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Research Article

Structural Analysis and Topological Characterization of Sudoku Nanosheet

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The physical and biological properties of chemical compounds are modelled using chemical graph theory. The geometric structure of chemical compounds can be modelled using a variety of topological indices derived from graph theory. The chemical structures, physicochemical characteristics, and biological activities are predicted by the topological indices using the real numbers derived from the molecular compound. The topological index's first use was to identify the physical characteristics of alkenes. A topological index is a molecular structure descriptor calculated from a chemical compound's molecular graph describing its topology. When applied to a chemical compound's molecular structure, it tells the theoretical properties. The chemical structure is studied as a graph, where elements are denoted as vertices, and chemical bonds are called edges. In this study, we have computed some novel topological indices named as modified neighborhood version of the forgotten topological index F_N^*, the neighborhood version of the first multiplicative Zagreb M_1^*, the neighborhood version of the second Zagreb index M_2^*, the neighborhood version of hyper-Zagreb index HM_N, the Sambor topological index $\mathrm{SO}(G)$, and the Sambor reduced topological index $\mathrm{SO}_{\mathrm{red}}(G)$ for the Sudoku nanosheet and derived formulas for them. Based on the derived formulas, the numerical results of the understudy nanosheet's physical and chemical properties are investigated. Our computed results are undoubtedly helpful in understanding the topology of the understudy nanosheet. These computed indices have the best correlation with acentric factor and entropy; therefore, they are effective in QSPRs and QSARs analysis with complete accuracy.

1. Introduction

The subject of intense research is the famous 2-dimensional nano-material graphene, the world's [1–3] lightest 2D material with a hexagonal grid. Since their inventions, carbon nanotubes have gained a lot of attention [4, 5]. Carbon nanotubes (CNTs) are made of carbon using nanometer diameters. The one-wall carbon nanotubes are a bore in the variety of nanometers by Iijima and Ichihashi [4], and Bethune et al. [5] independently. The thickness of the 2D nanostructure varies from 1 to 100 nm [6]. These 2D nanosheets have interesting physical, electronic, biological, and chemical properties that are essential for various applications. Therefore, it is critical to predicting these nanostructures to attain discrimination and bring about the network topology, meliorate, and their physical characteristics. Chemical graph theory is used to represent better and characterise molecules to understand chemical compounds' physical properties [7]. Graphs are mathematical structures that are used to model relationships. A Chemical graph is a basic calculable graph with atoms at the edge in an implicit system. In [8], Randic' gives the concept of finding a suitable path to reach the desire vertex.

A TI describes a lot of prominent properties of some chemical compounds. These are essential in biological and chemical science and engineering. Physicochemical characteristics or theoretical molecular descriptors are used as forecasters in QSAR modelling [9–11], whilst the expression QSPR models as replication variables [12–15]. Wiener [16] introduced the TI concept while functioning on paraffin's boiling point and set it as

a path number. From both a practical and theoretical standpoint, it is the first and maximum considered TI. It is described as the total distance of the distances between all pairs of vertices in graph G, with more information available in ref [17]. Degree-based TI is often used in chemical network graph theory, mainly in chemistry. Gutman et al. established the premature topological indices and the Zagreb indices [18–21], which have been used to investigate in molecular difficulty, boiling point, and chirality.

The discipline of graph theory is rapidly expanding and performing a vital function, cheminformatics, the investigation of various chemical formations and their physiochemical qualities that combine chemistry and mathematics, and information on technology. For example, Chemical network graph theory is the subsection of mathematics that deals with chemistry that uses the help of topological indices. Graph theory allows us to focus on the physiochemical aspects of the molecular graph (TIs). TIs are numerical numbers connected with various chemical structures in the molecular graph that forecast toxicological, organic, and physiochemical elements of chemical compounds present in the diagram. Furthermore, IT is for the isomorphic graphs to be the same. Period before, many researchers have functioned on TIs, see [22, 23]. The most common application of these TIs has been used most frequently to explore the evaluative construct movement and correlations in nature (QSAR and QSPR). In [24], Guo and Dong, gave the energy and analytical applications of chemical graphs. Li et al. [25] used some matrix techniques to obtain the eigenvalues and their multiplicity to find the kirchhoff index. In [26], Khan et al., established some-properties and applications of toxicities. Zaman et al. [27] determined the maximum H-index of Halin graph. The results on Cacti with maximal general sum-connectivity index are given in [28].

The degree of a vertex is an essential invariant in examining a graph. Calculate the number of edges with that vertex as an endpoint to get the degree.

