MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **92** (2024) 165–203
ISSN: 0340–6253
doi: 10.46793/match.92-1.165K

On Structure Sensitivity and Chemical Applicability of Some Novel Degree-Based Topological Indices

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(Received October 8, 2023)

Abstract

Numerous quantitative graph invariant-based topological indices have been developed in the literature and employed for correlation analysis in chemical graph theory. Among them, the degree-based topological indices are the most investigated molecular descriptors and have proven their usability in this area. Here, we focus on testing the structural properties and prediction potential of some novel degree-based topological indices. At the outset, computer testing for the considered topological indices is performed to calibrate their structure sensitivity and abruptness. After that, the correlation among the topological indices is also executed. In addition, QSPR analysis is performed for the octane isomers molecular database to investigate the physical and chemical significance of the considered topological indices.

1 Introduction

Let $G = (V(G), E(G))$ be an ordered pair that denotes a simple, connected and undirected graph where $V(G)$ and $E(G)$ represent the non-empty vertex set and edge set of the graph G, respectively. For a vertex $u \in V(G)$,

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the *degree* $d_G(u)$ is the total number of edges incident to vertex u [1]. An edge joining two distinct vertices u and v that belong to the set $E(G)$ is represented as $e = uv$ or vu.

Chemical graph theory (CGT) is a significant branch of mathematical chemistry that employs graph theory and chemistry. CGT constitutes the mathematical models (known as QSPR[†] and QSAR[‡]) to predict the physico-chemical properties and biological activities of the chemical networks/compounds. *Topological indices/descriptors* are numeric quantities obtained from the molecular graph of a chemical structure and perform the imperative character in the development of QSPR and QSAR studies [2]. These descriptors are availed significantly to study the topology of an underlying graph in various fields of network science and mathematical chemistry. Mathematically, a topological index TI is the function $TI : \Omega \to \mathbb{R}$ such that $TI(G_1) = TI(G_2)$ for every pair of two isomorphic graphs G_1 and G_2 where Ω is the set of all simple, connected and undirected graphs with n vertices and $\mathbb{R}$ is the set of real numbers.

The first most theoretically studied topological index from an application point of view is the *Wiener index* which was proposed by H. Wiener in 1947 [3]. It is a distance-based topological index which is defined as the sum of the distances between all pairs of vertices of a graph and has applicability to predict the boiling points of paraffin. Later, several other distance-based topological indices such as hyper-Wiener [4], Szeged [5] and Mostar [6] indices were proposed and have extended this class.

Another important class of topological index is the degree-based topological index. These indices are one of the most employable topological descriptors in QSPR/QSAR studies. In general terms, a degree-based topological index [7] is defined as

$$TI(G) = \sum_{uv \in E(G)} f(d_G(u), d_G(v)), \tag{1}$$

where function $f(x, y) \geq 0$ with symmetric property $f(x, y) = f(y, x)$.

Now, we discuss some well-known degree-based topological indices in

[†]Quantitative structure-property relationship
[‡]Quantitative structure-activity relationship

detail. In 1972, I. Gutman and N. Trinajstić proposed one of the oldest degree-based topological indices, namely the Zagreb indices. The *first Zagreb index* is the sum of degrees of all the vertices of a graph, that is

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

whereas the *second Zagreb index* is mathematically expressed as

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

Gutman and Trinajstić investigated the expressions associated with the first and second Zagreb indices while working on the total π-electron energy of the conjugated system [8]. The *second modified Zagreb index* (${}^mM_2$) was proposed by Miličević et al. in 2004 [9]. The function associated with the ${}^mM_2$ index is reversed to the second Zagreb index. It is defined as

$${}^mM_2(G) = \sum_{uv \in E(G)} \frac{1}{d_G(u) d_G(v)}.$$

The elements in the contribution of the Zagreb indices (M_1 and M_2) prioritize the internal (interior) vertices and edges based on their weights in comparison to the terminal (outer) edges and vertices of the graph. However, the ${}^mM_2$ index reports higher weights to outer vertices and edges than to internal edges and vertices of the molecular graph [9]. The same article reported the forgotten index [7] as the cubic sum of the degrees of all the vertices of the graph. But, it was not noticed for almost 40 years. In the year 2015, B. Furtula and I. Gutman reconsidered the *forgotten index* [10] and proposed it as

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

Milan Randić proposed the branch connectivity index in 1975 to estimate the degree of branching in the carbon-atom skeleton of saturated hydrocarbons [11]. It was named the *Randić index* or *branching/connectivity*

index and defined as

$$R_{-1/2}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) d_G(v)}}.$$

The $R_{-1/2}$ index has countless applications in drug design and discovery perspective. The reciprocal (or inverse) Randić index ($RR_{-1/2}$) first appeared in the paper [12], where the relation between maximum eigenvalue of the graph and $RR_{-1/2}$ was shown. It disappeared from the attention of chemists and mathematicians for almost 20 years. Later, Gutman et al. proposed the *reciprocal* (or *inverse*) *Randić index* in 2014 [13], and it is mathematically formulated as

$$RR_{-1/2}(G) = \sum_{uv \in E(G)} \sqrt{d_G(u) d_G(v)}.$$

It is a special case for $\alpha = 1/2$ of the very famous *general Randić index* $\sum_{uv \in E(G)} (d_G(u) d_G(v))^{\alpha}$, where $\alpha \in \mathbb{R}$ (see [14, 15]). Being motivated by the advancement and applicability of the Randić index in various areas of science and technology, B. Zhou and N. Trinajstić proposed the *sum-connectivity index* (*SCI*) in 2009 [16]. It is defined as

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

Several research articles on mathematical properties and chemical applicability of *SCI* index are reported in the literature [16, 17].

Among 148 discrete Adriatic indices, the *symmetric division deg index* (*SDD*) is one of the most important bond-additive descriptor [18]. It was commenced by D. Vukičević in 2010 and defined as

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

The *SDD* index has proved to be a good predictor of the total surface area of polychlorobiphenyls (PCB) [18]. It has shown a dominating nature over several other degree-based topological indices in the QSPR study [19].

Favron et al. introduced the *harmonic index* in 1993 [12], and it is defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_G(u) + d_G(v)}.$$

Some relations of the harmonic index with the eigenvalues of a graph were reported in the article [12]. Generalization of the harmonic index and some associated mathematical results were discussed in [20, 21].

In the year 2010, D. Vukičević proposed the *inverse sum* (*indeg*) *index* (*ISI*) in the same article where the *SDD* index was introduced [18]. The *ISI* index is mathematically described as

$$ISI(G) = \sum_{uv \in E(G)} \frac{d_G(u) d_G(v)}{d_G(u) + d_G(v)}.$$

It is a bond-additive descriptor that belongs to the class of the Adriatic indices and predicts the total surface area of octane isomers [18].

A graph theoretical descriptor based on the connectivity between atoms and bounds of the molecule was introduced by Estrada et al. in 1998 [22] and named the *atom-bond connectivity index*. It is defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u) d_G(v)}}.$$

The ABC index has performed good correlation with the enthalpy of formations of alkanes [22].

The *augmented Zagreb index* (AZI) was put forward by Furtula et al. in 2010 [23] while investigating the applicability of the generalized atom-bond connectivity index. The AZI index is defined as

$$AZI(G) = \sum_{uv \in E(G)} \Big(\frac{d_G(u) d_G(v)}{d_G(u) + d_G(v) - 2} \Big)^3.$$

It was claimed in this article that the AZI index demonstrates a good correlation with the heat of formation of octane [23, 24].

The hyper-Zagreb indices are a generalization of the Zagreb indices.

The definition of the *first hyper-Zagreb index* [25] is expressed as

$$HM_1(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))^2$$

and the *second hyper-Zagreb index* [26] is mathematically formulated as

$$HM_2(G) = \sum_{uv \in E(G)} (d_G(u) d_G(v))^2.$$

In the year 2009, D. Vukičević and B. Furtula introduced a novel topological index based on the geometric and arithmetic means of the end-vertex degrees of an edge [27]. They named it as *geometric-arithmetic index* (GA) and defined it as

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_G(u) d_G(v)}}{d_G(u) + d_G(v)}.$$

The QSPR analysis of the GA index with the physico-chemical properties of octane isomers was performed in the article [27] to assess the usability of the index.

Being inspired by the competency of the geometric-arithmetic index, an alternate form of the GA index by reciprocating its numerator and denominator was proposed by Shegehalli and Kanabur in 2015 [28]. They called it the *arithmetic-geometric index* (AG) and described it as

$$AG(G) = \sum_{uv \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u) d_G(v)}}.$$

I. Gutman recently introduced the *Sombor index* [29] to provide a geometrical approach to degree-based topological indices, and mathematically defined it as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}.$$

The function corresponding to the Sombor index is the distance of the $(d_G(u), d_G(v))$ from the origin $(0, 0)$ in the 2D-Cartesian plane where u and

v are two distinct vertices and there is an edge $e = uv$ or vu associated with them in the graph G. The investigations of mathematical and theoretical properties and chemical applicability of the Sombor index can be seen in articles [30, 31].

The *modified Sombor index* was proposed by V.R. Kulli [32] in 2021. It is symbolized by ${}^{m}SO$ and described as follows

$$ {}^{m}SO(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)^2 + d_G(v)^2}}. $$

Inspired by the advancement and applicability of the Sombor index, V.R. Kulli recently proposed the *Nirmala index* [33] and defined it as

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

Further, Kulli et al. [34] introduced the *first inverse Nirmala index* (IN_1) and *second inverse Nirmala index* (IN_2) in 2021, and defined them as follows

$$ IN_1(G) = \sum_{uv \in E(G)} \sqrt{\frac{1}{d_G(u)} + \frac{1}{d_G(v)}} $$

and

$$ IN_2(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\frac{1}{d_G(u)} + \frac{1}{d_G(v)}}}. $$

Motivated by the work and progress of the GA index, V.R. Kulli introduced two degree-based indices namely, *Geometric-Quadratic* (GQ) and *Quadratic-Geometric* (QG) indices in 2022 [35], and they are defined as follows

$$ GQ(G) = \sum_{uv \in E(G)} \frac{\sqrt{2d_G(u)d_G(v)}}{\sqrt{d_G(u)^2 + d_G(v)^2}} $$

and

$$ QG(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_G(u)^2 + d_G(v)^2}}{\sqrt{2d_G(u)d_G(v)}}. $$

The M-polynomial-based derivation formulas to compute the different Nirmala-

type indices and GQ-QG indices are proposed in articles [36, 37]. Very recently, the chemical applicability of the GQ and QG indices and the Nirmala indices-based entropy measures are reported in the articles [38, 39].

Methodology

Our primary objective of this research article is to investigate the smoothness (structure sensitivity and abruptness) and chemical applicability of some novel degree-based topological indices. In particular, we focus our investigation on degree-based topological indices namely N, IN_1, IN_2, ${}^mM_2$, F, $RR_{-1/2}$, SDD, ISI, HM_1, HM_2, AG, SO, ${}^mSO$, GQ and QG. Section 2 comprises the computation of the two measures of smoothness such as structure sensitivity and abruptness of the considered degree-based topological indices for the data set of trees having $n = 4$ to 10 vertices. The obtained numerical results are tabulated in a table and their comparison is demonstrated using the bar graphs. The correlation among the considered topological indices is presented for 106 trees with 10 vertices in Section 3. The outcomes are shown using a correlation graph and the obtained correlation coefficients are listed in a table. Furthermore, in Section 4, the QSPR analysis for the eleven physico-chemical properties of octane isomers is executed to check the applicability of the considered topological indices with the help of linear regression models. At last, Section 5 is reserved for the conclusion.

2 Smoothness of the topological indices

Several parameters were propounded to diminish the randomness in the construction of a new topological index [19, 40]. Those are essential to satisfy such a molecular descriptor. Smoothness is one of them which states that the value of a molecular descriptor should uniformly change with gradual changes in molecular structure. But, an inspection of this property is hard to accomplish, therefore researchers disregard it very often. In this section, we investigate the smoothness of some novel degree-based topological indices and perform the comparison with the exiting

results of some well-known topological indices. Two novel graph structural measures namely *structure sensitivity* (denoted as SS) and *abruptness* (symbolized as Abr) were proposed in [41] to inspect the smoothness of a molecular descriptor. In recent literature, the structure sensitivity (SS) of eigenvalue-based topological indices and smoothness of graph energy in chemical graphs were investigated in the articles [42] and [43], respectively. We now sketch an exiting algorithm to calculate the SS and Abr of a topological index of a given class of connected graphs [41]. The steps are

Step-1 Consider a graph G in the class of connected graphs Ω and calculate its topological index $TI(G)$.

