.1922	41.48	296.2	24.64	21.76	– 56.79
2-Methyl heptane	117.647	163.663	39.2316	39.68	288	24.8	20.6	– 109.04
3-Methyl heptane	118.925	161.832	39.1001	39.83	292	25.6	21.17	– 120.5
3-Methyl heptane	117.709	162.105	39.1174	39.67	290	25.6	21	– 120.95
3-Ethyl hexane	118.53	160.07	38.94	39.4	292	25.74	21.51	
2,2-Dimethyl hexane	10.84	164.28	39.25	37.29	279	25.6	19.6	– 121.18
2,3-Dimethyl hexane	115.607	160.39	38.98	38.79	293	26.6	20.99	
2,4-Dimethyl hexane	109.42	163.09	39.13	37.76	282	25.8	20.05	– 137.5
2,5-Dimethyl hexane	109.1	164.69	39.25	37.86	279	25	19.73	– 91.2
3,3-Dimethyl hexane	111.96	160.87	39	37.93	290.84	27.2	20.63	– 126.1
3,4-Dimethyl hexane	117.72	158.81	38.84	39.02	298	27.4	21.64	
3-Ethyl-2-methyl pentane	115.65	158.79	38.83	38.52	295	27.4	21.52	– 114.96
3-Ethyl-3-methyl pentane	118.25	157.02	38.71	37.99	305	28	21.99	– 90.87
2,2,3-Trimethyl pentane	109.84	159.52	38.92	36.91	294	28.2	20.67	– 112.27
2,2,4-Trimethyl pentane	99.23	165.08	39.26	35.13	271.15	25.5	18.77	– 107.38
2,3,3-Trimethyl pentane	114.76	157.29	38.76	37.22	303	29	21.56	– 100.7
2,3,4-Trimethyl pentane	113.46	158.85	38.86	37.61	295	27.6	21.14	– 109.21
Nonane	150.76	178.71	43.84	46.44	322	22.74	22.92	– 53.52
2-Methyl octane	143.26	179.77	43.87	44.65	315	23.6	21.88	– 80.4
3-Methyl octane	144.18	177.5	43.72	44.75	318	23.7	22.34	– 107.64
4-Methyl octane	142.48	178.15	43.76	44.75	318.3	23.06	22.34	– 113.2
3-Ethyl heptane	143	176.41	43.64	44.81	318	23.98	22.81	– 114.9
4-Ethyl heptane	141.2	175.68	43.69	44.81	318.3	23.98	22.81	
2,2-Dimethyl heptane	132.69	180.5	43.91	42.28	302	22.8	20.8	– 113
2,3-Dimethyl heptane	140.5	176.65	43.63	43.79	315	23.79	22.34	– 116
2,4-Dimethyl heptane	133.5	179.12	43.73	42.87	306	22.7	23.3	
2,5-Dimethyl heptane	136	179.37	43.84	43.87	307.8	22.7	21.3	

Table 9 continued

Alkanes	bp (°C)	mv (cm^3)	mr (cm^3)	hv (kJ)	ct (°C)	cp (atm)	st (dyne/cm)	mp (°C)
2,6-Dimethyl heptane	135.21	180.91	43.92	42.82	306	23.7	20.83	– 102.9
3,3-Dimethyl heptane	137.3	176.897	43.687	42.66	314	24.19	22.01	
3,4-Dimethyl heptane	140.6	175.349	43.5473	43.84	322.7	24.77	22.8	
3,5-Dimethyl heptane	136	177.386	43.6379	42.98	312.3	23.59	21.77	
4,4-Dimethyl heptane	135.2	176.897	43.6022	42.66	317.8	24.18	22.01	
3-Ethyl-2-methyl hexane	138	175.445	43.655	43.84	322.7	24.77	22.8	
4-Ethyl-2-methyl hexane	133.8	177.386	43.6472	42.98	330.3	25.56	21.77	
3-Ethyl-3-methyl hexane	140.6	173.077	43.268	44.04	327.2	25.66	23.22	
2,2,4-Trimethyl hexane	126.54	179.22	43.7638	40.57	301	23.39	20.51	– 120
2,2,5-Trimethyl hexane	124.084	181.346	43.9356	40.17	296.6	22.41	20.04	– 105.78
2,3,3-Trimethyl hexane	137.68	173.78	43.4347	42.23	326.1	25.56	22.41	– 116.8
2,3,4-Trimethyl hexane	139	173.498	43.4917	42.93	324.2	25.46	22.8	
2,3,5-Trimethyl hexane	131.34	177.656	43.6474	41.42	309.4	23.49	21.27	– 127.8
3,3,4-Trimethyl hexane	140.46	172.055	43.3407	42.28	330.6	26.45	23.27	– 101.2
3,3-Diethyl pentane	146.168	170.185	43.1134	43.36	342.8	26.94	23.75	– 33.11
2,2-Dimethyl-3-ethyl pentane	133.83	174.537	43.4571	42.02	322.6	25.96	22.38	– 99.2
2,3-Dimethyl-3-ethyl pentane	142	170.093	42.9542	42.55	338.6	26.94	23.87	
2,4-Dimethyl-3-ethyl pentane	136.73	173.804	43.4037	42.93	324.2	25.46	22.8	– 122.2
2,2,3,3-Tetramethyl pentane	140.274	169.495	43.2147	41	334.5	27.04	23.38	– 99
2,2,3,4-Tetramethyl pentane	133.016	173.557	43.4359	41	319.6	25.66	21.8	– 121.09
2,2,4,4-Tetramethyl pentane	122.284	178.256	43.8747	38.1	301.6	24.58	20.37	– 66.54
2,3,3,4-Tetramethyl pentane	141.551	169.928	43.2016	41.75	334.5	26.85	23.31	– 102.12

$$\mathrm{mp} = -142.0736 + [\mathrm{ND}_5(G)]2.2172$$

6. ND_6 index:

$$\mathrm{bp} = 35.3191 + [\mathrm{ND}_6(G)]0.5065$$
$$\mathrm{ct} = 187.4769 + [\mathrm{ND}_6(G)]0.6782$$
$$\mathrm{cp} = 30.8960 - [\mathrm{ND}_6(G)]0.0291$$
$$\mathrm{mv} = 127.7664 + [\mathrm{ND}_6(G)]0.2304$$
$$\mathrm{mr} = 28.1203 + [\mathrm{ND}_6(G)]0.0754$$
$$\mathrm{hv} = 29.6437 + [\mathrm{ND}_6(G)]0.0609$$
$$\mathrm{st} = 16.9413 + [\mathrm{ND}_6(G)]0.0266$$
$$\mathrm{mp} = -123.8778 + [\mathrm{ND}_6(G)]0.1045$$

The statistical parameters like previous discussion are used in Tables 11, 12, 13, 14, 15 and 16 to interpret the above regression models, where N denotes the total number of alkanes under consideration.