The vertex degree v of any graph G expressed by $d_G(v)$, that is detailed as the total amount of edges linked with a confers vertex v. Besides, we define

$$\alpha_G(n) = \sum_{m \in N_G(n)} d_G(m), \tag{1}$$

where

$$N_G(n) = \{m \in V(G): \quad mn \in E(G)\}. \tag{2}$$

Let F_N^* denote the modified neighborhood version of the forgotten topological index and is defined as follows [18]:

$$F_N^*(G) = \sum_{mn \in E(G)} \left[\alpha_G(m)^2 + \alpha_G(n)^2\right]. \tag{3}$$

Let M_1^* denote the first multiplicative Zagreb index, which is defined as follows [29]:

$$M_1^*(G) = \sum_{mn \in E(G)} \left[\alpha_G(m) + \alpha_G(n)\right]. \tag{4}$$

Let M_2^* denote the second Zagreb index, which is defined in [29] as follows:

$$M_2^*(G) = \sum_{mn \in E(G)} \alpha_G(m) \times \alpha_G(n). \tag{5}$$

The neighborhood form of the hyper-Zagreb index is expressed by HM_N, moreover, represented as follows [30]:

$$\mathrm{HM}_N(G) = \sum_{mn \in E(G)} \left[\alpha_G(m) + \alpha_G(n)\right]^2. \tag{6}$$

The Sambor index $\mathrm{SO}(G)$ and reduced Sambor index $\mathrm{SO}_{\mathrm{red}}(G)$ are introduced by Gutman in [31], which are defined as follows:

$$\begin{aligned} \mathrm{SO}(G) &= \sum_{mn \in E(G)} \sqrt{\alpha_G(m)^2 + \alpha_G(n)^2}, \\ \mathrm{SO}_{\mathrm{red}}(G) &= \sum_{mn \in E(G)} \sqrt{\left[(\alpha_m - 1)^2 + (\alpha_n - 1)^2\right]}. \end{aligned} \tag{7}$$

Let AZI denote the Argumanted Zagreb topological index, which is defined by [32] as follows:

$$\mathrm{AZI}(G) = \sum_{mn \in E(G)} \left(\frac{\alpha_G(m) \times \alpha_G(n)}{\alpha_G(m) + \alpha_G(n) - 2}\right). \tag{8}$$

For a few essentials values $n \geq 2$, the Sudoku nanosheet ($\mathrm{SK}_{n\times n}$) is a graphical description of the Sudoku puzzle in the form of a $n \times n$ grid chording of n^2 cells, where every single cell is a precise graph of nodes with four vertices of degree 5, 4 vertices of degree 7, and 1 vertex of degree 8. Besides, Sudoku graphs $|V(\mathrm{SK}_{n\times n})| = 9n^2$, belong to the number of vertices and $|E(\mathrm{SK}_{n\times n})| = n(34n - 6)$ are the number of edges, accordingly. For $n = 3$, the Sudoku nanosheet $\mathrm{SK}_{3\times 3}$ is demonstrated in Figure 1. In Table 1, we ciphered the consequence for the linked number-based partition of edges for $n \geq 3$ of the Sudoku graph $\mathrm{SK}_{n\times n}$.

1.1. Main Results on Sudoku Nanosheet $SK_{(r\times r)}$

Theorem 1. *Assume that G denotes the Sudoku nanosheet, then the Modified neighborhood version of forgotten topological index of G is*

$$F_N^*(G) = 392r^4 + 3540r^2 + 1852r + 144. \tag{9}$$

Proof. By definition of $F_N^*(G)$ and Table 1, we have

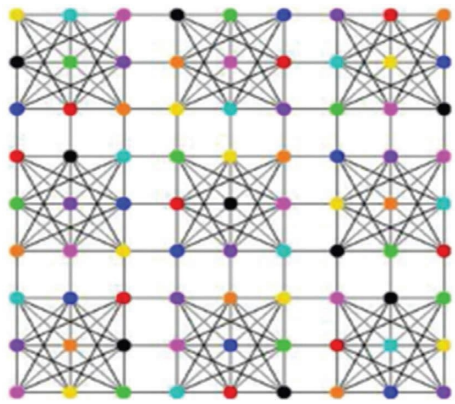

Figure 1: The Sudoku nanosheet $SK_{n\times n}$ for $r = 3$.

Table 1: Edge partition of Sudoku nanosheet $SK_{n\times n}$.

α_i	Edge partition	Frequency
α_1	$\alpha_{(5,7)}$	8
α_2	$\alpha_{(5,8)}$	12
α_3	$\alpha_{(6,6)}$	$4r-4$
α_4	$\alpha_{(4,7)}$	$8r$
α_5	$\alpha_{(6,8)}$	$32r-40$
α_6	$\alpha_{(7,7)}$	$4r^4$
α_7	$\alpha_{(7,8)}$	$20r^2-36r+20$
α_8	$\alpha_{(8,8)}$	$10r^2-14r+4$

$$\begin{aligned}
F_N^*(G) &= \sum_{mn\in E(G)} \left[\alpha_G(m)^2 + \alpha_G(n)^2\right] \\
&= \left|\alpha_{(5,7)}\right|(25+49) + \left|\alpha_{(5,8)}\right|(25+64) + \left|\alpha_{(6,6)}\right|(36+36) + \left|\alpha_{(4,7)}\right|(16+49) + \left|\alpha_{(6,8)}\right|(36+64) \\
&\quad + \left|\alpha_{(7,7)}\right|(49+49) + \left|\alpha_{(7,8)}\right|(49+64) + \left|\alpha_{(8,8)}\right|(64+64) \\
&= (8)(74) + (12)(89) + (4r-4)(72) + (8r)(65) + (32r-40)(100) + 4r^4(98) \\
&\quad + \left(20r^2 - 36r + 20\right)(113) + 10r^2 - 14r + 4(128) \\
&= 392r^4 + 3540r^2 + 1852r + 144.
\end{aligned} \tag{10}$$

