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Modeling Porphyrazine Properties: Entropy and Topological Indices through Linear Regression

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ABSTRACT: In this study, we examined topological-index-based entropy measures for subdivided cage networks. In particular, we compute several entropies: Randic, atom bond connection, first, second, Hyper, and redefining Zagreb. We used the linear fit method to analyze the graphical behavior of the different entropy metrics. The results provide insights into the complex connectivity and structural characteristics of the porphyrazine structure by highlighting trends in the distribution of entropy values and their interactions. This study enhances our understanding of the dynamics of porphyrazine structures and offers a visual framework for analyzing their behavior.

Keywords: Topological indices, por-phyrazine structure, Zagreb index, redefined Zagreb index.

Contents

1. Introduction

By combining chemical principles with mathematical ideas and methods, mathematical chemistry is an interdisciplinary field that investigates a variety of chemical processes. The use of quantitative frameworks bridges the gap between theoretical models and empirical data to help comprehend and interpret chemical processes. Statistical analysis, linear algebra, graph theory, and differential equations are some of the techniques used in mathematical chemistry.

Topological indices are numerical quantities that can be computed from the topology or a molecular graph of a chemical compound. They offer a method for identifying molecular structural characteristics that are unaffected by atomic details or spatial arrangements. To understand the many chemical and physical properties of molecules, one must have a solid understanding of topological features, such as cycles, branching patterns, and molecular connections, all of which are included in these indices. In computational chemistry, chemoinformatics, and quantitative structure-activity relationship (QSAR) investigations, topological indices are frequently employed to forecast molecular characteristics, such as reactivity, solubility, and biological activity, based on their structural aspects.

The study of molecular structures and bonding is crucial to mathematical chemistry. Graph theory is essential to this field of study because molecules are represented as graphs, with atoms as nodes τ and chemical bonds as edges $E(G)$. The total number of edges incident to vertex r is its degree, denoted as ξ_τ. It aids researchers in examining the characteristics, forecasting actions, and deciphering intricate chemical structures. [1] Salamat et al. (2021) computed a number of degree-based indices. To recognize and produce new Researchers can use the ideas and techniques of graph theory to better understand molecules with specific properties and functions. This understanding can be applied to the general three-dimensional form of molecules, arrangement of bonds, and interactions between atoms [2] (Zhao et al., 2023). The concepts and techniques of graph theory have shed light on the symmetry, coupling, and reaction mechanisms of molecules. Furthermore, it is easier to predict and produce new compounds

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with the necessary qualities when mathematical tools are used to understand the relationship between structure and features [3] (Estrada et al. 1998).

Entropy quantifies the level of uncertainty or randomness in a graph structure. By considering the distribution of vertices and edges as well as their connection patterns, this metric assesses the level of disorder or complexity inside the network.

A novel entropy metric proposed by Lu et al. (2022) [4] to help us comprehend the structural features of weighted graphs captures the intricacy and unpredictability of the weighted networks. They discussed the regression model for different chemical structures in [5] HAVARE BC (Çolakoğlu Havare and Havare 2019). In addition to describing its possible use in a number of domains, including network research, pattern recognition, and data mining, this study provides a thorough theoretical foundation for estimating edge-weighted graph entropy. [6] Ghani et al. discussed entropy in 2023. The conclusions of this research advance graph theory and offer new perspectives for the investigation of complex networks.

The design and characterization of graphite carbon nitride-based materials, particularly in photocatalysis and energy storage applications, are greatly influenced by the conclusions of this study. The topic of topological indices was covered by Salamat et al. (2021). These discoveries provide important new insights into the characteristics, behavior, and performance of these materials, enabling better engineering and optimization to increase their efficacy and efficiency in a variety of practical applications. Computed entropy in many networks. As a result, the research findings expand technologies in the areas of energy storage, environmental sanitation, and renewable energy production, which may pave the way for the further development of clean and sustainable energy sources.

To predict and describe a range of physicochemical properties of breast cancer treatments, including bioactivity, toxicity, and solubility, [7] Rauf et al. (2022) employed entropy indices as descriptors. The topological indices of different graphs have been discussed by Ghani et al. (2023). This study helps to develop computational tools and approaches for drug discovery and design in the treatment of breast cancer by shedding light on the relationship between these entropy indices and the physiochemical characteristics of breast cancer drugs through meticulous data analysis and statistical modeling.