Several interesting observations on the data presented in Table 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15 and 16 can be made. From Table 3, the correlation coefficient of ND_1 index with entropy, acentric factor and DHVAP for octane isomers are found to be good (Fig. 1). Specially, it is strongly correlated with acentric factor having correlation coefficient $r = -0.9904$. Also, the correlation of this index is good for the physical properties of 67 alkanes except for cp and mp having correlation coefficient values -0.6941 and 0.2516, respectively. The range of correlation coefficient values lies from 0.7436 to 0.8981.

The QSPR analysis of ND_2 index reveals that this index is suitable to predict entropy, acentric factor and DHVAP of octane isomers (Fig. 2). In addition, one can say from Table 12 that, this index have remarkably good correlations with the physical properties of alkanes except mp. The correlation coefficients lies from 0.809 to 0.9638 except mp ($r = 0.2862$). Surprisingly, the correlation of ND_2 with hv is very high with correlation coefficient value 0.9638.

Table 13 shows that ND_3 index is inadequate for any structure property correlation in the case of alkanes having the correlation coefficient values from 0.2036 to 0.7318. But, from Table 5, we can see that ND_3 is well correlated with entropy and acentric factor with correlation coefficients -0.9387 and -0.9765 respectively.

The QSPR analysis of ND_4 index shows that this index is well correlated with entropy, acentric factor, DHVAP, and HVAP for octane isomers (Table 6). Table 14 shows that ND_4 index is inadequate for structure property correlation in case of alkanes except cp and hv having correlation coefficients -0.8634 and 0.8679, respectively.

Table 10 Topological indices for 67 alkanes

Alkanes	ND_1	ND_2	ND_3	ND_4	ND_5	ND_6
Butane	7.899	1.303	114	1.149	6.333	28
2-Methyl propane	9	1.225	16	2 1	6	36
Pentane	11.827	1.65	228	1.394	8.5	44
2-Methyl butane	13.757	1.518	344	1.181	8.667	60
2,2-Dimethyl propane	16	1.414	512	1	8	80
Hexane	15.827	2.004	356	1.644	10.5	60
2-Methyl pentane	17.723	1.89	498	1.467	10.65	76
3-Methyl pentane	18.474	1.837	576	1.412	11.367	84
2,2-Methyl butane	21.579	1.694	860	1.187	11.05	114
2,3-Dimethyl butane	20.492	1.73	730	1.233	11.067	102
Heptane	19.827	2.357	484	1.894	12.5	76
2-Methyl hexane	21.786	2.248	642	1.721	12.517	92
3-Methyl hexane	22.496	2.212	748	1.702	13.25	100
3-Ethyl pentane	23.182	2.173	864	1.673	14	108
2,2-Dimethyl pentane	25.586	2.082	1062	1.497	12.85	130
2,3-Dimethyl pentane	25.193	2.066	1020	1.492	13.733	126
2,4-Dimethyl pentane	23.654	2.144	816	1.563	12.667	108
3,3-Dimethyl pentane	31.129	2.381	1504	1.718	15.933	164
Octane	23.827	2.711	612	2.144	14.5	92
2-Methyl heptane	25.786	2.601	770	1.971	14.517	108
3-Methyl heptane	26.559	2.569	892	1.956	15.117	116
3-Methyl heptane	26.518	2.588	920	1.991	15.133	116
3-Ethyl hexane	24.451	2.658	682	2.097	15.483	106
2,2-Dimethyl hexane	29.706	2.443	1224	1.754	14.6	146
2,3-Dimethyl hexane	29.266	2.444	1212	1.784	15.533	142
2,4-Dimethyl hexane	28.478	2.469	1086	1.799	15.183	132
2,5-Dimethyl hexane	27.801	2.495	946	1.802	14.433	124
3,3-Dimethyl hexane	31.129	2.381	1504	1.718	15.933	164
3,4-Dimethyl hexane	29.94	2.404	1332	1.753	16.333	150
3-Ethyl-2-methyl pentane	29.902	2.415	1372	1.77	16.29	150
3-Ethyl-3-methyl pentane	32.526	2.301	1778	1.645	17.364	182
2,2,3-Trimethyl pentane	33.88	2.252	1832	1.527	16.107	192
2,3,3-Trimethyl pentane	34.627	2.214	1976	1.489	16.681	202
2,3,4-Trimethyl pentane	31.907	2.308	1530	1.589	16.057	168
Nonane	27.827	3.064	740	2.394	16.5	108
2-Methyl octane	29.786	2.955	898	2.221	16.517	124
3-Methyl octane	30.559	2.923	1020	2.206	17.117	132
4-Methyl octane	29.116	3.004	888	2.323	16.917	123
3-Ethyl heptane	31.318	2.909	1200	2.218	17.667	140
4-Ethyl heptane	30.292	2.985	1152	2.342	17.6	136
2,2-Dimethyl heptane	33.706	2.796	1352	2.004	16.6	162
2,3-Dimethyl heptane	33.329	2.802	1356	2.038	17.4	158
2,4-Dimethyl heptane	32.499	2.844	1258	2.089	17.067	148
2,5-Dimethyl heptane	32.574	2.817	1196	2.036	17.033	148