Step-2 Construct the set $S(G) = \{\Gamma \in \Omega | GED(\Gamma, G) = 2\}$, where GED is the *graph edit distance* between two graphs. Readers may see references [19, 41, 44] for more details about the graph edit distance and construction of set $S(G)$.

Step-3 For all $H \in S(G)$, calculate the topological index $TI(H)$. Then, the structure sensitivity and abruptness of topological index (TI) for the graph G is computed by the following mathematical expressions:

$$SS(TI, G) = \frac{1}{|S(G)|} \sum_{H \in S(G)} \left| \frac{TI(H) - TI(G)}{TI(G)} \right|$$

and

$$Abr(TI, G) = \max_{H \in S(G)} \left| \frac{TI(H) - TI(G)}{TI(G)} \right|$$

where $|S(G)|$ is the total number of graphs in the set $S(G)$.

Step-4 Average of SS and Abr values of a topological index calculated $\forall\, G \in \Omega$ is the total structure sensitivity and abruptness of a topological index (TI) in a class of connected graphs Ω. That is

$$SS(TI) = \frac{1}{|\Omega|} \sum_{G \in \Omega} SS(TI, G)$$

and

$$Abr(TI) = \frac{1}{|\Omega|} \sum_{G \in \Omega} Abr(TI, G)$$

where $|\Omega|$ is the total number of graphs in the set Ω.

For the goodness of a topological index, it is important that the SS value should be as high as possible, and simultaneously the Abr value should be as small as possible. More details on these two measures could be explored in [41, 44, 45] where the computer testing of the smoothness of some distance-based and degree-based indices was examined on the data sets of trees of different vertex sizes. Next, we design a pseudocode mentioned in Algorithm 1 of the Supplementary Information Section[§] to compute the SS and Abr values efficiently using the above-mentioned 4-step algorithm. For that, the computation of the considered degree-based topological indices is performed using Python 3.11. And, the graph edit distance (GED) between two graphs G_1 and G_2 is obtained by implementing the function $nx.graph\_edit\_distance(G_1, G_2)$ using `import networkx as nx` command available in `NetworkX` package in Python. At last, Algorithm 1 is implemented in MATLAB R2029a software to compute the structure sensitivity and abruptness of the degree-based topological indices N, IN_1, IN_2, ${}^mM_2$, F, $RR_{-1/2}$, SDD, ISI, HM_1, HM_2, AG, SO, ${}^mSO$, GQ and QG on the data sets of trees having $n = 4$ to 10 vertices. For a comparative perspective, the SS and Abr values for the M_1, M_2, $R_{-1/2}$, SCI, H, AZI, ABC and GA indices are comprised from reference [41] and are listed in Table 3 of the Supplementary Information Section. Our obtained computational values of structure sensitivity and abruptness are cataloged in Table 1. The comparisons among the results of SS and Abr values of topological indices cataloged in Tables 1 and 3 are demonstrated in Figures 1–3 and Figures 7–9 (Please see Supplementary Information Section) through bar graphs for the class of trees with $n = 4$ to 10 vertices.

Table 1 and Figures 1–3 stimulate us to arrive at the following observations. The second hyper-Zagreb, forgotten and first hyper-Zagreb indices have the maximum, second maximum and third maximum structure sensitivity values, respectively. One can observe from Tables 1 and 3, and Figure 9 that for $n = 10$ vertices trees, $SS(HM_2) = 0.285$, $SS(F) = 0.192$

[§]Supplementary Information Section, associated MATLAB script files and input data sets may be found at https://github.com/1267Virendra/Structure-Sensitivity-and-Chemical-Applicability.

Table 1. Structure sensitivity (SS) and abruptness (Abr) of different topological indices of trees from $n = 4$ to 10 vertices.

Topological Indices		$n = 4$	$n = 5$	$n = 6$	$n = 7$	$n = 8$	$n = 9$	$n = 10$
N	SS	0.0937	0.0898	0.0701	0.0579	0.0480	0.0413	0.0356
	Abr	0.0937	0.0997	0.1037	0.0945	0.0884	0.0823	0.0776
IN_1	SS	0.0042	0.0031	0.0028	0.0028	0.0026	0.0025	0.0024
	Abr	0.0042	0.0039	0.0041	0.0047	0.0051	0.0055	0.0058
IN_2	SS	0.0134	0.0107	0.0098	0.0206	0.0091	0.0086	0.0083
	Abr	0.0134	0.0132	0.0142	0.0938	0.0181	0.0196	0.021
${}^{m}M_2$	SS	0.225	0.2106	0.1627	0.1278	0.1005	0.0817	0.0671
	Abr	0.225	0.2315	0.2234	0.1967	0.1741	0.1580	0.1429
F	SS	0.5333	0.4851	0.3653	0.3044	0.2533	0.2205	0.1918
	Abr	0.5333	0.5641	0.5917	0.5527	0.5166	0.4888	0.4675
$RR_{-1/2}$	SS	0.0735	0.0790	0.0689	0.0605	0.0563	0.0480	0.0434
	Abr	0.0735	0.0830	0.0986	0.7166	0.1336	0.1063	0.1061
SDD	SS	0.3643	0.3152	0.2359	0.1913	0.1546	0.1319	0.112
	Abr	0.3643	0.3642	0.3652	0.3266	0.2995	0.2773	0.256
ISI	SS	0.0364	0.0306	0.0284	0.0269	0.0261	0.0246	0.0237
	Abr	0.0364	0.0372	0.0414	0.0454	0.0523	0.0568	0.0604
HM_1	SS	0.3517	0.3463	0.2762	0.2364	0.2017	0.1775	0.1565
	Abr	0.3517	0.3917	0.4301	0.4147	0.4002	0.3885	0.3782
HM_2	SS	0.1181	0.2502	0.3135	0.31702	0.3163	0.2990	0.2847
	Abr	0.1181	0.2847	0.4994	0.6256	0.7323	0.8113	0.8599
AG	SS	0.1044	0.0958	0.0727	0.0591	0.0477	0.0403	0.0339
	Abr	0.1044	0.1087	0.1077	0.0958	0.0876	0.0805	0.0738
SO	SS	0.2649	0.2417	0.1835	0.1569	0.1246	0.1073	0.0926
	Abr	0.2649	0.2730	0.2803	0.2875	0.2362	0.2204	0.2075
${}^{m}SO$	SS	0.2777	0.2614	0.2013	0.0095	0.1261	0.1035	0.0861
	Abr	0.2777	0.2789	0.2751	0.2383	0.2187	0.1962	0.1779
GQ	SS	0.1834	0.1652	0.1221	0.0955	0.0751	0.0619	0.0513
	Abr	0.1834	0.1787	0.1693	0.1430	0.1296	0.1159	0.1042
QG	SS	0.1806	0.1581	0.1181	0.0949	0.0763	0.0645	0.0544
	Abr	0.1806	0.1787	0.1762	0.1547	0.1408	0.1293	0.1184

and $SS(HM_1) = 0.157$, followed by $SS(AZI) = 0.118$ $SS(SDD) = 0.112$ $SS(M_2) = 0.103$, $SS(SO) = 0.093$, $SS({}^{m}SO) = 0.086$, $SS(M_1) = 0.073$, $SS({}^{m}M_2) = 0.067$and $SS(H) = 0.067$, etc. The considered degree-based indices maintain the following inequality relation:

$$\begin{aligned} SS(HM_2) > SS(F) > SS(HM_1) > SS(AZI) > SS(SDD) > SS(M_2) > SS(SO) \\ > SS({}^{m}SO) > SS(M_1) > SS({}^{m}M_2) > SS(H) > SS(QG) > SS(GQ) \\ > SS(RR_{-1/2}) > SS(N) > SS(SCI) > SS(R_{-1/2}) \approx SS(AG) > SS(GA) \\ > SS(ABC) > SS(ISI) > SS(IN_2) > SS(IN_1). \end{aligned}$$

Similar results can be obtained from Tables 1, 3 and Figures 1, 7 and 8 for the cases when $4 \leq n \leq 9$. In this context, HM_1 and F indices display their supremacy over other considered topological indices.

On the other hand, the topological indices with the minimum abruptness are the first and second inverse Nirmala indices. For instance $n = 10$, Table 1 and Figure 9 quantify that $Abr(IN_1) = 0.006$, $Abr(IN_2) = 0.021$, followed by $Abr(ABC) = 0.057$, $Abr(ISI) = 0.0604$, $Abr(GA) = 0.0671$, $Abr(R_{-1/2}) = 0.071$ and $Abr(SCI) = 0.0714$, etc. Abruptness of the degree-based topological indices under investigation preserves the following inequality relationship:

$$Abr(IN_1) < Abr(IN_2) < Abr(ABC) < Abr(ISI) < Abr(GA) < Abr(R_{-1/2}) < Abr(SCI) < Abr(AG) < Abr(N) < Abr(RR_{-1/2}) < Abr(GQ) < Abr(QG) < Abr(H) < Abr({}^{m}M_2) < Abr(M_1) < Abr({}^{m}SO) < Abr(Abr) < Abr(AZI) < Abr(SDD) < Abr(M_2) < Abr(HM_1) < Abr(F) < Abr(HM_2).$$

Further, Figures 1 and 2 show that the structure sensitivity of the topo-

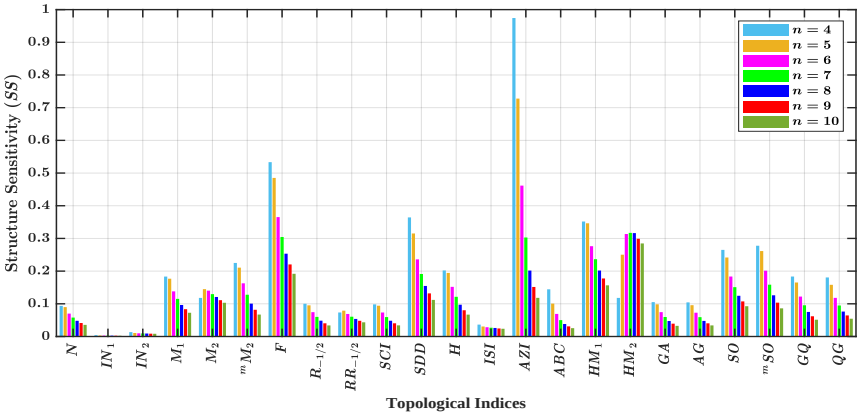

Figure 1. Comparison of structure sensitivity (SS)

logical indices apart from HM_2, decreases as we increase the value of n but it does not hold for the case of abruptness.

Unfortunately, the topological indices which have the greatest structure sensitivity attain the highest abruptness which leads to a contradiction to

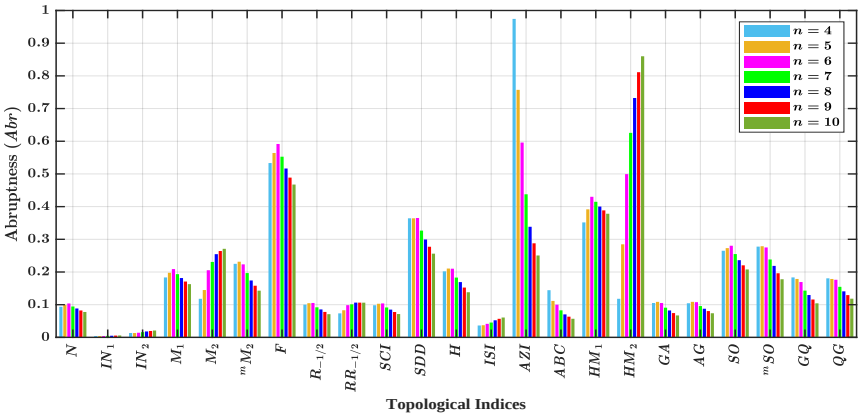

Figure 2. Comparison of abruptness (Abr).