Mathematical chemistry uses graph invariants, numerical values derived from molecular graphs, to describe the significant characteristics of organic components [8] (Gao et al. 2017) [9] Imran et al. 2018). A type of topological index, degree-based indices are frequently used to forecast several physicochemical characteristics of chemical compounds, including stability, energy dissipation, boiling point, bioactivity, and many more. [10] According to Randic (1975) and [11] Siddiqui, Imran, and Ahmad (2016), these indices are essential for understanding the properties and actions of chemicals under various conditions. The significance of these indices in real-world chemical applications makes them essential in theoretical chemistry. Several molecular graphs, such as chemical graph products, carbon nanotubes, and generalized bridge molecular networks, were thoroughly examined by [12,13,14] Zhang et al. (Zhang et al. 2018). [15] Ravi et al. (2023) discussed QSPR analysis. According to Zhang, Muhammad Awais, and Javaid (2019), they most likely looked into the mathematical properties and traits of these various types of molecular structures in their study, highlighting how topological indices could offer helpful information about their connections, forms, and other crucial components. A physical investigation of heat production and entropy in cerium oxide was also presented by [16] Zhang et al. (Zhang et al. 2022).

2. Preliminaries

In communication theory, Shannon first proposed the idea of information entropy [17,18] (Shannon 1948). Nevertheless, it was eventually found that information entropy applies to molecular networks among other domains [19,20,21,22] (Bonchev 2003; Karreman 1955; Rashevsky 1955). Information entropy is used in chemistry for two primary reasons. First, it can be used to assess the complexity of chemical structures as structural descriptors (Bonchev, 1995). [23] According to Castellano and Torrens (2015), this application is useful for classifying natural and synthetic chemicals, numerically differentiating isomers of organic molecules, and establishing relationships between structural and physicochemical characteristics [24] (Bonchev and Trinajsti 1977). Second, physicochemical process analysis and information transmission simulations can benefit from the use of information entropy.

The numerous topological indices are listed in Table 1

Table 1: Degree-based topological Indices

Topological Index	Notation	Formula
Randic	$R(G)$	$R(G) = \sum\limits_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$
Atom Bond Connectivity	$ABC(G)$	$ABC(G) = \sum\limits_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$
Geometric Arithmetic	$GA(G)$	$GA(G) = \sum\limits_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$
First Zagreb	$M_1(G)$	$M_1(G) = \sum\limits_{v \in V(G)} {d_v}^2 = \sum\limits_{uv \in E(G)} d_u + d_v$
Second Zagreb	$M_2(G)$	$M_2(G) = \sum\limits_{uv \in E(G)} d_u d_v$
Hyper Zagreb	$HM(G)$	$HM(G) = \sum\limits_{uv \in E(G)} (d_u + d_v)^2$
Forgotten	$F(G)$	$F(G) = \sum\limits_{uv \in E(G)} \left({d_u}^2 + {d_v}^2\right)$
Third Zagreb	$M_3(G)$	$M_3(G) = \sum\limits_{uv \in E(G)} \lvert d_u - d_v \rvert$
First Redefined Zagreb	$\operatorname{Re} ZG_1(G)$	$\operatorname{Re} ZG_1(G) = \sum\limits_{uv \in E(G)} \frac{d_u + d_v}{\sqrt{d_u d_v}}$
Second Redefined Zagreb	$\operatorname{Re} ZG_2(G)$	$\operatorname{Re} ZG_2(G) = \sum\limits_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}$
Third Redefined Zagreb	$\operatorname{Re} ZG_3(G)$	$\operatorname{Re} ZG_3(G) = \sum\limits_{uv \in E(G)} \frac{(d_u + d_v)^2}{\sqrt{d_u d_v}}$