Table 10 continued

Alkanes	ND_1	ND_2	ND_3	ND_4	ND_5	ND_6
2,6-Dimethyl heptane	31.745	2.845	1056	2.049	16.533	140
3,3-Dimethyl heptane	35.25	2.742	1666	1.975	17.683	180
3,4-Dimethyl heptane	34.012	2.782	1524	2.045	18.133	166
3,5-Dimethyl heptane	34.179	2.768	1536	2.009	17.862	160
4,4-Dimethyl heptane	35.182	2.771	1728	2.029	17.667	180
3-Ethyl-2-methyl hexane	34.02	2.795	1586	2.063	18.017	166
4-Ethyl-2-methyl hexane	33.282	2.809	1416	2.063	17.667	156
3-Ethyl-3-methyl hexane	36.621	2.693	2026	1.958	19.04	198
2,2,4-Trimethyl hexane	36.422	2.672	1728	1.837	17.195	186
2,2,5-Trimethyl hexane	35.771	2.692	1548	1.837	16.433	178
2,2,4-Trimethyl pentane	31.552	2.346	1436	1.606	14.752	162
2,3,3-Trimethyl hexane	38.722	2.605	2224	1.802	18.357	218
2,3,4-Trimethyl hexane	36.695	2.647	1866	1.851	18.6	192
2,3,5-Trimethyl hexane	35.293	2.703	1572	1.883	17.4	174
3,3,4-Trimethyl hexane	39.364	2.563	2358	1.767	19.24	226
3,3-Diethyl pentane	37.947	2.621	2360	1.897	20.5	216
2,2-Dimethyl-3-ethyl pentane	38.596	2.609	2256	1.817	18.583	216
2,3-Dimethyl-3-ethyl pentane	40.044	2.533	2560	1.741	19.833	236
2,4-Dimethyl-3-ethyl pentane	36.626	2.666	1952	1.879	18.517	192
2,2,3,3-Tetramethyl pentane	44.158	2.395	3122	1.528	19.107	282
2,2,3,4-Tetramethyl pentane	40.595	2.502	2416	1.635	18.383	234
2,2,4,4-Tetramethyl pentane	39.482	2.555	2120	1.658	16.75	216
2,3,3,4-Tetramethyl pentane	42.141	2.445	2760	1.585	19.167	238

Table 11 Statical parameters of linear QSPR model for $ND_1(G)$

Physical properties	N	c	m	r	SE	F	SF
bp	67	− 8.8069	4.0114	0.8160	22.8878	129.5828	4.01E−17
ct	67	135.4475	5.1317	0.8981	20.2494	270.9371	7.17E−25
cp	67	34.6560	− 0.2721	− 0.6941	2.2736	60.4267	7.37E−11
mv	65	100.8619	2.0398	0.8233	10.1969	132.5481	3.86E−17
mr	65	20.1480	0.6398	0.8683	2.6501	193.0535	7.53E−21
hv	65	21.8703	0.5616	0.7436	3.6618	77.9195	1.29E−12
st	64	14.3557	0.2177	0.7782	1.2448	95.1879	3.83E−14
mp	52	− 131.654	0.7933	0.2516	26.4042	3.3806	0.07191

Table 12 Statical parameters of linear QSPR model for $ND_2(G)$

Physical properties	N	c	m	r	SE	F	SF
bp	67	− 95.9303	84.2834	0.9020	22.8878	129.5828	4.01E−17
ct	67	47.6081	98.1177	0.9033	20.2494	270.9371	7.17E−25
cp	67	43.8159	− 7.0529	− 0.9465	2.2737	60.4267	7.37E−11
mv	65	50.7515	45.1187	0.9415	10.1969	132.5481	3.86E−17
mr	65	6.7917	13.1956	0.9259	2.6501	193.0535	7.53E−21
hv	65	3.9821	14.0794	0.9638	3.6618	77.9195	1.29E−−12
st	64	9.6530	4.5432	0.8090	1.1652	117.4079	6.13E−16
mp	52	− 150.622	17.6077	0.2862	26.1414	4.4595	0.039726

Table 13 Statical parameters of linear QSPR model for ND$_3$(G)

Physical properties	N	c	m	r	SE	F	SF
bp	67	60.7738	0.0372	0.6238	30.9524	41.3958	1.71E−08
ct	67	220.3722	0.0508	0.7318	31.3747	74.9341	2E−12
cp	67	29.0689	−0.0019	−0.3904	2.9077	11.6902	0.00109
mv	65	140.8691	0.0159	0.5684	14.7809	30.0655	7.86E−07
mr	65	32.2248	0.0054	0.6418	4.0973	44.1193	8.37E−09
hv	65	32.9914	0.0043	0.5041	4.7298	21.4635	1.86E−05
st	64	18.2408	0.0020	0.6448	1.5151	44.1117	8.93E−09
mp	52	−118.9098	0.0078	0.2036	26.7107	2.1626	0.147672

Table 14 Statical parameters of linear QSPR model for ND$_4(G)$

Physical properties	N	c	m	r	SE	F	SF
bp	67	−69.6148	100.5729	0.7947	24.0365	111.4291	9.91E−16
ct	67	86.3449	112.5233	0.7649	29.6545	91.6399	4.91E−14
cp	67	42.1443	−8.7145	−0.8634	1.5934	190.369	5.52E−21
mv	65	75.6867	48.0647	0.7785	11.2749	96.942	2.29E−14
mr	65	14.6003	13.7704	0.7500	3.5339	80.9956	6.48E−13
hv	65	9.3610	16.3338	0.8679	2.7207	192.2597	8.3E−21
st	64	12.1161	4.8742	0.6760	1.4605	52.1868	8.8E−10
mp	52	−146.0101	21.4463	0.2525	26.3985	3.4038	0.070974

Table 15 Statical parameters of linear QSPR model for ND$_5(G)$

Physical properties	N	c	m	r	SE	F	SF
bp	67	−62.0831	11.0891	0.9166	15.8369	341.4188	1.44E−27
ct	67	73.9689	13.7538	0.9779	9.6226	1422.6559	6.55E−46
cp	67	38.1279	−0.7430	−0.7700	2.0151	94.6835	2.61E−14
mv	65	74.7263	5.5594	0.8881	8.2565	235.2645	6.02E−23
mr	65	12.0902	1.7348	0.9319	1.9378	415.896	1.91E−29
hv	65	11.8876	1.7079	0.8950	2.443	253.5998	9.12E−24
st	64	10.2382	0.6757	0.9267	0.7446	377.2765	4.73E−28
mp	52	−142.0736	2.2172	0.2790	26.4042	3.3806	0.07191