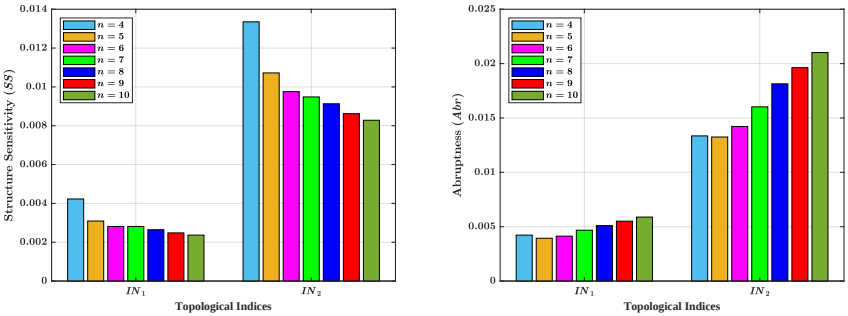

Figure 3. Comparison of structure sensitivity and abruptness for IN_1 and IN_2.

the fact that the SS value of topological indices should be as large as possible and simultaneously their Abr value should be as small as possible [41]. Apart from the IN_1 and IN_2, the results for the considered novel degree-based indices (such as N, ${}^{m}M_2$, F, $RR_{-1/2}$, SDD, ISI, HM_1, HM_2, AG, SO, ${}^{m}SO$, GQ and QG indices) are average and comparable than that of the exiting outcomes [41] of the well-known degree-based indices, namely M_1, M_2, $R_{-1/2}$, SCI, H, AZ, ABC and GA indices.

3 Correlation among the topological indices

Performing the correlation among the topological indices reveals their degree of independence from each other and it can determine the existence of any relationships between them. Here, we test the correlation among the considered degree-based topological indices on the data set of all trees with 10 vertices (106 trees). The obtained values of correlation coefficients are listed in Table 4 of the Supplementary Information Section. Figure 4 designates the correlation graph which depicts the strong correlation between the topological indices. In Figure 4, the correlation graph shows that the vertices representing the considered topological indices and there is an edge between two vertices if the obtained higher correlation coefficient between the associated topological indices is $0.9900 \leq |R| < 1$. From Figure 4, It is evident that the first inverse Nirmala (IN_1), augmented Zagreb (AZI) and first hyper-Zagreb (HM_2) indices do not correlate with any other topological index while the rest of the topological indices correlate with one or more topological indices. The topological indices that are strongly correlated with each other may convey the same graph structural information and can function similarly in this context.

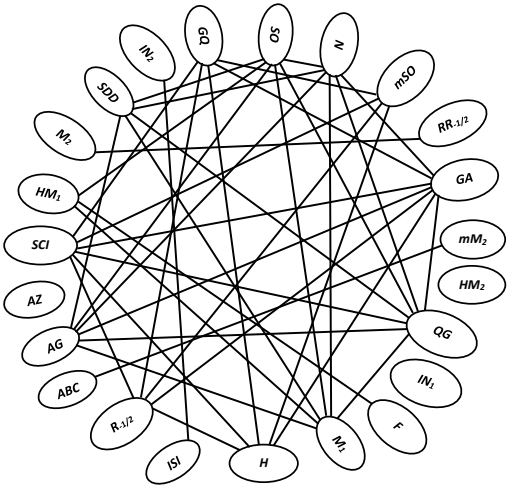

Figure 4. Correlation graph for the degree-based topological indices.

4 QSPR analysis: Applicability of the topological indices

In this segment, we perform the QSPR analysis of considered degree-based topological indices with the physico-chemical properties of octane isomers and compare the obtained results. The tested values of the eleven physico-chemical properties, such as boiling points (BP), critical temperature (CT), critical pressure (CP), heats of vaporization (HV), molar refraction (MR), molar volume (MV), surface tension, melting point (MP), standard heats of formations (DHFORM), density (DENS) and total surface area (TSA) of octane isomers are listed in Table 2. The values of the physico-chemical properties are comprised from the following web source `https://web.archive.org/web/20180912171255if_/http://www.moleculardescriptors.eu/index.htm` and reference [46]. The topological indices of the octane isomers are computed using a Python script. We catalog the estimated values of the topological indices (namely, N, IN_1, IN_2, ${}^mM_2$, SDD, ISI, HM_1, HM_2, AG, SO, ${}^mSO$, GQ and QG) in Table 5 of the Supplementary Information Section, and the rest of the other indices are incorporated from the article [46].

The linear regression model

$$P = a\ TI + b \tag{2}$$

is executed to investigate the prediction power of the topological indices. In Equation 2, the dependent variable P represents the physico-chemical property, the independent variable TI denotes the topological index, and the constants a and b are the slope and intercept of the fitting line, respectively. Next, we perform the linear regression model among the physico-chemical properties and the considered different degree-based topological indices using MATLAB R2019a software. The obtained best-fit linear regression models and associated statistical parameters are defined as follows:

Table 2. Physical properties of octane isomers

Physical properties → / Octane isomers ↓	BP	CT	CP	HV	MR	MV	ST	MP	DHFORM	DENS	TSA
n-Octane	125.6650	296.2000	24.6400	41.4800	39.1922	162.6050	21.7600	216.3000	4.1400	0.7025	415.3000
2-Methyl heptane	117.6470	288.0000	24.8000	39.6800	39.2316	163.6530	20.6000	164.1600	3.0600	0.6980	407.8500
3-Methyl heptane	118.9250	292.0000	25.6000	39.8300	39.1001	161.8450	21.1700	152.6000	3.2900	0.7058	397.3400
4-Methyl heptane	117.7090	290.0000	25.6000	39.6700	39.1174	162.1200	21.0000	152.0000	4.0000	0.7046	396.0400
3-Ethyl hexane	118.5340	292.0000	25.7400	39.4000	38.9400	160.0760	21.5100	–	3.5900	0.7136	379.0400
2,2-Dimethyl hexane	106.8400	279.0000	25.6000	37.2900	39.2500	164.2890	19.6000	151.9700	2.5600	0.6953	405.1100
2,3-Dimethyl hexane	115.6070	293.0000	26.6000	38.7900	38.9800	160.4130	20.9900	–	4.2300	0.7121	384.9300
2,4-Dimethyl hexane	109.4290	282.0000	25.8000	37.7600	39.1300	163.0930	20.0500	–	2.8000	0.7004	388.1100
2,5-Dimethyl hexane	109.1030	279.0000	25.0000	37.8600	39.2500	164.7150	19.7300	182.0000	2.5000	0.6935	395.0800
3,3-Dimethyl hexane	111.9690	290.8400	27.2000	37.9300	39.0000	160.8870	20.6300	147.0000	3.1700	0.7100	389.7900
3,4-Dimethyl hexane	117.7250	298.0000	27.4000	39.0200	38.8400	158.6530	21.6400	–	4.9700	0.7200	376.9100
3-Ethyl-2-methyl pentane	115.4500	295.0000	27.4000	38.5200	38.8300	158.8070	21.5200	158.2000	5.0800	0.7193	368.1000
3-Ethyl-3-methyl pentane	118.2590	305.0000	28.9000	37.9900	38.7100	157.0390	21.9900	182.2000	4.7600	0.7274	366.9900
2,2,3-Trimethyl pentane	109.841	294.0000	28.2000	36.9100	38.9200	159.51700	20.6700	160.8900	4.0900	0.7161	371.7500
2,2,4-Trimethyl pentane	99.2380	271.1500	25.5000	35.1300	39.2600	165.0960	18.7700	165.8000	3.1300	0.6919	392.1900
2,3,3-Trimethyl pentane	114.7600	303.0000	29.0000	37.2200	38.7600	157.2980	21.5600	172.2200	4.5200	0.7262	377.4000
2,3,4-Trimethyl pentane	113.467	295.0000	27.6000	37.6100	38.8600	158.8510	21.1400	163.9000	4.3200	0.7191	368.9300

(i) Linear regression model for boiling point (BP):

$$BP = 0.7829 \times AZI + 78.5600, R = 0.9176,\ R^2 = 0.8421,$$

$$Adj\text{-}R^2 = 0.8315, RMSE = 2.4730,\ \ SSE = 91.7100.$$

(ii) Linear regression model for critical temperature (CT):

$$CT = -339.3000 \times IN_1 + 2809.0000, R = -0.7378, R^2 = 0.5443,$$
$$Adj\text{-}R^2 = 0.5140, RMSE = 6.1260,\ \ SSE = 562.8000.$$

(iii) Linear regression model for critical pressure (CP):

$$CP = 8.2400 \times ISI - 27.6800, R = 0.9532, R^2 = 0.9086,$$
$$Adj\text{-}R^2 = 0.9025, RMSE = 0.4368,\ \ SSE = 2.8620.$$

(iv) Linear regression model for heats of vaporization (HV):

$$HV = 3.9210 \times GQ + 14.3500, R = 0.9661, R^2 = 0.9334,$$
$$Adj\text{-}R^2 = 0.9290, RMSE = 0.3859,\ \ SSE = 2.2340.$$

(v) Linear regression model for molar refraction (MR):

$$MR = 9.4650 \times IN_1 - 31.2200, R = 0.9824, R^2 = 0.9652,$$
$$Adj\text{-}R^2 = 0.9628,\ \ RMSE = 0.0355,\ \ SSE = 0.0189.$$

(vi) Linear regression model for molar volume (MV):

$$MV = 127.4000 \times IN_1 - 784.1000, R = 0.9503, R^2 = 0.9031,$$
$$Adj\text{-}R^2 = 0.8967,\ \ RMSE = 0.8230,\ \ SSE = 10.1600.$$

(vii) Linear regression model for surface tension (ST):

$$ST = 0.1001 \times AZI + 16.3000,\ \ R = 0.8064,\ \ R^2 = 0.6503,$$
$$Adj\text{-}R^2 = 0.6270,\ \ RMSE = 0.5354,\ \ SSE = 4.2990.$$

(viii) Linear regression model for melting point (MP):

$$MP = 43.1100 \times SCI + 20.1600,\ R = 0.3206,\ R^2 = 0.1028,$$
$$Adj\text{-}R^2 = 0.0212,\ RMSE = 18.3000,\ SSE = 3684.0000.$$

(ix) Linear regression model for standard enthalpy of formation (DHFORM):

$$DHFORM = -33.2600 \times IN_1 + 250.6000,\ R = 0.7642,$$
$$R^2 = 0.5842,\ Adj\text{-}R^2 = 0.5564,\ RMSE = 0.5537,\ SSE = 4.599.$$

(x) Linear regression model for density (DENS):

$$DENS = -0.5612 \times IN_1 - 779.8000,\ R = -0.9512,\ R^2 = 0.9047,$$
$$Adj\text{-}R^2 = 0.8984,\ RMSE = 0.0036,\ SSE = 0.0002.$$

(xi) Linear regression model for total surface area (TSA):

$$TSA = -233.1000 \times IN_2 + 1954.0000,\ R = -0.9369,\ R^2 = 0.8778,$$
$$Adj\text{-}R^2 = 0.8696,\ RMSE = 5.2880,\ SSE = 419.4000.$$

The above-mentioned statistical parameters R, R^2, Adj$-R^2$, $RMSE$ and SSE represent the correlation between the dependent and independent variables, the square of the correlation coefficient, adjusted R^2, the root mean squared error and the sum of squared error, respectively. For more details, readers may see the reference [47]. The higher value of R^2 (close to 1) together with the lower $RMSE$ (close to 0) value depict the goodness of the regression model. The best-fit linear regression models defined above corresponding to the topological indices that have higher prediction power to forecast the physico-chemical properties of the octane isomers are demonstrated in Figures 5 and 6. The rest of the others performed linear regression models and corresponding statistical parameters for all the considered indices are cataloged in Tables 6–16 of the Supplementary Information Section.