Theorem 2. *Assume that G denotes the Sudoku nanosheet, then the Neighborhood version of first multiplicative Zagreb index is* $M_1^*(G) = 56r^4 + 460r^2 - 180r + 8$

Proof. By using the definition of M_1^* and Table 1, we can write as follows:

$$\begin{aligned}
M_1^*(G) &= \sum_{mn\in E(G)} \left[\alpha_G(m) + \alpha_G(n)\right] \\
&= \sum_{mn\in E(5,7)} \left[\alpha_G(u) + \alpha_G(v)\right] + \sum_{mn\in E(5,8)} \left[\alpha_G(u) + \alpha_G(v)\right] \\
&\quad + \sum_{mn\in E(6,6)} \left[\alpha_G(u) + \alpha_G(v)\right] + \sum_{mn\in E(4,7)} \left[\alpha_G(u) + \alpha_G(v)\right] \\
&\quad + \sum_{mn\in E(6,8)} \left[\alpha_G(u) + \alpha_G(v)\right] + \sum_{mn\in E(7,7)} \left[\alpha_G(u) + \alpha_G(v)\right] \\
&\quad + \sum_{mn\in E(7,8)} \left[\alpha_G(u) + \alpha_G(v)\right] + \sum_{mn\in E(8,8)} \left[\alpha_G(u) + \alpha_G(v)\right]
\end{aligned}$$

$$
\begin{aligned}
&= \left|\alpha_{(5,7)}\right|(5+7) + \left|\alpha_{(5,8)}\right|(5+8) + \left|\alpha_{(6,6)}\right|(6+6) + \left|\alpha_{(4,7)}\right|(4+7) \\
&\quad + \left|\alpha_{(6,8)}\right|(6+8) + \left|\alpha_{(7,7)}\right|(7+7) + \left|\alpha_{(7,8)}\right|(7+8) + \left|\alpha_{(8,8)}\right|(8+8) \\
&= 12(8) + 13(12) + 12(4r-4) + 11(8r) + 14(32r-40) + 14\left(4r^4\right) \\
&\quad + 15\left(20r^2 - 36r + 20\right) + 16\left(10r^2 - 14r + 4\right) \\
M_1^*(G) &= 56r^4 + 460r^2 - 180r + 8.
\end{aligned} \tag{11}
$$

□

Theorem 3. *Assume that G denotes the Sudoku nanosheet, then the Neighborhood version of second Zagreb index is* $M_2^*(G) = 196r^4 + 1760r^2 - 1008r + 72$

Proof. According to the definition of M_2^* and Table 1, we can write as follows:

$$
\begin{aligned}
M_2^*(G) &= \sum_{mn\in E(G)} \left[\alpha_G(m) \times \alpha_G(n)\right] \\
&= \sum_{mn\in E(5,7)} \left[\alpha_G(m) \times \alpha_G(n)\right] + \sum_{mn\in E(5,8)} \left[\alpha_G(m) \times \alpha_G(n)\right] \\
&\quad + \sum_{mn\in E(6,6)} \left[\alpha_G(m) \times \alpha_G(n)\right] + \sum_{mn\in E(4,7)} \left[\alpha_G(m) \times \alpha_G(n)\right] \\
&\quad + \sum_{mn\in E(6,6)} \left[\alpha_G(m) \times \alpha_G(n)\right] + \sum_{mn\in E(7,7)} \left[\alpha_G(m) \times \alpha_G(n)\right] \\
&\quad + \sum_{mn\in E(7,8)} \left[\alpha_G(m) \times \alpha_G(n)\right] + \sum_{mn\in E(7,7)} \left[\alpha_G(m) \times \alpha_G(n)\right] \\
&= \left|\alpha_{(5,7)}\right|(5\times 7) + \left|\alpha_{(5,8)}\right|(5\times 8) + \left|\alpha_{(6,6)}\right|(6\times 6) + \left|\alpha_{(4,7)}\right|(4\times 7) \\
&\quad + \left|\alpha_{(6,8)}\right|(6\times 8) + \left|\alpha_{(7,7)}\right|(7\times 7) + \left|\alpha_{(7,8)}\right|(7\times 8) + \left|\alpha_{(8,8)}\right|(8\times 8) \\
&= 280 + 480 + 144r - 144 + 224r + 1536r - 1920 + 196r^4 \\
&\quad + 1120r^2 - 2016 + 1120 + 640r^2 - 896r + 256 \\
M_2^*(G) &= 196r^4 + 1760r^2 - 1008r + 72.
\end{aligned} \tag{12}
$$

□

Theorem 4. *Assume that G denotes the Sudoku nanosheet, then the Neighborhood version of hyper-Zagreb index is* $HM_N(G) = 784r^4 + 7060r^2 - 3868r + 288$.