Table 16 Statistical parameters of linear QSPR model for ND$_6(G)$

Physical properties	N	c	m	r	SE	F	SF
bp	67	35.3191	0.5065	0.6791	29.0691	55.6291	2.67E−10
ct	67	187.4769	0.6782	0.7823	28.6755	102.5177	5.42E−15
cp	67	30.8960	−0.0291	−0.4892	2.7546	20.4495	2.66E−05
mv	65	127.7664	0.2304	0.6393	13.8148	43.5369	9.97E−09
mr	65	28.1203	0.0754	0.7033	3.7979	61.6774	6.44E−11
hv	65	29.6437	0.0609	0.5551	4.5554	28.0552	1.6E−06
st	64	16.9413	0.0266	0.6646	1.4811	49.0453	2.12E−09
mp	52	−123.8778	0.1045	0.2192	26.619	2.5225	0.118536

From Table 7, one can say that ND_5 does not sound so good except CP having correlation coefficient 0.8478. But this index can be considered as an useful tool to predict the physical properties of alkanes except cp and mp. This index is suitable to model bp, ct, mv, mr, hv, st with correlation coefficients 0.9166, 0.9779, 0.8881, 0.9319, 0.8950, and 0.9267, respectively.

The QSPR analysis of ND_6 index reveals that the correlation coefficient of this index with the physical properties of alkanes are very poor (Table 16). The range of correlation coefficient values lies from 0.2192 to 0.7823. But, when we look into the Table 8, we can say that this index has the ability to model entropy, acentric factor, and DHVAP for octane isomers.

Now we compare the modelling ability of the novel indices with some well-known and mostly used indices that include: First Zagreb index (M_1), second Zagreb index (M_2), Forgotten topological index (F), Sum connectivity index (SCI), Randić index (R), symmetric division deg index (SDD), Weiner index (W) [47], hyper Weiner index [37] (WW), terminal Wiener index (TW) [18], Schultz index (Sc) [41], first (S_1) and second status connectivity index (S_2) [34], Gutman index (GI) [16], degree distance index (DD) [6], inverse sum indeg status (ISIS) index [7], total eccentricity connectivity index (TECI) [1], first Zagreb eccentricity connectivity Index (ZECI_1) [13], first (ξ_1) and second eccentricity connectivity index (ξ_2) [29,46], connective eccentricity index (CEI) [29,46], vertex adjacency energy (E) [17], Laplacian energy (LE) [21], atom bond connectivity index (ABC) [8], augmented Zagreb index (AZI) [11], geometric arithmetic index (GA) [45], harmonic index (H) [9], Ashwini Index (A) [33], SM-index (SM) [42], vertex Zagreb energy ($Z_1 E$) [26], forgotten energy (FE) [26], harmonic energy (HE) [26], geometric-arithmetic energy (GAE) [40], degree-sum energy (DSE) [35], sum-connectivity energy (SCE) [48], and Randić energy (RE) [3]. From Tables 3, 4, 5, 6, 7 to 8, it is clear that among six new indices, the ND_1 index can model acentric factor of octane isomers with excellent accuracy. To investigate the predictability of different well-established descriptors for acentric factor of octanes, linear regression analysis is performed and the outcomes are reported in Tables 17, 18, 19 and 20. From those findings, several observations can be made. The modulus of the correlation coefficient and the F value of ND_1 index is significantly high compared to the existing indices listed in Tables 17, table:comp2, table:comp3 and 20. The standard error and the SF value of the ND_1 index is lower than that of the indices reported in Tables 17, 18, 19 and 20. Thus, it can be concluded that the ND_1 index is efficient in predicting acentric factor of octanes with high accuracy compared to several well-known and mostly utilised molecular descriptors.

Now we are going to compare the new descriptors with the existing descriptors in structure-property modelling for 67 alkanes. Statistical parameters of linear regression models of different degree based indices, distance based indices and spectral indices are reported in [24,26,42]. We listed the correlation coefficients of those models in Tables 21, 22 and 23 for critical temperature (ct), critical pressure (cp) and surface tension (st). Form Tables 11, 12, 13, 14, 15 16, 21, 22, 23, one can draw the following observations. Among all the newly proposed indices and the already existing indices listed in Tables 21, 22 and 23, the ND_5 index has remarkable correlation with ct and st, whereas for cp, the ND_2 index sounds the best. The rest parameters [24,26,42] are also in favour of ND_2 and ND_5 indices. Therefore, we can conclude that ND_2 and ND_5 indices outperform several well-established and mostly utilised descriptors in modelling cp, ct, and st for alkanes.

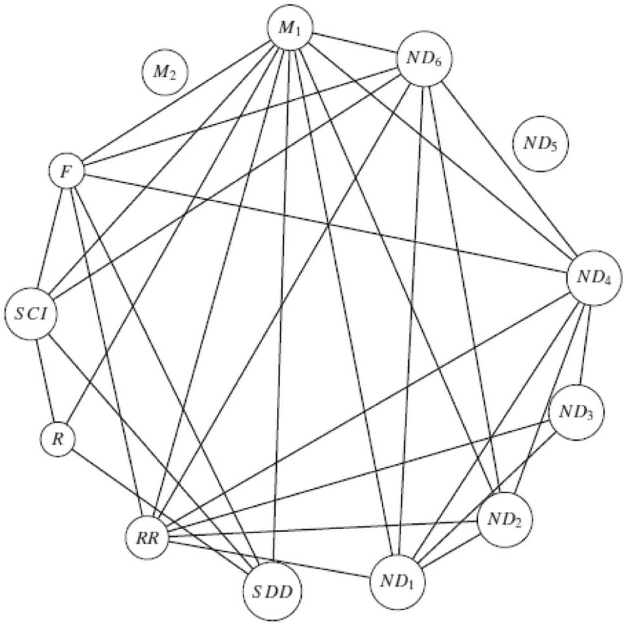


Fig. 7 Correlation graph of novel indices with some well-known indices for decane isomer

Correlation with some well-known indices

In this section, we investigate the correlation between the new indices and some well-known indices for octane isomers. It is clear from Table 24, that the new indices have a high correlation with the well-established indices except ND_5 index. Highest correlation coefficient ($r = 0.9977$) is between ND_1 and M_2. From Table 25, one can say that ND_5 has significantly low correlation coefficient with other indices. So we can conclude that ND_5 is independent among five indices. A correlation graph (Fig. 7) is drawn considering indices as vertices and two vertices are adjacent if and only if $|r| \geq 0.95$.