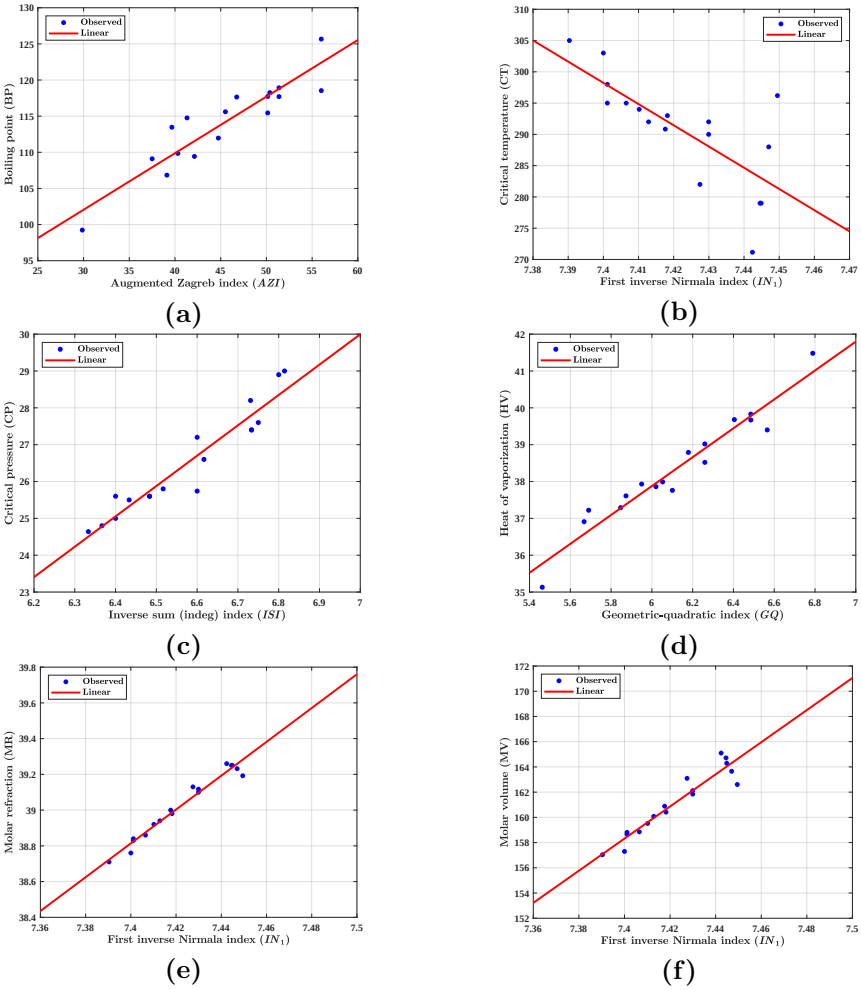

Figure 5. Plots of linear regression models having strong correlation between physico-chemical properties and topological indices of octane isomers: (a) BP vs. AZI (b) CT vs. IN_1 (c) CP vs. ISI (d) HV vs. GQ (e) MR vs. IN_1 (f) MV vs. IN_1.

Now, we present the comparative study of the considered degree-based topological indices depending on the correlation coefficient (R) obtained from the linear regression models, as shown in Tables 6–16 of Supplementary Information Section. The topological indices preserve the following ordering relations corresponding to R-values with each physico-chemical

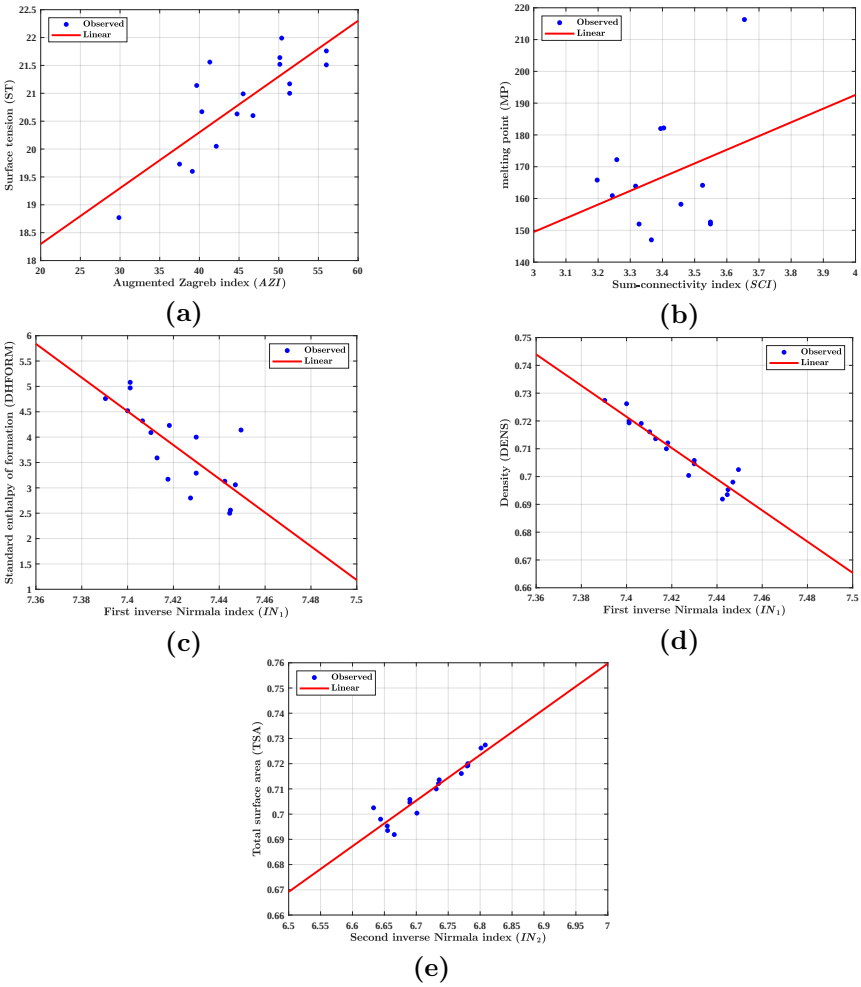

Figure 6. Graphical representation of linear regression models those obtain strong correlation between physico-chemical properties and topological indices of octane isomers: (a) ST vs. AZI (b) MP vs. SCI (c) DHFORM vs IN_1 (d) DENS vs IN_1 (e) TSA vs. IN_2.

property.

(i) Boiling point (BP):

$$ISI < IN_2 < IN_1 < HM_2 < M_2 < RR_{-1/2} < HM_1 < F < M_1 < N$$

$$< SO < SCI < {}^{m}SO < GQ < H < R_{-1/2} < GA < SDD < QG$$
$$< AG < {}^{m}M_2 < ABC < AZI,$$

(ii) Critical temperature (CT):

$$HM_1 < F < M_1 < N < SO < RR_{-1/2} < SCI < GQ < {}^{m}SO$$
$$< H < GA < M_2 < R_{-1/2} < QG < AG < SDD < HM_2 < {}^{m}M_2$$
$$< ABC < AZI < ISI < IN_2 < IN_1,$$

(iii) Critical pressure (CP):

$$AZI < M_2 < ABC < {}^{m}M_2 < SDD < AG < QG < R_{-1/2} < H$$
$$< GA < {}^{m}SO < GQ < SCI < SO < N < F < M_1 < HM_1$$
$$< RR_{-1/2} < M_2 < IN_1 < IN_2 < HM_2 < ISI,$$

(iv) Heats of vaporization (HV):

$$IN_1 < IN_2 < ISI < SDD < HM_2 < M_2 < RR_{-1/2} < HM_1 < AZI$$
$$< F < ABC < {}^{m}M_2 < M_1 < SO < N < AG < R_{-1/2} < H < QG$$
$$< SCI < {}^{m}SO < GA < GQ,$$

(v) Molar refraction (MR):

$$SDD < AG < QG < R_{-1/2} < GA < H < GQ < {}^{m}SO < {}^{m}M_2$$
$$< ABC < SCI < SO < N < AZI < F < M_1 < HM_1 < RR_{-1/2}$$
$$< M_2 < HM_2 < ISI < IN_2 < IN_1,$$

(vi) Molar volume (MV):

$$QG < AG < R_{-1/2} < GA < SDD < H < GQ < {}^{m}SO < SCI$$
$$< SO < N < {}^{m}M_2 < ABC < F < M_1 < HM_1 < AZI < RR_{-1/2}$$
$$< M_2 < HM_2 < ISI < IN_2 < IN_1,$$

(vii) Surface tension (ST):

$$M_2 < RR_{-1/2} < HM_2 < HM_1 < F < M_1 < N < SO < SCI < {}^mSO < GQ < ISI < H < GA < R_{-1/2} < QG < AG < SDD < IN_2 < IN_1 < {}^mM_2 < ABC < AZI,$$

(viii) Standard enthalpy of formation (DHFORM):

$$SO < N < F < M_1 < SCI < {}^mSO < H < GQ < R_{-1/2} < GA < HM_1 < QG < AG < SDD < RR_{-1/2} < {}^mM_2 < ABC < M_2 < AZI < HM_2 < ISI < IN_2 < IN_1,$$

(ix) Density (DENS):

$$AG < SDD < QG < R_{-1/2} < GA < H < GQ < {}^mSO < SCI < SO < {}^mM_2 < N < ABC < F < M_1 < AZI < HM_1 < RR_{-1/2} < M_2 < HM_2 < ISI < IN_2 < IN_1,$$

(x) Total surface area (TSA):

$$AZI < ABC < {}^mM_2 < SDD < AG < QG < GA < R_{-1/2} < H < GQ < {}^mSO < SCI < SO < F < N < M_1 < HM_1 < RR_{-1/2} < M_2 < HM_2 < IN_1 < ISI < IN_2.$$

Above obtained (i)-(x) ordering relations, Tables 6–16 and Figures 5 and 6 stimulate us to make the following intriguing observations related to the prediction capability of the topological indices. The observations are discussed as follows:

(i) Augmented Zagreb index (AZI) index shows a good correlation with the boiling points (BP) and surface tension (ST) of octane isomers and obtains the R-values 0.9127 and 0.8064, respectively.

(ii) First inverse Nirmala index (IN_1) observes the higher correlation

with the critical temperature (CT), molar refraction (MR), molar volume (MV), standard heats of formation (DHFORM) and density (DENS) of octane isomers and have correlation coefficients (R) -0.7378, 0.9824, 0.9503, 0.7642 and -0.9512, respectively.

(iii) Inverse sum (indeg) index (ISI) demonstrates good prediction power to forecast the critical pressure (CP) with R-value 0.9532.

(iv) Geometric-quadratic index (GQ) obtains the high correlation with the heats of vaporization (HV) and have R-value 0.9661.

(v) Second Nirmala index (IN_1) shows a strong correlation to predict the total surface area (TSA) with R-value -0.9369.

(vi) No topological index performs a good correlation with melting point (MP). Therefore in this case, we may not assert any conclusion about it.

Given the above discussion, among all the considered degree-based topological indices, the novel indices such as IN_1, IN_2, ISI and GQ indices are better predictors and show their domination nature over other degree-based topological indices for most of the considered physico-chemical properties of octane isomers.

5 Conclusion

This article aimed to investigate the smoothness and chemical applicability of some novel degree-based topological indices and their inter-correlation among each other.

In the context of smoothness, among all the considered topological indices, the second hyper Zagreb index (HM_2) obtained the higher SS-value followed by F, HM_1 and AZI indices, and the first Zagreb index (IN_1) showed the lower SS-value. However, the same observation was observed reverse in the case of abruptness. The obtained results concerning the (SS) and (Abr) of most of the considered novel degree-based topological indices are almost average and comparable with the existing results of the article [41].

The executed correlation analysis among the degree-based topological indices shows that the indices having a correlation coefficient $0.9900 \leq R < 1$ among each other are strongly correlated. It suggests that two well-correlated indices are dependent on each other and possess the same structural features and chemical applicability. Therefore, one should carry forward the topological index among them which shows a good prediction power and structural features.

The performed QSPR analysis for the physico-chemical properties of octane isomers calibrate that among the considered novel topological indices the IN_1 index predicts the CT, MR, MV, DHFORM and DENS properties of the octane isomers significantly. Further, the GQ, ISI and IN_2 indices obtain a good correlation with HV, CP and TSA properties, respectively. The augmented Zagreb index (AZI) somewhat performs a better correlation with BP and ST properties. Furthermore, apart from BP for all the considered properties, the obtained results for the SO, SDD, and N indices are fable in comparison to the IN_1, IN_2, and ISI indices.

Given the results associated with the discussed properties of the novel topological indices, one may consider these indices as strong contenders for future experimentation in this area.

***Acknowledgment*:** We sincerely thank the anonymous referees for the thorough reviews of this article and for their valuable suggestions and comments which have helped us to improve the quality of the article. Moreover, the first author (Virendra Kumar) is grateful to the UNIVERSITY GRANTS COMMISSION, Ministry of Human Resource Development, India for awarding the Senior Research Fellowship (SRF) with reference to UGC-Ref. No.: 1127/(CSIR-UGC NET JUNE 2019) dated 11-December-2019. The second author (Dr. Shibsankar Das) is obliged to the Science and Engineering Research Board (SERB), Department of Science and Technology (DST), Government of India for financially supporting this work through the SERB's research project sanction order number: EEQ/2022/000313, dated 20-January-2023.