Proof. According to the definition of HM_N and Table 1, we can write as follows:

$$
\begin{aligned}
\mathrm{HM}_N(G) &= \sum_{mn\in E(G)} \left[\alpha_G(m) + \alpha_G(n)\right]^2, \\
\mathrm{HM}_N(G) &= \sum_{mn\in E(5,7)} \left[\alpha_G(m) + \alpha_G(n)\right]^2 + \sum_{mn\in E(5,8)} \left[\alpha_G(m) + \alpha_G(n)\right]^2 \\
&\quad + \sum_{mn\in E(6,6)} \left[\alpha_G(m) + \alpha_G(n)\right]^2 + \sum_{mn\in E(4,7)} \left[\alpha_G(m) + \alpha_G(n)\right]^2 \\
&\quad + \sum_{mn\in E(6,8)} \left[\alpha_G(m) + \alpha_G(n)\right]^2 + \sum_{mn\in E(7,7)} \left[\alpha_G(m) + \alpha_G(n)\right]^2 \\
&\quad + \sum_{mn\in E(7,8)} \left[\alpha_G(m) + \alpha_G(n)\right]^2 + \sum_{mn\in E(8,8)} \left[\alpha_G(m) + \alpha_G(n)\right]^2,
\end{aligned} \tag{13}
$$

$$
\begin{aligned}
\mathrm{HM}_N(G) &= \left|\alpha_{(5,7)}\right|(5+7)^2 + \left|\alpha_{(5,8)}\right|(5+8)^2 + \left|\alpha_{(6,6)}\right|(6+6)^2 + \left|\alpha_{(4,7)}\right|(4+7)^2 \\
&\quad + \left|\alpha_{(6,8)}\right|(6+8)^2 + \left|\alpha_{(7,7)}\right|(7+7)^2 + \left|\alpha_{(7,8)}\right|(7+8)^2 + \left|\alpha_{(8,8)}\right|(8+8)^2 \\
&= 1152 + 2028 + 576r - 576 + 968r + 6272r - 7840 + 784r^4 + 4500r^2 - 8100r + 4500 + 2560r^2 - 3584r + 1024 \\
&= 784r^4 + 7060r^2 - 3868r + 288.
\end{aligned}
$$

□

Theorem 5. *Assume that G denotes the Sudoku nanosheet, then the sambor index is*

$$\mathrm{SO}(G) = 39.59r^4 + 325.73r^2 - 122.631r + 5.919. \tag{14}$$

Proof. According to the definition of $\mathrm{S0}(G)$ and Table 1, we have

$$\begin{aligned}
\mathrm{S0}(G) &= \sum_{mn\in E(G)} \sqrt{\alpha_G(m)^2 + \alpha_G(n)^2} \\
&= \sqrt{25+49}\,(8) + \sqrt{25+64}\,(12) + \sqrt{36+36}\,(4r-4) + \sqrt{16+49}\,(8r) \\
&\quad + \sqrt{36+64}\,(32r-40) + \sqrt{49+49}\left(4r^4\right) + \sqrt{49+64}\left(20r^2-36r+20\right) + \sqrt{64+64}\left(10r^2-14r+4\right) \\
&= \sqrt{74}(8) + \sqrt{89}(12) + 6\sqrt{2}(4r-4) + \sqrt{65}(8r) + (10)(32r-40) + 7\sqrt{2}\left(4r^4\right) \\
&\quad + \sqrt{113}\left(20r^2-36r+20\right) + 8\sqrt{2}\left(10r^2-14r+4\right) \\
\mathrm{S0}(G) &= 39.59r^4 + 325.73r^2 - 122.631r + 5.91.
\end{aligned} \tag{15}$$

□

Theorem 6. *Assume that G denotes the Sudoku nanosheet, then the reduced sambor index is* $S0_{red}(G) = 33.941r^4 + 218.331r^2 - 113.275r + 6.049$.

Proof. Through analysis of the definition of $\mathrm{SO}_{\mathrm{red}}(G)$ as well as Table 1, we can write as follows:

$$\begin{aligned}
\mathrm{S0}_{\mathrm{red}}(G) &= \sum_{mn\in E(G)} \sqrt{\left[(\alpha_m-1)^2 + (\alpha_n-1)^2\right]} \\
&\quad + \sqrt{16+36}\,(8) + \sqrt{16+49}\,(12) + \sqrt{25+25}\,(4r-4) + \sqrt{9+36}\,(8r) \\
&\quad + \sqrt{25+49}\,(32r-40) + \sqrt{36+36}\left(4r^4\right) + \sqrt{36+49}\left(20r^2-36r+20\right) + \sqrt{49+49}\left(10r^2-14r+4\right) \\
&= \sqrt{52}(8) + \sqrt{65}(12) + \sqrt{50}(4r-4) + \sqrt{45}\,(8r) + \sqrt{74}(32r-40) + \sqrt{72}\left(4r^4\right) \\
&\quad + \sqrt{85}\left(20r^2-36r+20\right) + \sqrt{98}\left(10r^2-14r+4\right) \\
&= 33.941r^4 + 218.331r^2 - 113.275r + 6.049.
\end{aligned} \tag{16}$$