Table 17 Statical parameters of linear QSPR model of acentric factor for some degree based indices

Topological indices	*c*	*m*	*r*	SE	*F*	SF
M_1	0.6996	−0.0118	0.9731	0.0084	285.064	1.28E−11
M_2	0.6076	−0.0088	−0.9864	0.006	577.1626	5.57E−14
F	0.4701	−0.0016	0.965	0.0096	216.9488	1E−10
SCI	−0.4	0.2165	0.9299	0.0134	102.2326	2.36E−08
R	−0.3694	0.1934	0.9042	0.0156	71.7338	2.62E−07
SDD	0.5346	−0.0101	0.901	0.0158	69.0429	3.38E−07

Table 18 Statical parameters of linear QSPR model of acentric factor for some distance based indices

Topological indices	*c*	*m*	*r*	SE	*F*	SF
W	−0.032	0.0053	0.9656	0.0095	220.4186	8.91E−11
WW	0.1666	0.0012	0.9458	0.0119	135.5882	3.18E−09
TW	0.4257	−0.0041	0.897	0.0162	65.928	4.57E−07
Sc	−0.0308	0.0014	0.9514	0.0112	152.6589	1.35E−09
S_1	0.06608	0.0012	0.8866	0.0169	58.7816	9.58E−07
S_2	0.2104	7.02E−05	0.8808	0.0173	55.3582	1.4E−06
GI	0.2151	0.0007	0.6826	0.0267	13.9565	0.0018
DD	0.1441	0.0008	0.6906	0.0264	14.5858	0.0015
$ISIS$	0.0638	0.005	0.9669	0.0093	230.3191	6.41E−11

Table 19 Statical parameters of linear QSPR model of acentric factor for some eccentricity based indices

Topological indices	*c*	*m*	*r*	SE	*F*	SF
TECI	0.1453	0.006	0.9392	0.0125	119.8089	7.7E−09
ZECI$_1$	0.2433	0.0007	0.9216	0.0142	90.2098	5.6E−08
ξ_1	0.167	0.0033	0.9357	0.0129	112.5135	1.2E−08
ξ_2	0.2554	0.0008	0.9149	0.0147	82.1992	1.05E−07
CEI	0.4997	−0.0398	0.9492	0.0115	145.6681	1.89E−09

Table 20 Statical parameters of linear QSPR model of acentric factor for some graph energies

Graph energies	*c*	*m*	*r*	SE	*F*	SF
E	−0.0059	0.03956	0.7163	0.0255	16.8571	0.0008
LE	0.9693	−0.0576	0.9124	0.0149	79.5214	1.32E−07

Table 21 Correlation coefficients of some degree based indices with different physical properties for 67 alkanes

Physical properties	M_1	M_2	*F*	*R*	ABC	AZI	GA	*H*	SCI
ct	0.856	0.898	0.704	0.962	0.850	0.85	0.964	0.908	0.963
cp	0.686	0.688	0.486	0.911	0.743	0.718	0.913	0.878	0.920
st	0.329	0.777	0.595	0.909	0.7	0.834	0.9	0.847	0.901

Table 22 Correlation coefficients of some distance based indices with different physical properties for 67 alkanes

Physical properties	*W*	TW	WW	DD	GI	*A*	SM
ct	0.899	0.620	0.809	0.809	0.807	0.459	0.326
cp	0.899	0.475	0.636	0.890	0.889	0.381	0.288
st	0.815	0.481	0.555	0.716	0.711	0.320	0.198

Table 23 Correlation coefficients of some graph energies with different physical properties for 67 alkanes

Physical properties	E	Z_1E	FE	HE	GAE	DSE	LE	SCE	RE
ct	0.936	0.855	0.525	0.808	0.833	0.638	0.935	0.883	0.749
cp	0.006	0.030	0.024	0.018	0.020	0.045	0.014	0.025	0.035
st	0.871	0.727	0.369	0.804	0.767	0.540	0.834	0.847	0.667

Table 24 Correlation with some well-known indices

	M_1	M_2	F	SCI	R	RR	SDD
ND_1	− 0.86958	− 0.8295	0.995406	0.817435	0.946941	0.741367	0.937806
ND_2	0.892937	0.857255	− 0.99282	− 0.83834	− 0.95286	− 0.71895	− 0.93683
ND_3	− 0.75331	− 0.70235	0.953983	0.691599	0.865993	0.746587	0.861531
ND_4	0.955051	0.933136	− 0.97643	− 0.9137	− 0.97717	− 0.6806	− 0.95874
ND_5	− 0.29763	− 0.22396	0.665973	0.198425	0.471285	0.56989	0.461035
ND_6	− 0.89201	− 0.85372	0.994895	0.848793	0.964237	0.739059	0.959608

Table 25 Correlation among new indices

	ND_1	ND_2	ND_3	ND_4	ND_5	ND_6
ND_1	1					
ND_2	− 0.98906	1				
ND_3	0.976497	− 0.94568	1			
ND_4	− 0.95818	0.980133	− 0.87983	1		
ND_5	0.719609	− 0.68604	0.825766	− 0.54476	1	
ND_6	0.992599	− 0.97954	0.962921	−0.95487	0.675576	1

Degeneracy

The objective of a topological index is to encipher the structural property as much as possible. Different structural formulae should be distinguished by a good topological descriptor. A major drawback of most topological indices is their degeneracy, i.e., two or more isomers possess the same topological index. Topological indices having high discriminating power captures more structural information. We use the measure of degeneracy known as sensitivity introduced by Konstantinova [28], which is defined as follows:

$$S_I = \frac{N - N_I}{N},$$

where N is the total number of isomers considered and N_I is the number of them that cannot be distinguished by the topological index I. As S_I increases, the isomer-discrimination power of topological indices increases. The vertex degree-based topological indices have more discriminating power in comparison with other classes of molecular descriptors. For octane and decane isomers, the newly introduced indices exhibit better response compared to some well-known degree-based indices (Table 26).