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SUPPLEMENTARY MATERIALS TO On Structure Sensitivity and Chemical Applicability of Some Novel Degree-based Topological Indices

Table 3. Structure sensitivity (SS) and abruptness (Abr) of different topological indices of trees from $n = 4$ to 10 vertices.

Topological Indices		$n = 4$	$n = 5$	$n = 6$	$n = 7$	$n = 8$	$n = 9$	$n = 10$
M_1	SS	0.1833	0.1768	0.1381	0.1151	0.0964	0.0835	0.0726
	Abr	0.1833	0.19762	0.2090	0.1934	0.1815	0.1708	0.1623
M_2	SS	0.1181	0.1448	0.1403	0.1296	0.1209	0.1111	0.1032
	Abr	0.1181	0.1448	0.2054	0.2308	0.2546	0.2642	0.2706
$R_{-1/2}$	SS	0.1002	0.0953	0.0744	0.0599	0.0484	0.0404	0.0339
	Abr	0.1002	0.1046	0.1053	0.0919	0.0855	0.0779	0.0709
SCI	SS	0.0983	0.0942	0.0734	0.0594	0.0482	0.0404	0.0341
	Abr	0.0983	0.1028	0.1039	0.0915	0.0849	0.0776	0.0714
H	SS	0.2020	0.1945	0.1519	0.1214	0.0972	0.0803	0.0669
	Abr	0.2020	0.2106	0.2101	0.1829	0.1691	0.1524	0.1381
AZI	SS	0.9742	0.7278	0.4616	0.3029	0.2017	0.1515	0.1182
	Abr	0.9742	0.7572	0.5960	0.4378	0.3384	0.2878	0.2506
ABC	SS	0.1443	0.1007	0.0691	0.0501	0.0382	0.0309	0.0255
	Abr	0.1443	0.1115	0.1000	0.08274	0.0704	0.0634	0.0569
GA	SS	0.1052	0.0984	0.0746	0.0596	0.0474	0.0393	0.0326
	Abr	0.1052	0.1086	0.1051	0.0908	0.0823	0.0743	0.0671

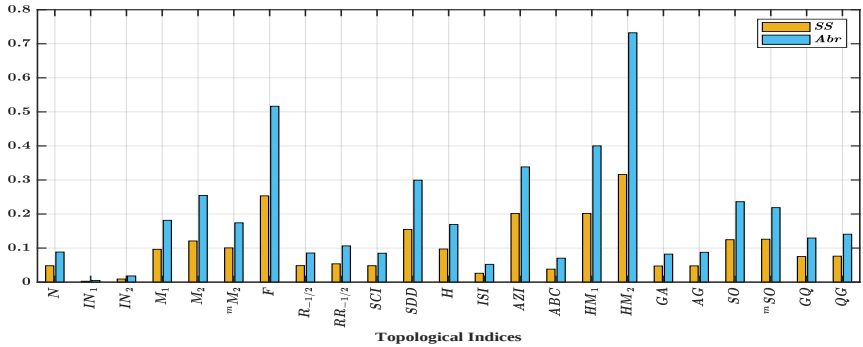

Figure 7. Comparison of SS and Abr of different topological indices for the data set of 23 trees with 8 vertices.

Algorithm 1 A pseudocode, implemented in MATLAB R2019a, to compute the structure sensitivity (SS) and abruptness (Abr) of topological indices (TIs) for a data set of trees of given vertex.

Require: Ω={Set of all trees with given number of vertices}
$A = Zeroes(|\Omega|, 23)$
$B = Zeroes(|\Omega|, 23)$
$C = Zeroes(1, 23)$
$D = Zeroes(1, 23)$
for $i = 1 : |\Omega|$ (for a tree T_i in n-vertex trees data set Ω) **do**
    $S = \{$Trees with $GED = 2$ from tree $T_i\}$ ▷ use Python networkx package to compute GED
    $E = [23\ TIs \text{ of tree } T_i]_{1\times 23}$ ▷ calculate TIs of tree T_i
    $F = [23\ TIs \text{ of the trees in set } S]_{23\times|S|}$ ▷ compute topological indices
    $G = Zeroes(23, |S|)$
    $H = Zeroes(1, 23)$
    $I = Zeroes(1, 23)$
    for $j = 1 : 23$ **do** ▷ Implementation of Step-3
        $p = 0$
        for $k = 1 : |S|$ **do**
            $q = |\frac{F(j,k)-E(j)}{E(j)}|$
            $p = q + p$
            $G(j, k) = q$
        end for
        $SS(T_i, TIs) = \frac{p}{|S|}$
        $Abr(T_i, TIs) = \max(G(j);:)$
        $H(j) = SS(T_i, TIs)$ ▷ Give all 23 SS-values of each TIs for a tree T_i
        $I(j) = Abr(T_i, TIs)$ ▷ Give all 23 Abr-values of each TIs for a tree T_i
    end for
    $disp(H)$
    $disp(I)$
    $A(i,:) = H(1,:)$
    $B(i,:) = I(1,:)$
end for
$disp(A)$
$disp(B)$
for $l = 1 : 23$ **do** ▷ Implementation of Step-4
    $r = 0$
    $t = 0$
    for $m = 1 : |\Omega|$ **do**
        $r = A(l, m) + r$
        $t = B(l, m) + t$
    end for ▷ To obtain the average of SS and Abr values of all the T_i
    $SS(\Omega, TIs) = \frac{r}{|\Omega|}$
    $Abr(\Omega, TIs) = \frac{t}{|\Omega|}$
    $C(l) = SS(\Omega, TIs)$
    $D(l) = Abr(\Omega, TIs)$
end for
$disp(C)$ ▷ Give all 23 SS-values of each TIs for data set Ω
$disp(D)$ ▷ Give all 23 Abr-values of each TIs for data set Ω

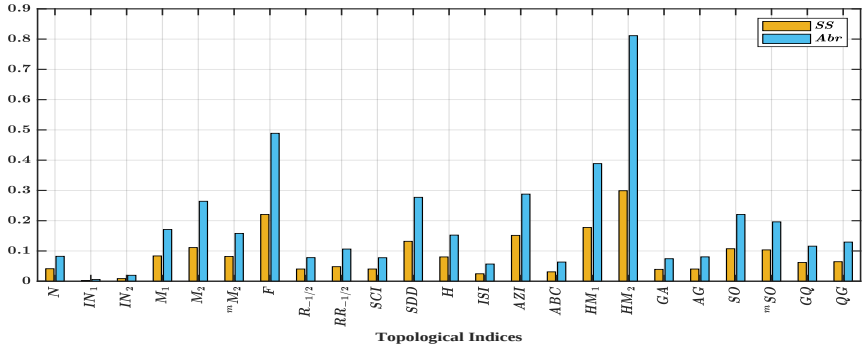

Figure 8. Comparison of SS and Abr of different topological indices for the data set of 47 trees with 9 vertices.

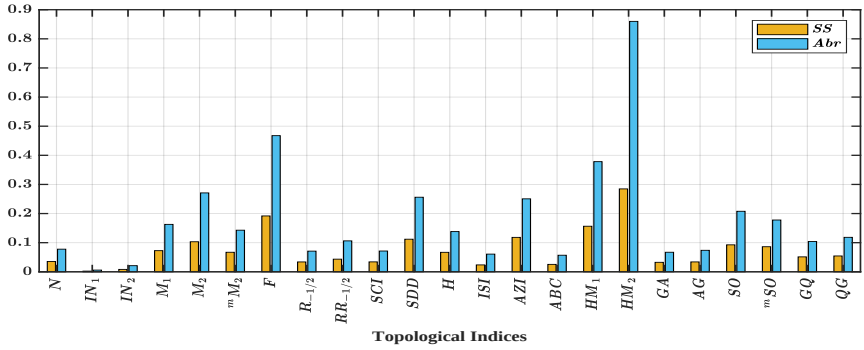

Figure 9. Comparison of SS and Abr of different topological indices for the data set of 106 trees with 10 vertices.

Table 4. Correlation coefficient among the different degree-based topological indices of decane isomers.

	N	IN_1	IN_2	M_1	M_2	${}^mM_2$	F	$R_{-1/2}$	$RR_{-1/2}$	SCI	SDD	H	ISI	AZI	ABC	HM_1	HM_2	GA	AG	SO	${}^mSO$	GQ	QG
N	1																						
IN_1	0.1437	1																					
IN_2	−0.0099	−0.9789	1																				
M_1	**0.9977**	0.1515	−0.0228	1																			
M_2	0.9527	−0.1462	0.2817	0.9497	1																		
${}^mM_2$	−0.9423	−0.2888	0.1256	−0.9221	−0.8501	1																	
F	0.9709	0.2319	−0.1223	0.9841	0.8995	−0.8705	1																
$R_{-1/2}$	−0.9831	−0.1843	0.0309	−0.9694	−0.9217	0.9855	−0.9222	1															
$RR_{-1/2}$	0.9806	−0.0473	0.1842	0.9764	**0.9927**	−0.8974	0.9310	−0.9576	1														
SCI	−0.9889	−0.1479	−0.0020	−0.9767	−0.9385	0.9757	−0.9292	**0.9986**	−0.9704	1													
SDD	**0.9902**	0.2688	−0.1378	**0.9917**	0.9060	−0.9429	0.9840	−0.9726	0.9454	−0.9738	1												
H	−0.9739	−0.1567	0.0001	−0.9567	−0.9197	0.9866	−0.9001	**0.9983**	−0.9542	**0.9967**	−0.9577	1											
ISI	0.0591	−0.9517	**0.9943**	0.0429	0.3469	0.0414	−0.0644	−0.0468	0.2506	−0.0776	−0.0691	−0.0786	1										
AZI	−0.8453	−0.4406	0.3163	−0.8223	−0.6895	0.9476	−0.7822	0.9063	−0.7639	0.8897	−0.8650	0.9087	0.2466	1									
ABC	0.9346	0.2954	−0.1323	0.9132	0.8393	**-0.9996**	0.8599	−0.9818	0.8883	−0.9711	0.9541	−0.9838	−0.0482	−0.9541	1								
HM_1	0.9814	0.1733	−0.0578	**0.9921**	0.9285	−0.8792	**0.9974**	−0.9349	0.9541	−0.9436	0.949	−0.9158	0.0021	−0.7779	0.8685	1							
HM_2	0.8652	−0.2612	0.4128	0.8583	0.9655	−0.7708	0.7804	−0.8412	0.9339	−0.8591	0.8027	−0.8444	0.4855	−0.5592	0.7588	0.8301	1						
GA	**-0.9916**	−0.1941	0.0485	−0.9815	−0.9284	0.9745	−0.9413	**0.9969**	−0.9641	0.9981	−0.9824	**0.9925**	−0.0258	0.8974	−0.9697	−0.9523	−0.8409	1					
AG	**0.9945**	0.2451	−0.1083	**0.9920**	0.9173	−0.9579	0.9728	−0.9850	0.9555	−0.9861	**0.9978**	−0.9737	−0.0371	−0.8796	0.9513	0.9772	0.8195	**-0.9925**	1				
SO	**0.9968**	0.1839	−0.0562	**0.9994**	0.9390	−0.9255	0.9864	−0.9696	0.9691	−0.9757	**0.9949**	−0.9559	0.0095	−0.8331	0.9169	**0.9924**	0.8428	−0.9823	**0.9944**	1			
${}^mSO$	−0.9619	−0.1228	−0.0356	−0.9415	−0.9161	0.9831	−0.8761	**0.9931**	−0.9490	**0.9916**	−0.9397	**0.9982**	−0.1144	0.9075	−0.9813	−0.8948	−0.8453	0.9846	−0.9591	−0.9398	1		
GQ	−0.9824	−0.1515	0.0029	−0.9678	−0.9301	0.9759	−0.9149	**0.9965**	−0.9637	**0.9979**	−0.9646	**0.9967**	−0.0719	0.9015	−0.9724	−0.9301	−0.8482	**0.9967**	−0.9796	−0.9673	**0.9935**	1	
QG	**0.9952**	0.2326	−0.0936	**0.9909**	0.9213	−0.9631	0.9667	−0.9832	0.9589	**-0.9904**	**0.9955**	−0.9795	−0.0217	−0.8851	0.9569	0.9727	0.8258	**-0.9957**	**0.9996**	**0.9929**	−0.9665	−0.9851	1