□

Theorem 7. *Assume that G denotes the Sudoku nanosheet, then the Argumented Zagreb Index is* $AZI(G) = 272.33r^4 + 2553.6r^2 - 1738.966r + 153.955$

Proof. Through analysis of the definition of $\mathrm{AZI}(G)$ as well as Table 1, we have

$$\begin{aligned}
&\left(\frac{5\times 7}{5+7-2}\right)^3(8) + \left(\frac{5\times 8}{5+8-2}\right)^3(12) + \left(\frac{6\times 6}{6+6-2}\right)^3(4r-4) + \left(\frac{4\times 7}{4+7-2}\right)^3(8r) + \left(\frac{6\times 8}{6+8-2}\right)^3 \\
&\quad \cdot (32r-40) + \left(\frac{7\times 7}{7+7-2}\right)^3\left(4r^4\right) + \left(\frac{7\times 8}{7+8-2}\right)^3\left(20r^2-36r+20\right) + \left(\frac{8\times 8}{8+8-2}\right)^3\left(10r^2-14r+4\right) \\
&= 343 + 576.979 + 186.624r - 186.624 + 240.89r + 2048r - 2560 + 272.33r^4 \\
&\quad + 1598.6r^2 - 2877.48 + 1598.6 + 955r^2 - 1337r + 382 \\
&= 272.33r^4 + 2553.6r^2 - 1738.966r + 153.955.
\end{aligned} \tag{17}$$

□

2. Comparison and Concluding Remarks

This study ciphered a few novel topological indices for $\mathrm{SK}_{(r\times r)}$ and their formulas. The knowing topological indices are the modified neighborhood version of Forgotten topological index F_N^*, the neighborhood version of the first multiplicative Zagreb M_1^*, the neighborhood version of the second Zagreb index M_2^*, the neighborhood version of

Table 2: Numerical table corresponding with the structure of the Sudoku graph.

[r]	$F_N^*(G)$	$M_1^*(G)$	$M_2^*(G)$	$HM_N(G)$	$SO(G)$	$SO_{red}(G)$	$AZI(G)$
[1]	2134	344	1020	4264	248.608	145.046	1240.919
[2]	16872	2384	8232	33336	1697.017	1195.879	11247.703
[3]	58200	8144	28764	115728	5776.386	4380.424	39978.187
[4]	149728	20984	74376	288480	14862.115	11735.141	103772.171
[5]	324384	45608	161532	647448	32279.764	26111.074	225505.375
[6]	624504	88064	311400	1247304	62305.053	51173.851	434589.43
[7]	1101832	155744	549852	2201536	110163.862	91403.684	766971.923
[8]	1817520	257384	907464	3632448	182032.231	152095.369	1265136.307
[9]	2842128	403064	1419516	5681160	285036.36	239358.286	1978101.991
[10]	4255624	604208	2125992	8507608	427252.609	360116.39	2961424.295

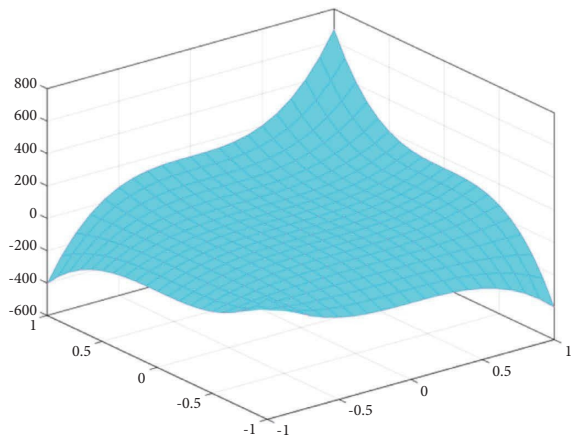

Figure 2: The correlation of r and FN*.

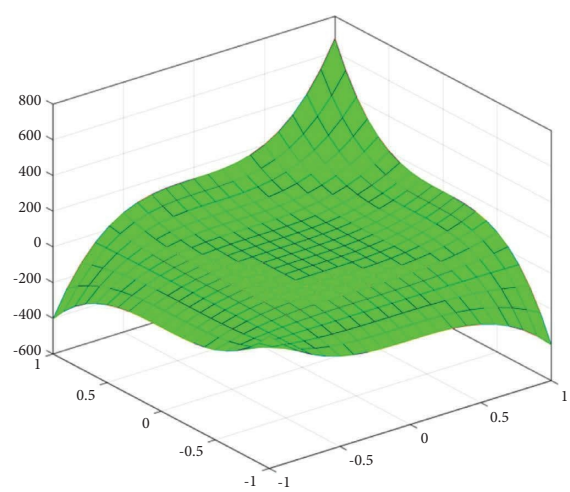

Figure 3: The correlation of r and $M_1{}^*$.