Table 26 Measure of sensitivity (S_I) of different indices for octane and decane isomers

Topological indices	Sensityvity (S_I)	
	Octane	Decane
ND_1	**1.000**	**1.000**
ND_2	**1.000**	**1.000**
ND_3	**1.000**	**0.96**
ND_4	**1.000**	**0.987**
ND_5	**1.000**	**0.92**
ND_6	**0.833**	**0.613**
R	0.889	0.667
RR	0.889	0.653
SCI	0.889	0.64
SDD	0.889	0.547
M_2	0.722	0.28
F	0.389	0.133
M_1	0.333	0.107

Sensitivity of the newly proposed descriptors are made bold to highlight the supremacy of the newly introduced indices in comparison to the already existing well-established indices

Applications

QSPR analysis is a powerful investigation for breaking down a molecule into a series of numerical values describing its relevant physico-chemical properties and biological activities. Descriptors having the strongest correlation in this study give information about essential functional groups of compounds under consideration. Accordingly, we can regulate pharmacological action or physico-chemical properties of drugs by modifying certain groups in the structure of medications. It is usually very costly to test a compound using a wet lab, but the QSPR study allow that cost to be reduced. This is generally used to analyze biological activities with specific properties associated with the structures and is helpful in understanding how molecular attributes in a drug effect biological activities. QSPR approaches can be used to develop models which can predict properties or activities of organic chemical. An efficient way of encoding structures with determined topological index is, therefore, necessary for the construction of accurate models. The indices used for the creation of model can offer a chance to concentrate on particular characteristics that account for the activity or property of interest in the compounds. QSPR analysis of some newly designed indices using octane isomers and alkanes is performed in this work. It has been shown that these indices can be considered as useful molecular descriptors in QSPR research. They yield excellent correlation with S, Acent Fac, HVAP, DHVAP, CP for octane isomers and bp, ct, cp, mv, mr,hv, st, mp for alkanes. Their isomer discrimination ability is also remarkable for octane and decane isomers. These indices are an extension of some well-known degree-based topological indices namely R, SCI, SDD, and ReZG_3. Sometimes the predictive power of these indices is superior, sometimes little bit inferior than that of the old indices. But the degeneracy test on Table 26, assures the supremacy of newly designed indices in comparison to the old indices. It is worth discussing the mathematical properties of the novel descriptors discussed in the following section.

Mathematical properties

In this section, we discuss about some bounds of the newly proposed indices with some well-known indices. Throughout this section, we consider simple connected graph. We construct this section with some standard inequalities. We start with the following inequality.

Lemma 1 (Radon's inequality) *If $x_i, y_i > 0$, $i = 1, 2, \dots, n$, $t > 0$, then*

$$\frac{\sum_{i=1}^{n} x_i^{t+1}}{\sum_{i=1}^{n} y_i^{t}} \geq \frac{\left(\sum_{i=1}^{n} x_i\right)^{t+1}}{\left(\sum_{i=1}^{n} y_i\right)^{t}}, \tag{2}$$

where equality holds iff $x_i = k y_i$ for some constant k, $\forall i = 1, 2, \dots, n$.

Proposition 1 *For a graph G having m edges with neighborhood version of second Zagreb index $M_2^*(G)$ [31], we have*

$$\text{ND}_1(G) \leq \sqrt{m M_2^*(G)}, \tag{3}$$

where equality holds iff G is regular or complete bipartite graph.

Proof For a graph G, $M_2^*(G) = \sum_{uv \in E(G)} \delta_G(u)\delta_G(v)$. Now considering $x_i = 1$, $y_i = \delta_G(u)\delta_G(v)$, $t = \frac{1}{2}$, in (2), we obtain

$$\frac{\sum_{uv \in E(G)} 1}{\sum_{uv \in E(G)} (\delta_G(u)\delta_G(v))^{\frac{1}{2}}} \geq \frac{\left(\sum_{uv \in E(G)} 1\right)^{\frac{3}{2}}}{\left(\sum_{uv \in E(G)} \delta_G(u)\delta_G(v)\right)^{\frac{1}{2}}}. \tag{4}$$

Now using the definition of ND_1 and M_2^* indices, we can easily obtain the required bound (3). Equality in (4) holds iff $\delta_G(u)\delta_G(v) = k$, a constant $\forall uv \in E(G)$. So the equality in (3) holds iff G is regular or complete bipartite graph.

Lemma 2 *Let $\mathbf{x} = (x_1, x_2, \dots, x_n)$ and $\mathbf{y} = (y_1, y_2, \dots, y_n)$ be sequence of real numbers. Also let $\mathbf{z} = (z_1, z_2, \dots, z_n)$ and $\mathbf{w} = (w_1, w_2, \dots, w_n)$ be non-negative sequences. Then*

$$\sum_{i=1}^{n} w_i \sum_{i=1}^{n} Z_i x_i^2 + \sum_{i=1}^{n} z_i \sum_{i=1}^{n} w_i y_i^2 \geq 2 \sum_{i=1}^{n} z_i x_i \sum_{i=1}^{n} w_i y_i, \tag{5}$$

In particular, if z_i and w_i are positive, then the equality holds iff $\mathbf{x} = \mathbf{y} = \mathbf{k}$, where $\mathbf{k} = (k, k, \dots, k)$, a constant sequence.

Proposition 2 *For a graph G having m edges with neighbourhood version of second Zagreb index $M_2^*(G)$, we have*

$$\text{ND}_1(G) \leq \frac{(m + M_2^*(G))}{2}, \tag{6}$$

where equality holds iff G is P_2.