Table 5. Topological indices of octane isomers

Topological indices → / Octane isomers ↓	N	IN_1	IN_2	${}^mM_2$	SDD	ISI	HM_1	HM_2	AG	SO	${}^mSO$	GQ	QG
Octane	13.4641	7.4495	6.6329	2.2500	15.0000	6.3333	98.0000	88.0000	7.1213	18.6143	2.6622	6.7889	7.2361
2-Methyl heptane	13.9681	7.4470	6.6439	2.0833	17.3333	6.3667	114.0000	106.0000	7.3907	20.6515	2.4177	6.4044	7.7409
3-Methyl heptane	13.9362	7.4299	6.6899	2.16667	16.6667	6.4833	116.0000	121.0000	7.3173	20.5024	2.4725	6.4850	7.6087
4-Methyl heptane	13.9362	7.4299	6.6899	2.1667	16.6667	6.4833	116.0000	121.0000	7.3173	20.5024	2.4725	6.4850	7.6087
3-Ethyl hexane	13.9043	7.4128	6.7358	2.2500	16.0000	6.6000	118.0000	136.0000	7.2438	20.3533	2.5272	6.5656	7.4766
2,2-Dimethyl hexane	14.8897	7.4448	6.6545	1.8750	21.7500	6.4000	152.0000	148.0000	7.8713	24.7344	2.1055	5.8468	8.6093
2,3-Dimethyl hexane	14.4176	7.4182	6.7347	2.0278	18.6667	6.6167	134.0000	164.0000	7.5454	22.3995	2.2625	6.1789	8.0319
2,4-Dimethyl hexane	14.4402	7.4274	6.7009	2.0000	19.0000	6.5167	132.0000	139.0000	7.5866	22.5395	2.2279	6.1005	8.1135
2,5-Dimethyl hexane	14.4721	7.4445	6.6550	1.9167	19.6667	6.4000	130.0000	124.0000	7.6600	22.6886	2.1732	6.0199	8.2456
3,3-Dimethyl hexane	14.8352	7.4176	6.7312	2.0000	20.5000	6.6000	156.0000	184.0000	7.7426	24.4914	2.1803	5.9497	8.3876
3,4-Dimethyl hexane	14.3857	7.4011	6.7806	2.1111	18.0000	6.7333	136.0000	179.0000	7.4719	22.2504	2.3173	6.2596	7.8997
3-Ethyl-2-methyl pentane	14.3857	7.4011	6.7806	2.1111	18.0000	6.7333	136.0000	179.0000	7.4719	22.2504	2.3173	6.2596	7.8997
3-Ethyl-3-methyl pentane	14.7807	7.3903	6.8080	2.1250	19.2500	6.8000	160.0000	220.0000	7.6139	24.2477	2.2550	6.0526	8.1659
2,2,3-Trimethyl pentane	15.3221	7.4102	6.7705	1.8333	22.8333	6.7309	174.0000	241.0000	7.9963	26.3732	1.9684	5.6676	8.8437
2,2,4-Trimethyl pentane	15.3937	7.4424	6.6655	1.7083	24.0833	6.4333	168.0000	166.0000	8.1407	26.7716	1.8610	5.4624	9.1141
2,3,3-Trimethyl pentane	15.2994	7.4000	6.8014	1.8750	22.2500	6.8143	176.0000	262.0000	7.9411	26.2789	1.9883	5.6898	8.7541
2,3,4-Trimethyl pentane	14.8989	7.4065	6.7796	1.8889	20.6667	6.7500	152.0000	207.0000	7.7735	24.2967	2.0525	5.8730	8.4550

Table 6. Statistical parameters of linear QSPR model for boiling point (BP) of octane isomers.

Linear Models	R	R^2	Adjusted$-R^2$	$RMSE$	SSE
$BP = -8.0910 \times N + 231.6000$	-0.7506	0.5633	0.5342	4.112	253.6000
$BP = -61.7500 \times IN_1 + 572.5000$	-0.1958	0.0384	-0.0258	6.1020	558.4000
$BP = 12.7500 \times IN_2 + 28.4200$	0.1246	0.0155	-0.0501	6.1740	571.7000
$BP = -1.7880 \times M_1 + 168.6000$	-0.7124	0.5076	0.4748	4.3660	286.0000
$BP = -0.7725 \times M_2 + 137.4000$	-0.4234	0.1793	0.1246	5.6370	476.6000
$BP = 34.3600 \times {}^mM_2 + 44.6300$	0.8824	0.7786	0.7639	2.9270	128.5000
$BP = -0.2487 \times F + 133.8000$	-0.6965	0.4851	0.4507	4.465	299.0000
$BP = 36.9200 \times R_{-1/2} - 21.3300$	0.84063	0.7067	0.6871	3.3700	170.3000
$BP = -5.2110 \times RR_{-1/2} + 187.7000$	-0.5622	0.3160	0.2704	5.1460	397.2000
$BP = 38.8200 \times SCI - 18.6100$	0.8151	0.6643	0.6419	3.6050	194.9000
$BP = -1.9840 \times SDD + 152.2000$	-0.8409	0.7071	0.6875	3.3680	170.1000
$BP = 20.5100 \times H + 44.7500$	0.8387	0.7034	0.6837	3.3880	172.2000
$BP = 3.4400 \times ISI + 91.5100$	0.0924	0.0085	-0.0576	6.1950	575.7000
$BP = 0.7829 \times AZI + 78.5600$	**0.9176**	**0.8421**	0.8315	2.4730	91.7100
$BP = -27.0200 \times ABC + 255.8000$	-0.8859	0.7849	0.7706	2.8860	124.9000
$BP = -0.1653 \times HM_1 + 137.2000$	-0.6318	0.3992	0.3591	4.8230	348.9000
$BP = -0.0319 \times HM_2 + 119.3000$	-0.2559	0.0655	0.0032	6.0150	542.7000
$BP = 22.2800 \times GA - 30.2700$	0.8408	0.7069	0.6874	3.3680	170.2000
$BP = -17.8600 \times AG + 249.9000$	-0.8414	0.7080	0.6885	3.3620	169.6000
$BP = -1.899 \times SO + 157.7000$	-0.7509	0.5638	0.5347	4.1090	253.3000
$BP = 23.1800 \times {}^mSO + 61.9600$	0.8347	0.6968	0.6766	3.4260	176.1000
$BP = 14.1400 \times GQ + 27.5400$	0.8376	0.7016	0.6817	3.3990	173.3000
$BP = -9.75405 \times QG + 193.4000$	-0.8414	0.7079	0.6884	3.3630	169.6000

Table 7. Statistical parameters of linear QSPR model for critical temperature (CT) of octane isomers.

Linear Models	R	R^2	Adjusted$-R^2$	$RMSE$	SSE
$CT = -1.9560 \times N + 319.2000$	-0.1244	0.0155	-0.0502	9.004	1216.0000
$CT = -339.3000 \times IN_1 + 2809.0000$	**-0.7378**	**0.5443**	0.5140	6.1260	562.8000
$CT = 106.6000 \times IN_2 - 425.6000$	0.7141	0.5100	0.4773	6.3520	605.3000
$CT = -0.2464 \times M_1 + 298.3000$	-0.0673	0.0045	-0.0618	9.0540	1230.0000
$CT = 0.7936 \times M_2 + 266.8000$	0.2982	0.0889	0.0282	8.6620	1125.0000
$CT = 26.7800 \times {}^mM_2 + 236.6000$	0.4717	0.2225	0.1706	8.0020	960.4000
$CT = -0.0321 \times F + 293.3000$	-0.0617	0.0038	-0.0626	9.0570	1231.0000
$CT = 19.2000 \times R_{-1/2} + 220.3000$	0.2997	0.0898	0.0292	8.6570	1124.0000
$CT = 1.9200 \times RR_{-1/2} + 263.7000$	0.1420	0.02016	-0.0452	8.9830	1210.0000
$CT = 16.5900 \times SCI + 234.1000$	0.2388	0.0570	-0.0058	8.8120	1165.0000
$CT = -1.0660 \times SDD + 311.2000$	-0.3098	0.0959	0.0357	8.6280	1117.0000
$CT = 10.4500 \times H + 255.4000$	0.2931	0.0859	0.0249	8.6760	1129.0000
$CT = 38.0300 \times ISI + 40.6700$	0.7007	0.4909	0.4570	6.4750	628.8000
$CT = 0.7581 \times AZI + 256.3000$	0.6092	0.3712	0.3292	7.1960	776.8000
$CT = -21.5100 \times ABC + 403.5000$	-0.4836	0.2338	0.1828	7.9430	946.4000
$CT = 0.0154 \times HM_1 + 288.6000$	0.0403	0.0016	-0.0649	9.0670	1233.0000
$CT = 0.0836 \times HM_2 + 277.1000$	0.4604	0.2119	0.1594	8.0560	973.4000
$CT = 11.3600 \times GA + 217.1000$	0.2940	0.0864	0.0255	8.6740	1128.0000
$CT = -9.4420 \times AG + 362.5000$	-0.3051	0.0931	0.0326	8.6420	1120.0000
$CT = -0.4847 \times SO + 301.9000$	-0.1314	0.0173	-0.0483	8.9960	1214.0000
$CT = 11.3700 \times {}^mSO + 265.2000$	0.2809	0.0789	0.0175	8.7090	1138.0000
$CT = 6.8810 \times GQ + 248.6000$	0.2794	0.0781	0.0166	8.7130	1139.000
$CT = -5.0920 \times QG + 332.2000$	-0.3011	0.0907	0.0301	8.6530	1123.0000

Table 8. Statistical parameters of linear QSPR model for critical pressure (CP) of octane isomers.

Linear Models	R	R^2	**Adjusted**$-R^2$	$RMSE$	SSE
$CP = 1.5340 \times N + 4.2380$	0.6127	0.3754	0.3338	1.1420	19.5700
$CP = -66.5700 \times IN_1 + 520.6000$	−0.9089	0.8261	0.8145	0.6026	5.4480
$CP = 22.4100 \times IN_2 - 124.1000$	0.9427	0.8886	0.8812	0.4823	3.4900
$CP = 0.3830 \times M_1 + 14.8400$	0.6571	0.4318	0.3939	1.0890	17.8000
$CP = 0.3792 \times M_2 + 15.0600$	0.8950	0.8010	0.7877	0.6447	6.2340
$CP = -2.0480 \times {}^mM_2 + 30.6500$	−0.2265	0.0513	−0.0119	1.4080	29.7200
$CP = -0.0536 \times F + 22.2700$	0.6465	0.4180	0.3792	1.1030	18.2300
$CP = -4.5330 \times R_{-1/2} + 43.1400$	−0.4443	0.1974	0.1439	1.2950	25.1400
$CP = 1.7490 \times RR_{-1/2} + 1.8210$	0.8121	0.6595	0.6369	0.8432	10.6700
$CP = -5.6400 \times SCI + 45.7900$	−0.5098	0.2599	0.2106	1.2430	23.1800
$CP = 0.2346 \times SDD + 22.0000$	0.4281	0.1832	0.1288	1.3060	25.5900
$CP = -2.5740 \times H + 35.2100$	−0.4531	0.2053	0.1523	1.2880	24.8900
$CP = 8.2400 \times ISI - 27.6800$	**0.9532**	**0.9086**	0.9025	0.4368	2.8620
$CP = -0.0134 \times AZI + 27.1100$	−0.0674	0.0045	−0.0618	1.4420	31.1800
$CP = 1.5100 \times ABC + 18.5900$	0.2132	0.0455	−0.0182	1.4120	29.9000
$CP = 0.0444 \times HM_1 + 20.3200$	0.7305	0.5336	0.5025	0.9869	14.6100
$CP = 0.0274 \times HM_2 + 22.0100$	0.9480	0.8987	0.8920	0.4599	3.1730
$CP = -2.7970 \times GA + 44.6300$	−0.4545	0.2065	0.1536	1.287	24.8600
$CP = 2.1520 \times AG + 10.1500$	0.4366	0.1907	0.1367	1.3000	25.3500
$CP = 0.3537 \times SO + 18.3900$	0.6020	0.3625	0.3200	1.1540	19.9700
$CP = -3.0240 \times {}^mSO + 33.3100$	−0.4689	0.2199	0.1678	1.2760	24.4400
$CP = -1.8630 \times GQ + 37.9100$	−0.4752	0.2258	0.1742	1.272	24.25
$CP = 1.1930 \times QG + 16.8100$	0.4431	0.1964	0.1428	1.2960	25.1800

Table 9. Statistical parameters of linear QSPR model for heats of vaporization (HV) of octane isomers.