hyper-Zagreb index HM_N. The Sambor topological index $SO(G)$ and the Sambor reduced topological index $SO_{red}(G)$. Our ciphered consequence is really beneficial in the apprehension of the topology and ameliorates the material characteristics of reserve $SK_{(r\times r)}$. As previously stated, the beyond-ciphered indices F_N^*, M_1^*, M_2^*, HM_N, SO and SO_{red} have the best tie-up with entropy and acentric factor; therefore, the particular dynamic in QSAR and QSPR anatomy with robust precision. Their ability to distinguish between isomer momentous as opposed to other degree-based indices is extraneous. Meanwhile, Table 2 and Figures 2–8 indicate that all the considered indices also increase when we increase. This implies that there is a direct proportion between r the considered indices. In Figure 9, we

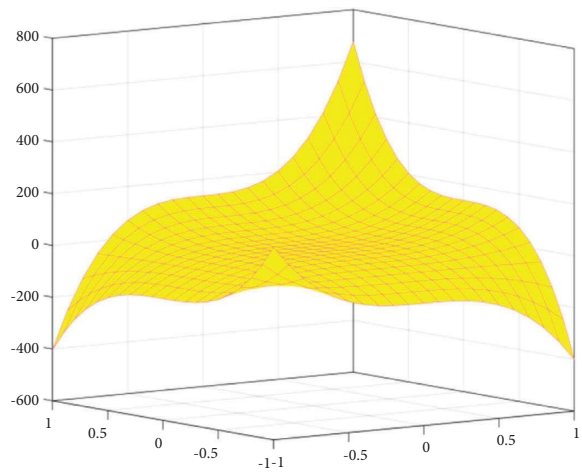

Figure 4: The correlation of r and $M_2{}^*$.

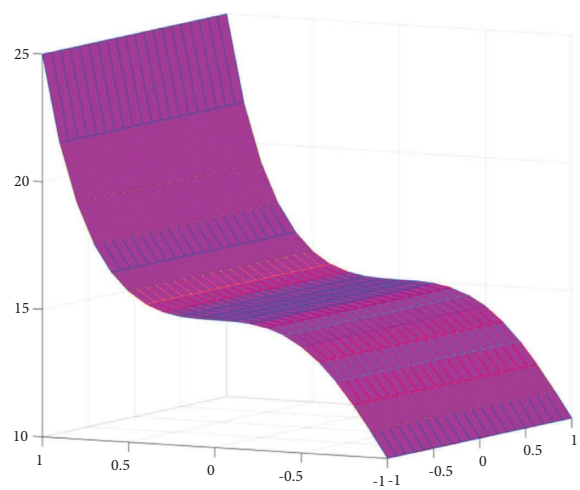

Figure 5: The correlation of r and HM_N.

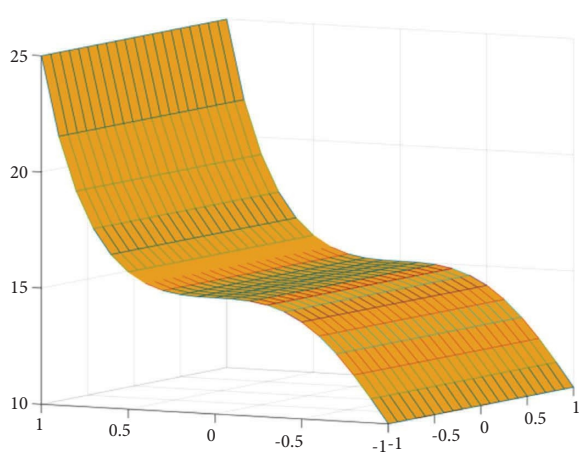

Figure 6: The correlation of r and $\mathrm{SO}(G)$.

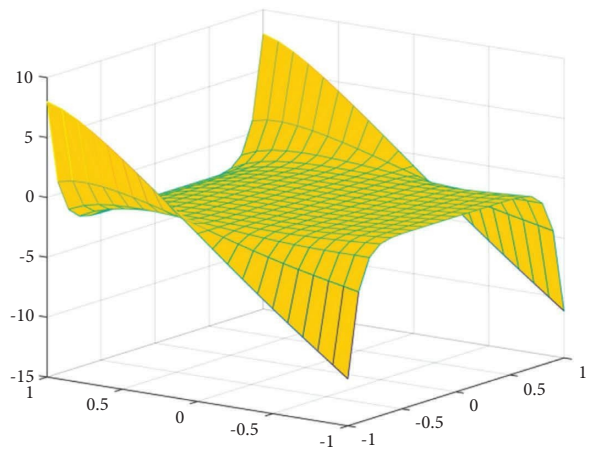

Figure 7: The correlation of r and $SO_{red}(G)$.