Proof Considering $x_i = \delta_G(u)\delta_G(v)$, $y_i = 1$, $z_i = 1$, $w_i = 1$, in (5), we get

$$\sum_{uv \in E(G)} 1 \sum_{uv \in E(G)} \delta_G(u)\delta_G(v) + \sum_{uv \in E(G)} 1 \sum_{uv \in E(G)} 1 \geq 2 \sum_{uv \in E(G)} \sqrt{\delta_G(u)\delta_G(v)} \sum_{uv \in E(G)} 1.$$

After using the definition of ND_1 and M_2^* indices we can obtain

$$m M_2^*(G) + m^2 \geq 2m\text{ND}_1(G).$$

After simplification, the required bound is obvious.

From Lemma 2, the equality in (6) holds iff $\delta_G(u)\delta_G(v) = 1 \forall uv \in E(G)$,i.e. G is P_2.

Remark By arithmetic mean $\geq$ geometric mean, we can write

$$\frac{(m + M_2^*(G))}{2} \geq \sqrt{mM_2^*(G)}.$$

So the upper bound of $\mathrm{ND}_1(G)$ obtained in Proposition 1, is better than that obtained in Proposition 2.

Proposition 3 *For a graph G having second Zagreb index $M_2(G)$, forgotten topological index $F(G)$, neighbourhood version of hyper Zagreb index $HM_N(G)$ [31], neighbourhood Zagreb index $M_N(G)$ [30], we have*

$$\mathrm{ND}_6(G) \leq \frac{F(G)}{2} + M_2(G) + \frac{HM_N(G)}{2} - M_N(G), \quad (7)$$

equality holds iff G is P_2.

Proof For a graph G, we have $M_N(G) = \sum_{v\in V(G)} \delta_G(v)^2 = \sum_{uv\in E(G)}[\delta_G(u)d_G(v) + \delta_G(v)d_G(u)]$, $HM_N(G) = \sum_{uv\in E(G)}[\delta_G(u) + \delta_G(v)]^2$. We know that for any two non-negative numbers x, y, arithmetic mean $\geq$ geometric mean, i.e., $\frac{x+y}{2} \geq \sqrt{xy}$, equality holds iff $x = y$. Now considering $x = d_G(u) + d_G(v)$, $y = \delta_G(u) + \delta_G(v)$, we get

$$\frac{[d_G(u) + d_G(v) + \delta_G(u) + \delta_G(v)]}{2} \geq \sqrt{(d_G(u) + d_G(v))(\delta_G(u) + \delta_G(v))},$$

squiring both sides, we have

$$4(d_G(u) + d_G(v))(\delta_G(u) + \delta_G(v)) \leq [d_G(u) + d_G(v) + \delta_G(u) + \delta_G(v)]^2,$$

which gives

$$2 \sum_{uv\in E(G)} [(d_G(u)\delta_G(u) + d_G(v)\delta_G(v))(d_G(u)\delta_G(v) + d_G(v)\delta_G(u))] \leq \sum_{uv\in E(G)} [d_G(u)^2 + d_G(v)^2] + 2 \sum_{uv\in E(G)} d_G(u)d_G(v) + \sum_{uv\in E(G)} [\delta_G(u)^2 + \delta_G(v)^2] + 2 \sum_{uv\in E(G)} \delta_G(u)\delta_G(v).$$

After simplifying and using the formulation of ND_6, F, M_2, HM_N, and M_N indices, the required bound is clear. The equality in (7) occurs iff $d_G(u) + d_G(v) = \delta_G(u) + \delta_G(v)$, i.e., G is P_2. Hence the proof. □

For a graph G consider

$$\Delta_N = \max\{\delta_G(v) : v \in V(G)\},$$
$$\delta_N = \min\{\delta_G(v) : v \in V(G)\}.$$

Thus $\delta_N \leq \delta_G(u) \leq \Delta_N$ for all $u \in V(G)$. Equality holds iff G is regular or complete bipartite graph. Clearly we have the following proposition.

Proposition 4 *For a graph G with m number of edges, we have the following bounds.*

(i) $m\delta_N \leq \mathrm{ND}_1(G) \leq m\Delta_N$,
(ii) $\frac{m}{\sqrt{2\Delta_N}} \leq \mathrm{ND}_2(G) \leq \frac{m}{\sqrt{2\delta_N}}$,
(iii) $2m\delta_N^3 \leq \mathrm{ND}_3(G) \leq 2m\Delta_N^3$,
(iv) $\frac{m}{\Delta_N} \leq \mathrm{ND}_4(G) \leq \frac{m}{\delta_N}$,
(v) $\frac{F_N^*(G)-2M_2^*(G)}{\delta_N^2} + 2m \leq \frac{F_N^*(G)-2M_2^*(G)}{\Delta_N^2} + 2m$,

where [31] $F_N^*(G) = \sum_{uv\in E(G)}[d_G(u)^2 + d_G(v)^2]$.

Equality holds in each case iff G is regular or complete bipartite graph.

Lemma 3 *Let a_i and b_i be two sequences of real numbers with $a_i \neq 0\,(i = 1, 2, \ldots, n)$ and such that $pa_i \leq b_i \leq Pa_i$. Then*

$$\sum_{i=1}^{n} b_i^2 + pP\sum_{i=1}^{n} a_i^2 \leq (P + p)\sum_{i=1}^{n} a_ib_i. \quad (8)$$

Equality holds iff either $b_i = pa_i$ or $b_i = Pa_i$ for every $i = 1, 2, \ldots, n$.

Proposition 5 *For a graph G with m edges having neighbourhood version of second Zagreb index $M_2^*(G)$, we have*

$$\mathrm{ND}_1(G) \geq \frac{M_2^*(G) + m\delta_N\Delta_N}{\delta_N + \Delta_N}$$

Equality holds iff G is regular or complete bipartite graph.