Linear Models	R	R^2	**Adjusted**$-R^2$	$RMSE$	SSE
$HV = -2.4330 \times N + 73.6600$	−0.9387	0.8811	0.8732	0.5157	3.9900
$HV = 12.8600 \times IN_1 - 57.1100$	0.1697	0.0288	−0.0359	32.5900	1.4740
$HV = -6.1490 \times IN_2 + 79.6800$	−0.2499	0.0625	$-3.359e-05$	1.448	31.4600
$HV = -0.5558 \times M_1 + 55.2900$	−0.9215	0.8492	0.8391	0.5809	5.0610
$HV = -0.3275 \times M_2 + 48.2400$	−0.7467	0.5576	0.5281	0.9948	14.8500
$HV = 8.4990 \times {}^mM_2 + 21.1700$	0.9081	0.8246	0.8130	0.6263	5.8840
$HV = -0.0777 \times F + 44.4900$	−0.9048	0.8187	0.8067	0.6368	6.082
$HV = 10.0800 \times R_{-1/2} + 1.3860$	0.9545	0.9110	0.9051	0.4462	2.9860
$HV = -1.8750 \times RR_{-1/2} + 64.8300$	−0.8417	0.7084	0.6889	0.8077	9.7850
$HV = 10.9600 \times SCI + 0.8975$	0.9569	0.9157	0.9101	0.4343	2.83
$HV = -0.5386 \times SDD + 48.700$	−0.9497	0.9020	0.8954	0.4683	3.2900
$HV = 5.6210 \times H + 19.3500$	0.9562	0.9143	0.9086	0.4378	2.8760
$HV = -2.5450 \times ISI + 55.0900$	−0.2844	0.0809	0.0196	1.4340	30.8400
$HV = 0.1806 \times AZI + 30.1600$	0.8804	0.7752	0.7602	0.7092	7.5440
$HV = -6.6460 \times ABC + 73.1900$	−0.9064	0.8215	0.8096	0.6319	5.9900
$HV = -0.0552 \times HM_1 + 46.0500$	−0.8772	0.7696	0.7542	0.7180	7.7320
$HV = -0.0184 \times HM_2 + 41.3700$	−0.6147	0.3779	0.3364	1.1800	20.8800
$HV = 6.1180 \times GA - 1.2970$	0.9606	0.9228	0.9176	0.4157	2.5920
$HV = -4.8660 \times AG + 75.3400$	−0.9538	0.9097	0.9037	0.4493	3.0280
$HV = -0.5691 \times SO + 51.4100$	−0.9361	0.8762	0.8680	0.5262	4.1530
$HV = 6.3990 \times {}^mSO + 23.9600$	0.9588	0.9192	0.9138	0.4251	2.7110
$HV = 3.9210 \times GQ + 14.3500$	**0.9661**	**0.9334**	0.9290	0.3859	2.2340
$HV = -2.6650 \times QG + 60.0300$	−0.9564	0.9147	0.9091	0.4367	2.8610

Table 10. Statistical parameters of linear QSPR model for molar refraction (MR) of octane isomers.

Linear Models	R	R^2	Adjusted$-R^2$	$RMSE$	SSE
$MR = -0.0909 \times N + 40.3400$	-0.2763	0.0763	0.0147	0.1827	0.5006
$MR = 9.4650 \times IN_1 - 31.2200$	**0.9824**	**0.9652**	0.9628	0.0355	0.0189
$MR = -3.0520 \times IN_2 + 59.5300$	-0.9762	0.9530	0.9498	0.0412	0.0255
$MR = -0.0252 \times M_1 + 39.7900$	-0.3284	0.1078	0.0484	0.1795	0.4835
$MR = -0.0375 \times M_2 + 40.1500$	-0.6723	0.4520	0.4155	0.1407	0.2970
$MR = -0.1629 \times {}^{m}M_2 + 39.3500$	-0.1369	0.0188	-0.0467	0.1883	0.5318
$MR = -0.0034 \times F + 39.2900$	-0.3083	0.0951	0.0347	0.1808	0.4904
$MR = 0.1207 \times R_{-1/2} + 38.5800$	0.0899	0.0081	-0.0580	0.1893	0.5376
$MR = -0.1548 \times RR_{-1/2} + 41.2100$	-0.5465	0.2987	0.2519	0.1592	0.3801
$MR = 0.2357 \times SCI + 38.2200$	0.1620	0.0263	-0.0387	0.1876	0.5277
$MR = -0.0042 \times SDD + 39.1000$	-0.0579	0.0033	-0.0631	0.1898	0.5402
$MR = 0.0765 \times H + 38.7600$	0.1024	0.0105	-0.0555	0.1891	0.5363
$MR = -1.1000 \times ISI + 46.2600$	-0.9676	0.9362	0.9320	0.0480	0.0346
$MR = -0.0073 \times AZI + 39.3500$	-0.2802	0.0785	0.0171	0.1825	0.4994
$MR = 0.1382 \times ABC + 38.3000$	0.1483	0.0219	-0.0432	0.1880	0.5301
$MR = -0.0033 \times HM_1 + 39.4900$	-0.4188	0.1754	0.1204	0.1726	0.4469
$MR = -0.0029 \times HM_2 + 39.5000$	-0.7667	0.5878	0.5604	0.1220	0.2234
$MR = 0.0747 \times GA + 38.5400$	0.0923	0.0085	-0.0576	0.1893	0.5374
$MR = -0.0447 \times AG + 39.3600$	-0.0689	0.0048	-0.0616	0.1896	0.5394
$MR = -0.0199 \times SO + 39.4800$	-0.2584	0.06677	0.0046	0.1836	0.5058
$MR = 0.1053 \times {}^{m}SO + 38.7800$	0.1241	0.0154	-0.0502	0.1886	0.5336
$MR = 0.0616 \times GQ + 38.6400$	0.1194	0.0143	-0.0515	0.1887	0.5342
$MR = -0.0273 \times QG + 39.2400$	-0.0772	0.0059	-0.0603	0.1895	0.5387

Table 11. Statistical parameters of linear QSPR model for molar volume (MV) of octane isomers.

Linear Models	R	R^2	Adjusted$-R^2$	$RMSE$	SSE
$MV = -0.9130 \times N + 174.4000$	-0.1993	0.0397	-0.0243	2.591	100.7000
$MV = 127.4000 \times IN_1 - 784.1000$	**0.9503**	**0.9031**	0.8967	0.8230	10.1600
$MV = -41.0400 \times IN_2 + 437.0000$	-0.9437	0.8906	0.8833	0.8746	11.4700
$MV = -0.2705 \times M_1 + 169.4000$	-0.2537	0.0644	0.0019	2.5580	98.1200
$MV = -0.4737 \times M_2 + 175.4000$	-0.6110	0.3733	0.3315	2.0930	65.7200
$MV = -3.4160 \times {}^{m}M_2 + 168.0000$	-0.2064	0.0426	-0.0212	2.5870	100.4000
$MV = -0.0363 \times F + 164.0000$	-0.2389	0.0571	-0.0058	2.5680	98.8900
$MV = 0.2273 \times R_{-1/2} + 160.3000$	0.0122	0.0001	-0.0665	2.6440	104.9000
$MV = -1.8700 \times RR_{-1/2} + 187.5000$	-0.4746	0.2253	0.1736	2.3270	81.2500
$MV = 1.6710 \times SCI + 155.4000$	0.0825	0.0068	-0.0594	2.6350	104.2000
$MV = 0.0152 \times SDD + 160.8000$	0.0151	0.0002	-0.0664	2.6440	104.9000
$MV = 0.2384 \times H + 160.3000$	0.0229	0.0005	-0.0661	2.6430	104.8000
$MV = -14.8000 \times ISI + 258.4000$	-0.9357	0.8756	0.8673	0.9327	13.0500
$MV = -0.1307 \times AZI + 167.1000$	-0.3604	0.1299	0.0719	2.4670	91.2500
$MV = 2.8380 \times ABC + 146.2000$	0.2190	0.0479	-0.0155	2.5800	99.8500
$MV = -0.0389 \times HM_1 + 166.5000$	-0.3504	0.1228	0.0643	2.4770	92.0000
$MV = -0.0385 \times HM_2 + 167.4000$	-0.7269	0.5284	0.4970	1.8160	49.4600
$MV = 0.1521 \times GA + 160.1000$	0.0135	0.0002	-0.0665	2.6440	104.9000
$MV = 0.0542 \times AG + 160.7000$	0.0060	$3.614e-05$	-0.0666	2.6440	104.9000
$MV = -0.1967 \times SO + 165.6000$	-0.1831	0.0335	-0.0309	2.5990	101.4000
$MV = 0.4938 \times {}^{m}SO + 160.0000$	0.0418	0.0018	-0.0648	2.6420	104.7000
$MV = 0.2628 \times GQ + 159.5000$	0.0366	0.0013	-0.0652	2.6420	104.7000
$MV = -0.0044 \times QG + 161.2000$	-0.0009	$8.07e-07$	-0.0667	2.6440	104.9000

Table 12. Statistical parameters of linear QSPR model for surface tension (ST) of octane isomers.

Linear Models	R	R^2	Adjusted$-R^2$	$RMSE$	SSE
$ST = -0.6265 \times N + 29.9400$	−0.3994	0.1595	0.1035	0.8300	10.3300
$ST = -28.8200 \times IN_1 + 234.8000$	−0.6281	0.3945	0.3542	0.7045	7.4440
$ST = 8.5520 \times IN_2 - 36.6300$	0.5743	0.3298	0.2851	0.7412	8.2400
$ST = -0.1260 \times M_1 + 24.6800$	−0.3452	0.1191	0.0604	0.8497	10.8300
$ST = 0.0087 \times M_2 + 20.5800$	0.0328	0.0011	−0.0655	0.9049	12.2800
$ST = 3.9850 \times {}^{m}M_2 + 12.7800$	0.7034	0.4948	0.4612	0.6435	6.2110
$ST = -0.0177 \times F + 22.2400$	−0.3414	0.1165	0.0576	0.8510	10.8600
$ST = 3.5730 \times R_{-1/2} + 7.7320$	0.5592	0.3127	0.2668	0.7506	8.4510
$ST = -0.1754 \times RR_{-1/2} + 23.3200$	−0.1300	0.0169	−0.0486	0.8977	12.0900
$ST = 3.4970 \times SCI + 8.8850$	0.5046	0.2546	0.2049	0.7816	9.1640
$ST = -0.1964 \times SDD + 24.6100$	−0.5720	0.3272	0.2823	0.7426	8.2720
$ST = 1.9650 \times H + 14.1900$	0.5524	0.3051	0.2588	0.7547	8.5430
$ST = 2.9630 \times ISI + 1.3560$	0.5472	0.2994	0.2527	0.7578	8.6130
$ST = 0.1001 \times AZI + 16.3000$	**0.8064**	**0.6503**	0.6270	0.5354	4.2990
$ST = -3.1620 \times ABC + 37.4200$	−0.7125	0.5076	0.4748	0.6353	6.0540
$ST = -0.0092 \times HM_1 + 22.1200$	−0.2407	0.0579	−0.0049	0.8787	11.5800
$ST = 0.0037 \times HM_2 + 20.2400$	0.2015	0.0406	−0.0233	0.8868	11.8000
$ST = 2.1480 \times GA + 6.9170$	0.5573	0.3106	0.2646	0.7517	8.4760
$ST = -1.7530 \times AG + 34.1700$	−0.5677	0.3223	0.2772	0.7453	8.3320
$ST = -0.1500 \times SO + 24.2800$	−0.4075	0.1661	0.1105	0.8268	10.2500
$ST = 2.1810 \times {}^{m}SO + 15.9300$	0.5398	0.2914	0.2442	0.7621	8.7120
$ST = 1.3340 \times GQ + 12.6800$	0.5429	0.2948	0.2478	0.7603	8.6700
$ST = -0.9516 \times QG + 28.5800$	−0.5641	0.3182	0.2728	0.7475	8.3820

Table 13. Statistical parameters of linear QSPR model for melting point (MP) of octane isomers.