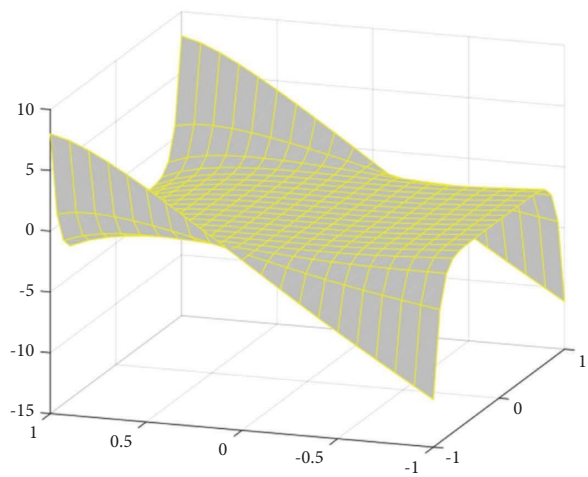

Figure 8: The correlation of r and AZI.

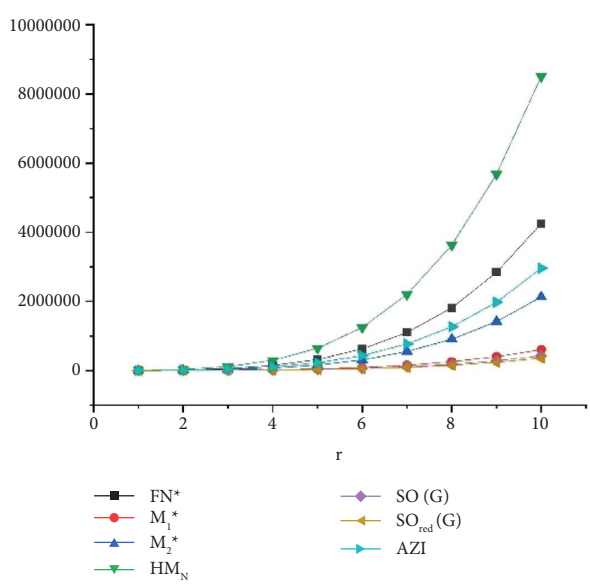

Figure 9: Correlation of r with obtained indices.

collate all the indices together, reflecting that HM_N they increase more speedily than other indices. Similarly, $SO_{red}(G)$ it increases slower than other indices.

Data Availability

There are no data associated with this article.

Additional Points

There is no code available for this article.

Conflicts of Interest

The authors declare that there are no conflicts of interest.

Authors' Contributions

All authors have equally contributed to this manuscript in all stages, from conceptualization to the write up of final draft.

References

[1] D. G. Papageorgiou, I. A. Kinloch, and R. J. Young, "Mechanical properties of graphene and graphene-based nanocomposites," *Progress in Materials Science*, vol. 90, pp. 75–127, 2017.

[2] S. Zaman, "Spectral analysis of three invariants associated to random walks on rounded networks with 2 n-pentagons," *International Journal of Computer Mathematics*, vol. 99, no. 3, pp. 465–485, 2022.

[3] G. Wang, L. Yan, S. Zaman, and M. Zhang, "The connective eccentricity index of graphs and its applications to octane isomers and benzenoid hydrocarbons," *International Journal of Quantum Chemistry*, vol. 120, no. 18, Article ID e26334, 2020.

[4] S. Iijima and T. Ichihashi, "Single-shell carbon nanotubes of 1 nm diameter," *Nature*, vol. 363, no. 6430, pp. 603–605, 1993.

[5] D. S. Bethune, C. H. Kiang, M. S. de Vries et al., "Cobalt-catalysed growth of carbon nanotubes with single-atomic-layer walls," *Nature*, vol. 363, no. 6430, pp. 605–607, 1993.

[6] J. N. Coleman, M. Lotya, A. O'Neill et al., "Two-dimensional nanosheets produced by liquid exfoliation of layered materials," *Science*, vol. 331, no. 6017, pp. 568–571, 2011.

[7] K. J. Burch, "Chapter 8—chemical applications of graph theory," in *Mathematical Physics in Theoretical Chemistry*, S. M. Blinder and J. E. House, Eds., pp. 261–294, Elsevier, Amsterdam, Netherlands, 2019.

[8] M. Randic, "Nenad trinajstic—pioneer of chemical graph theory," *Croatica Chemica Acta*, vol. 77, pp. 1–15, 2004.

[9] R. Todeschini and V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley, New York, NY, USA, 2009.

[10] A. Ullah, A. Zeb, and S. Zaman, "A new perspective on the modeling and topological characterization of H-naphtalenic nanosheets with applications," *Journal of Molecular Modelling*, vol. 28, no. 8, p. 211, 2022.

[11] U. Muhammad, A. Uzairu, and D. Ebuka Arthur, "Review on: quantitative structure activity relationship (QSAR) modeling," *Journal of Analytical & Pharmaceutical Research*, vol. 7, no. 2, p. 240, 2018.