Proof Putting $a_i = 1$, $b_i = \sqrt{\delta_G(u)\delta_G(v)}$, $p = \delta_N$, $P = \Delta_N$ in 8, we get

$$\sum_{uv\in E(G)} \delta_G(u)\delta_G(v) + \delta_N\Delta_N \sum_{uv\in E(G)} 1 \leq (\delta_N + \Delta_N) \sum_{uv\in E(G)} \sqrt{\delta_G(u)\delta_G(v)}.$$

Now applying the definition of $M_2^*(G)$, $\mathrm{ND}_1(G)$ in the above inequation, we obtain

$$M_2^*(G) + m\delta_N\Delta_N \leq (\delta_N + \Delta_N)\mathrm{ND}_1(G).$$

Which implies

$$\mathrm{ND}_1(G) \geq \frac{M_2^*(G) + m\delta_N\Delta_N}{\delta_N + \Delta_N}.$$

Equality holds iff $\sqrt{\delta_G(u)\delta_G(v)} = \delta_N$ or $\sqrt{\delta_G(u)\delta_G(v)} = \Delta_N$ for all $uv \in E(G)$, i.e. G is regular or complete bipartite graph. Hence the proof. □

Proposition 6 *For a graph G of size m with fifth version of geometric arithmetic index GA_5, and second Zagreb index $M_2(G)$, we have*

(i) $\mathrm{ND}_5(G) \geq \frac{2m^2}{GA_5}$,
(ii) $\mathrm{ND}_5(G) \geq \frac{4M_2(G)^2}{m\Delta_N^2} - 2m.$

Equality in both cases hold iff G is regular or complete bipartite graph.

Proof (i) For a graph G, we know that [14] $GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}$. Now by Cauchy–Schwarz inequality, we have

$$\left(\sum_{uv\in E(G)} 1\right)^2 = \left(\sum_{uv\in E(G)} \sqrt{\frac{\delta_G(u)+\delta_G(v)}{\sqrt{\delta_G(u)\delta_G(v)}}} \times \frac{1}{\sqrt{\frac{\delta_G(u)+\delta_G(v)}{\sqrt{\delta_G(u)\delta_G(v)}}}}\right)^2 \leq \sum_{uv\in E(G)} \frac{\delta_G(u)+\delta_G(v)}{\sqrt{\delta_G(u)\delta_G(v)}} \sum_{uv\in E(G)} \frac{\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}.$$

Thus,

$$2m^2 \leq GA_5(G) \sum_{uv\in E(G)} \frac{\delta_G(u)+\delta_G(v)}{\sqrt{\delta_G(u)\delta_G(v)}}. \tag{9}$$

We know that

$$\frac{\delta_G(u)}{\delta_G(v)} + \frac{\delta_G(v)}{\delta_G(u)} \geq \sqrt{\frac{\delta_G(u)}{\delta_G(v)}} + \sqrt{\frac{\delta_G(v)}{\delta_G(u)}}.$$

From 9, we obtain $2m^2 \leq GA_5(G)\mathrm{ND}_5(G)$, i.e.

$$\mathrm{ND}_5(G) \geq \frac{2m^2}{GA_5}.$$

Equality holds iff $\frac{\delta_G(u)+\delta_G(v)}{\sqrt{\delta_G(u)\delta_G(v)}} = k$, a constant $\forall uv \in E(G)$. That is, $\delta_G(u) =$ some constant $\times\ \delta_G(v)\ \forall uv \in E(G)$, i.e., G is regular or complete bipartite graph.

(ii) By Cauchy–Schwarz inequality, we have

$$\begin{aligned}\mathrm{ND}_5(G) &= \sum_{uv\in E(G)} \frac{[\delta_G(u)+\delta_G(v)]^2}{\delta_G(u)\delta_G(v)} - 2m \\ &\geq \frac{1}{\Delta_N^2} \sum_{uv\in E(G)} [\delta_G(u)+\delta_G(v)]^2 - 2m \\ &= \frac{1}{m\Delta_N^2} \sum_{uv\in E(G)} 1^2 \sum_{uv\in E(G)} [\delta_G(u)+\delta_G(v)]^2 - 2m \\ &\geq \frac{1}{m\Delta_N^2}[\sum_{uv\in E(G)} (\delta_G(u)+\delta_G(v))]^2 - 2m \\ &= \frac{4M_2(G)^2}{m\Delta_N^2} - 2m.\end{aligned}$$

Equality holds iff $\delta_G(u) = \Delta_N = \delta_G(v)$ and $\delta_G(u) + \delta_G(v) = c$, a constant occur simultaneously for all $uv \in E(G)$. That is, G is regular or complete bipartite graph.

Hence the proof □

It is obvious that, $\delta_G(u) \geq d_G(u)$ and $\delta_G(v) \geq d_G(v), \forall uv \in E(G)$. Equality appears for P_2 only. Keeping in mind this fact, we have the following proposition.

Proposition 7 *For a graph G, having Randic index $R(G)$, second Zagreb index $M_2(G)$, reciprocal Randic index $\mathrm{RR}(G)$, sum-connectivity index $\mathrm{SCI}(G)$, we have*

(i) $\mathrm{ND}_1(G) \geq \mathrm{RR}(G)$
(ii) $\mathrm{ND}_2(G) \geq \mathrm{SCI}(G)$
(ii) $\mathrm{ND}_3(G) \geq \mathrm{ReZG}_3(G)$
(iii) $\mathrm{ND}_4(G) \geq R(G)$
(iv) $\mathrm{ND}_5(G) \leq 2M_2(G)$
(v) $\mathrm{ND}_6(G) \leq 2M_2(G)$

Equality holds in each case iff G is P_2.

Conclusion

In this article, we have proposed some novel topological indices based on neighborhood degree sum of end vertices of edges. Their predictive ability have tested using octane isomers and alkanes from n-butanes to nonanes. These indices have demonstrated as useful molecular descriptors in QSPR study. These indices are an extension of some well established indices based on degree. The correlations between these new indices and the different properties and activities are often stronger, sometimes slightly weaker than the old indices. For octane isomers, the ND_1 index can model acentric factor with high precision compared to the existing indices under consideration. For alkanes, the ND_5 index is more effective in predicting *ct* and *st* compared to other well-known indices. The predictability of ND_2 index is remarkable for *cp* compared to the existing and often used topological indices. The sensitivity test (Table 26) confirms the supremacy of the novel indices compared to the old indices. We have also correlated these indices with other degree-based topological indices. This investigation on Tables 24, 25 concludes that ND_5 index is independent among all novel indices. This work ends with computing some bounds of these novel indices. For further research, these indices can be computed for various graph operations and some composite graphs and networks.

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