Linear Models	R	R^2	Adjusted$-R^2$	$RMSE$	SSE
$MP = -9.6450 \times N + 307.5000$	−0.3204	0.1027	0.0211	18.3	3684
$MP = 157.3000 \times IN_1 - 1001.0000$	0.1773	0.0314	−0.0566	19.0100	3977.0000
$MP = -51.5100 \times IN_2 + 512.8000$	−0.1810	0.03276	−0.0552	19.0000	3971.0000
$MP = -2.2010 \times M_1 + 234.6000$	−0.3154	0.0995	0.0176	18.3300	3697.0000
$MP = -1.3440 \times M_2 + 207.7000$	−0.2711	0.0735	−0.0108	18.6000	3804.0000
$MP = 30.9800 \times {}^{m}M_2 + 104.9000$	0.2719	0.0739	−0.0103	18.5900	3802.0000
$MP = -0.3014 \times F + 191.4000$	−0.3017	0.0910	0.0084	18.4200	3732.0000
$MP = 39.2700 \times R_{-1/2} + 23.4900$	0.3142	0.0987	0.0168	18.3400	3700.0000
$MP = -7.7220 \times RR_{-1/2} + 276.3000$	−0.3052	0.0932	0.0107	18.4000	3723.0000
$MP = 43.1100 \times SCI + 20.1600$	**0.3206**	**0.1028**	0.0212	18.3000	3684.0000
$MP = -2.0950 \times SDD + 207.9000$	−0.3108	0.0966	0.0145	18.3600	3709.0000
$MP = 21.9100 \times H + 93.4300$	0.3153	0.0994	0.0176	18.3300	3697.0000
$MP = -18.5900 \times ISI + 288.9000$	−0.1805	0.0326	−0.0554	19.0000	3972.0000
$MP = 0.6401 \times AZI + 138.4000$	0.2531	0.0640	−0.0210	18.6900	3843.0000
$MP = -24.1100 \times ABC + 293.9000$	−0.2697	0.0728	−0.0115	18.6000	3807.0000
$MP = -0.2158 \times HM_1 + 197.5000$	−0.2979	0.0888	0.0059	18.4400	3741.0000
$MP = -0.0685 \times HM_2 + 178.3000$	−0.2021	0.0408	−0.0464	18.9200	3938.0000
$MP = 23.6800 \times GA + 14.1200$	0.3139	0.0986	0.0166	18.3400	3701.0000
$MP = -18.8900 \times AG + 311.2000$	−0.3118	0.0972	0.0152	18.3600	3706.0000
$MP = -2.2330 \times SO + 218.8000$	−0.3152	0.0994	0.0175	18.3300	3698.0000
$MP = 25.0200 \times {}^{m}SO + 111.2000$	0.3179	0.1011	0.0194	18.3200	3691.0000
$MP = 15.1900 \times GQ + 74.5800$	0.3171	0.1006	0.0188	18.3200	3693.0000
$MP = -10.3400 \times QG + 251.7000$	−0.3128	0.0978	0.0158	18.3500	3704.0000

Table 14. Statistical parameters of linear QSPR model for standard enthalpy of formation (DHFORM) of octane isomers.

Linear Models	R	R^2	Adjusted$-R^2$	$RMSE$	SSE
$DHFORM = 0.0249 \times N + 3.4150$	0.0168	0.0003	−0.0664	0.8585	11.0600
$DHFORM = -33.2600 \times IN_1 + 250.6000$	**0.7642**	**0.5842**	0.5564	0.5537	4.599
$DHFORM = 10.6600 \times IN_2 - 67.8800$	0.7549	0.5699	0.5412	0.5631	4.7570
$DHFORM = 0.0209 \times M_1 + 3.1420$	0.0602	0.0036	−0.0628	0.8571	11.0200
$DHFORM = 0.0972 \times M_20.8439$	0.3861	0.1491	0.09233	0.7920	9.4100
$DHFORM = 1.5530 \times {}^mM_20.6357$	0.2890	0.0835	0.0224	0.8220	10.1300
$DHFORM = 0.0019 \times F + 3.6220$	0.0399	0.0016	−0.0649	0.8579	11.0400
$DHFORM = 0.7610 \times R_{-1/2} + 0.9849$	0.1256	0.0158	−0.0499	0.8518	10.8800
$DHFORM = 0.3326 \times RR_{-1/2} - 0.9179$	0.2599	0.0676	0.0054	0.8291	10.3100
$DHFORM = 0.4802 \times SCI + 2.1350$	0.0731	0.0053	−0.0609	0.8563	11.0000
$DHFORM = -0.0514 \times SDD + 4.7630$	−0.1578	0.0249	−0.0401	0.8479	104.0000
$DHFORM = 0.3952 \times H + 2.4400$	0.1171	0.0137	−0.0520	0.8527	10.9100
$DHFORM = 3.8350 \times ISI + -21.4400$	0.7468	0.5577	0.5282	0.5711	4.8920
$DHFORM = 0.0498 \times AZI + 1.5140$	0.4231	0.1790	0.1243	0.778	9.0790
$DHFORM = -1.2600 \times ABC + 10.3800$	−0.2994	0.0897	0.0289	0.8192	10.0700
$DHFORM = 0.0051 \times HM_1 + 3.0730$	0.1399	0.0196	−0.0458	0.8502	10.8400
$DHFORM = 0.0087 \times HM_2 + 2.3570$	0.5047	0.2547	0.2050	0.7413	8.2420
$DHFORM = 0.5037 \times GA + 0.5123$	0.1378	0.0189	−0.0464	0.8504	10.8500
$DHFORM = -0.4433 \times AG + 7.1460$	−0.1514	0.0229	−0.0422	0.8487	10.8100
$DHFORM = -0.0009 \times SO + 3.7980$	−0.0026	$6.783e-06$	−0.0667	0.8586	11.0600
$DHFORM = 0.3944 \times {}^mSO + 2.8900$	0.1029	0.0106	−0.0554	0.8541	10.9400
$DHFORM = 0.2851 \times GQ + 2.0320$	0.1224	0.0149	−0.0507	0.8522	10.8900
$DHFORM = -0.2347 \times QG + 5.6850$	−0.1467	0.0215	−0.0437	0.8493	10.8200

Table 15. Statistical parameters of linear QSPR model for density (DENS) of octane isomers.

Linear Models	R	R^2	Adjusted$-R^2$	$RMSE$	SSE
$DENS = 0.0042 \times N + 0.6486$	0.2068	0.0428	−0.0210	0.0114	0.0019
$DENS = -0.5612 \times IN_1 - 779.8000$	**−0.9512**	**0.9047**	0.8984	0.0036	0.0002
$DENS = 0.1810 \times IN_2 - 5.070$	0.9451	0.8933	0.8861	0.0038	0.0002
$DENS = 0.0012 \times M_1 + 0.6718$	0.2612	0.0682	0.0061	0.0112	0.0019
$DENS = 0.0021 \times M_2 + 0.6456$	0.6170	0.3807	0.3394	0.0092	0.0013
$DENS = 0.0145 \times {}^mM_2 + 0.6798$	0.1995	0.0398	−0.0242	0.0114	0.0019
$DENS = 0.0002 \times F + 0.6962$	0.2465	0.0608	−0.0018	0.0113	0.0019
$DENS = -0.0016 \times R_{-1/2} + 0.7151$	−0.0196	0.0004	−0.0663	0.0116	0.0020
$DENS = 0.0083 \times RR_{-1/2} + 0.5913$	0.4813	0.2316	0.1804	0.0102	0.0016
$DENS = -0.0080 \times SCI + 0.7366$	−0.0900	0.0081	−0.0580	0.0116	0.0020
$DENS = -3.354e-05 \times SDD + 0.7098$	−0.0076	$5.775e-05$	−0.0665	0.0116	0.0020
$DENS = -0.0014 \times H + 0.7139$	−0.0304	0.0009	−0.0657	0.0116	0.0020
$DENS = 0.0653 \times ISI + 0.2800$	0.9374	0.8786	0.8705	0.0041	0.0002
$DENS = 0.0006 \times AZI + 0.6836$	0.3532	0.1247	0.0664	0.0109	0.0018
$DENS = -0.0121 \times ABC + 0.7726$	−0.2120	0.0449	−0.0187	0.01138	0.0019
$DENS = 0.0002 \times HM_1 + 0.6848$	0.3577	0.1279	0.0698	0.0109	0.0018
$DENS = 0.0002 \times HM_2 + 0.6812$	0.7319	0.5356	0.5047	0.0079	0.0009
$DENS = -0.0011 \times GA + 0.7160$	−0.0212	0.0005	−0.0662	0.01164	0.0020
$DENS = 6.293e-05 \times AG + 0.7087$	0.0016	$2.512e-06$	−0.0667	0.0116	0.0020
$DENS = 0.0009 \times SO + 0.6885$	0.1907	0.0342	−0.0302	2.5880	100.5000
$DENS = -0.0026 \times {}^mSO + 0.7149$	−0.0493	0.0024	−0.0641	0.0116	0.0020
$DENS = -0.0014 \times GQ + 0.7178$	−0.0445	0.0019	−0.0646	0.0116	0.0020
$DENS = 0.0002 \times QG + 0.7077$	0.0085	$7.297e-05$	−0.0666	0.0116	0.0020

Table 16. Statistical parameters of linear QSPR model for total surface area (TSA) of octane isomers.

Linear Models	$\boldsymbol{R}$	$\boldsymbol{R^2}$	**Adjusted**$-\boldsymbol{R^2}$	$\boldsymbol{RMSE}$	$\boldsymbol{SSE}$
$TSA = -12.7700 \times N + 572.5000$	-0.4875	0.2376	0.1868	13.2100	2616.0000
$TSA = 709.0000 \times IN_1 - 4875.0000$	0.9249	0.8554	0.8458	5.7510	5.7510
$TSA = -233.1000 \times IN_2 + 1954.0000$	$\mathbf{-0.9369}$	**0.8778**	0.8696	5.2880	419.4000
$TSA = -3.1620 \times M_1 + 483.4000$	-0.5183	0.2687	0.2199	12.9300	2510.0000
$TSA = -3.4050 \times M_2 + 489.9000$	-0.7679	0.5896	0.5623	9.6890	1408.0000
$TSA = 14.4300 \times {}^{m}M_2 + 357.9000$	0.1525	0.0233	-0.0419	14.9500	3352.0000
$TSA = -0.4099 \times F + 419.5000$	-0.4721	0.2229	0.1711	13.3300	2667.0000
$TSA = 37.8000 \times R_{-1/2} + 248.4000$	0.3541	0.1254	0.0671	14.1500	3001.0000
$TSA = -15.6900 \times RR_{-1/2} + 608.6000$	-0.6962	0.4848	0.4504	10.8600	1768.0000
$TSA = 47.7600 \times SCI + 223.8000$	0.4124	0.1701	0.1148	13.7800	2848.0000
$TSA = 1.7160 \times SDD + 420.0000$	-0.2992	0.0895	0.0288	14.4300	3124.0000
$TSA = 21.9700 \times H + 312.8000$	0.3696	0.1366	0.0791	14.0500	2963.0000
$TSA = -84.6500 \times ISI + 943.8000$	-0.9357	0.8755	0.8672	5.3370	427.3000
$TSA = 0.0992 \times AZI + 382.6000$	0.0478	0.0023	-0.0642	15.1100	3424.0000
$TSA = -10.8300 \times ABC + 443.9000$	-0.1460	0.0213	-0.0439	14.9600	3358.0000
$TSA = -0.3602 \times HM_1 + 437.3000$	-0.5663	0.3206	0.2754	12.4700	2331.0000
$TSA = -0.2400 \times HM_2 + 426.4000$	-0.7929	0.6288	0.6040	9.2150	1274.0000
$TSA = 22.1300 \times GA + 243.7000$	0.3436	0.1180	0.0592	14.2000	3027.0000
$TSA = -16.1900 \times AG + 510.2000$	-0.3139	0.0985	0.0384	14.3600	3094.0000
$TSA = -2.8260 \times SO + 451.9000$	-0.4596	0.2112	0.1587	13.4300	2707.0000
$TSA = 26.6700 \times {}^{m}SO + 327.1000$	0.3951	0.1561	0.0998	13.8900	2896.0000
$TSA = 15.4100 \times GQ + 292.8000$	0.3754	0.1409	0.0836	14.0200	2948.0000
$TSA = -9.1370 \times QG + 461.4000$	-0.3242	0.1051	0.0455	14.3100	3071.0000