[12] C. Nantasenamat, C. Isarankura-Na-Ayudhya, T. Naenna, and V. Prachayasittikul, "A practical overview of quantitative structure-activity relationship," *EXCLI Journal*, vol. 8, 2009.

[13] A. Ullah, M. Qasim, S. Zaman, and A. Khan, "Computational and comparative aspects of two carbon nanosheets with respect to some novel topological indices," *Ain Shams Engineering Journal*, vol. 13, no. 4, Article ID 101672, 2022.

[14] D. Joudaki and F. Shafiei, "QSPR models to predict thermodynamic properties of cycloalkanes using molecular descriptors and GA-MLR method," *Current Computer-Aided Drug Design*, vol. 16, no. 1, pp. 6–16, 2020.

[15] J. Dinar, Z. Hussain, S. Zaman, and S. Ur Rehman, "Wiener index for an intuitionistic fuzzy graph and its application in water pipeline network," *Ain Shams Engineering Journal*, vol. 14, no. 1, Article ID 101826, 2023.

[16] H. Wiener, "Structural determination of paraffin boiling points," *Journal of the American Chemical Society*, vol. 69, no. 1, pp. 17–20, 1947.

[17] R. Janoschek, "Mathematik um konstitutionsformeln: mathematical concepts in organic chemistry. Von I. Gutman und O. E. Polansky. Springer-Verlag, Berlin—Heidelberg—New York—Tokyo 1986. 28 Abb., X, 212 S., DM 128,-. ISBN 3-540-16235-6," *Nachrichten aus Chemie, Technik und Laboratorium*, vol. 35, no. 1, pp. 34–41, 1987.

[18] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons," *Chemical Physics Letters*, vol. 17, no. 4, pp. 535–538, 1972.

[19] B. Furtula, I. Gutman, and M. Dehmer, "On structure-sensitivity of degree-based topological indices," *Applied Mathematics and Computation*, vol. 219, no. 17, pp. 8973–8978, 2013.

[20] P. Ali, S. A. K. Kirmani, O. Al Rugaie, and F. Azam, "Degree-based topological indices and polynomials of hyaluronic acid-curcumin conjugates," *Saudi Pharmaceutical Journal*, vol. 28, no. 9, pp. 1093–1100, 2020.

[21] Y. C. Kwun, A. Ali, W. Nazeer, M. Ahmad Chaudhary, and S. M. Kang, "M-polynomials and degree-based topological indices of triangular, hourglass, and jagged-rectangle benzenoid systems," *Journal of Chemistry*, vol. 2018, Article ID 8213950, 8 pages, 2018.

[22] S. Hayat and M. Imran, "Computation of topological indices of certain networks," *Applied Mathematics and Computation*, vol. 240, pp. 213–228, 2014.

[23] W. Gao, M. Younas, A. Farooq, A. Mahboob, and W. Nazeer, "M-polynomials and degree-based topological indices of the crystallographic structure of molecules," *Biomolecules*, vol. 8, no. 4, p. 107, 2018.

[24] S. Guo and S. Dong, "Graphene nanosheet: synthesis, molecular engineering, thin film, hybrids, and energy and analytical applications," *Chemical Society Reviews*, vol. 40, no. 5, pp. 2644–2672, 2011.

[25] Q. Li, S. Zaman, W. Sun, and J. Alam, "Study on the normalized Laplacian of a penta-graphene with applications," *International Journal of Quantum Chemistry*, vol. 120, no. 9, Article ID e26154, 2020.

[26] I. Khan, K. Saeed, and I. Khan, "Nanoparticles: properties, applications and toxicities," *Arabian Journal of Chemistry*, vol. 12, no. 7, pp. 908–931, 2019.

[27] S. Zaman, F. A. Abolaban, A. Ahmad, and M. A. Asim, "Maximum $ H $-index of bipartite network with some given parameters," *AIMS Mathematics*, vol. 6, no. 5, pp. 5165–5175, 2021.

[28] S. Zaman, "Cacti with maximal general sum-connectivity index," *Journal of Applied Mathematics and Computing*, vol. 65, no. 1-2, pp. 147–160, 2021.

[29] I. Gutman, B. Ruščić, N. Trinajstić, and C. F. Wilcox, "Graph theory and molecular orbitals. XII. Acyclic polyenes," *The*

Journal of Chemical Physics, vol. 62, no. 9, pp. 3399–3405, 1975.

[30] K. Pattabiraman and M. Vijayaragavan, "Hyper Zagreb indices and its coindices of graphs," *Bulletin of International Mathematical Virtual Institute*, vol. 7, no. 1, pp. 31–41, 2017.

[31] I. Gutman, "Some basic properties of Sombor indices," *Open Journal of Discrete Applied Mathematics*, vol. 4, no. 1, pp. 1–3, 2021.

[32] B. Furtula, A. Graovac, and D. Vukičević, "Augmented Zagreb index," *Journal of Mathematical Chemistry*, vol. 48, no. 2, pp. 370–380, 2010.