The base of the logarithm in this discussion is assumed to be e. A graph G's vertex set, edge set, and edge weight are represented by the variablesG_V, G_E, and$G(rs)$ Previous research has calculated a number of graph entropies using graph order, vertex degrees, and characteristic polynomials. [25] According to Manzoor, Siddiqui, and Ahmad (2020), graph entropies based on independent sets, matchings, and vertex degrees have been the subject of recent studies. Several connections between Hosoya entropy and graph complexity were proposed by Dehmer and Mowshowitz [26] (Cao and Dehmer 2015). [?,28] Additional sources for research and analysis include Morowitz (1955), Shannon (2001), and Sol and Valverde (2004).

$$ENT_{\tau}(G) = -\sum_{r' s' \in E_i(G)} \frac{\tau\left(r' s'\right)}{\sum\limits_{r s \in E_i(G)} \tau(r s)} \log\left[\frac{\tau\left(r' s'\right)}{\sum\limits_{r s \in E_i(G)} \tau(r s)}\right] \text{———}(1)$$

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Entropy of Randic: After inserting the values from Table 1 into Equation 1 and performing simplifications, the final expression is as follows:

$$ENT_{R_a}(G) = \log(R_a) - \frac{1}{R_a}\sum_{i=1}^{m}\sum_{r s \in G_i} \log\left[\psi_r \times \psi_s\right]^{\psi_r \times \psi_s} \text{———}(2)$$

Entropy of atom-bond connectivity: The following is the final expression following simplifications and the entry of the values from Table 1 into Equation 1:

$$ENT_{ABC}(G) = \log(ABC) - \frac{1}{ABC}\sum_{i=1}^{m}\sum_{r s \in G_i} \log\left[\sqrt{\frac{\psi_r + \psi_s - 2}{\psi_r * \psi_s}}\right]^{\sqrt{\frac{\psi_r + \psi_s - 2}{\psi_r * \psi_s}}} \text{———}(3)$$

The entropy of geometric arithmetic: Following simplifications and the entry of the values from Table 1 into Equation 1, the resultant expression is as follows:

$$ENT_{GA}(G) = \log(GA) - \frac{1}{GA}\sum_{i=1}^{m}\sum_{r\,s\in G_i}\log\left[\frac{2\sqrt{\psi_r\times\psi_s}}{\psi_r+\psi_s}\right]^{\frac{2\sqrt{\psi_r\times\psi_s}}{\psi_r+\psi_s}} \text{———(4)}$$

Zagreb's first entropy: Following simplifications and the entry of the values from Table 1 into Equation 1, the resultant expression is as follows:

$$ENT_{M_1}(G) = \log(M_1) - \frac{1}{M_1}\sum_{i=1}^{m}\sum_{r\,s\in G_i}\log\left[\psi_r+\psi_s\right]^{\psi_r+\psi_s} \text{———(5)}$$

Zagreb's second entropy: Following simplifications and the entry of the values from Table 1 into Equation 1, the resultant expression is as follows:

$$ENT_{M_2}(G) = \log(M_2) - \frac{1}{M_2}\sum_{i=1}^{m}\sum_{r\,s\in G_i}\log\left[\psi_r\times\psi_s\right]^{\psi_r\times\psi_s} \text{———(6)}$$

Zagreb hyper-entropy: Following simplifications and the entry of the values from Table 1 into Equation 1, the resultant expression is as follows:

$$ENT_{HM}(G) = \log(HM) - \frac{1}{HM}\sum_{i=1}^{m}\sum_{r\,s\in G_i}\log\left[(\psi_r\times\psi_s)^2\right]^{(\psi_r\times\psi_s)^2} \text{———(7)}$$

Entropy forgotten: The following is the final expression following simplifications and the entry of the values from Table 1 into Equation 1:

$$ENT_{F}(G) = \log(F) - \frac{1}{F}\sum_{i=1}^{m}\sum_{r\,s\in G_i}\log\left[\left({\psi_r}^2+{\psi_s}^2\right)\right]^{\left({\psi_r}^2+{\psi_s}^2\right)} \text{———(8)}$$

Zagreb's third entropy: Following simplifications and the entry of the values from Table 1 into Equation 1, the resultant expression is as follows:

$$ENT_{M_3}(G) = \log(M_3) - \frac{1}{M_3}\sum_{i=1}^{m}\sum_{r\,s\in G_i}\log\left[(\psi_r-\psi_s)\right]^{(\psi_r-\psi_s)} \text{———(9)}$$

The first Redefined Zagreb entropy: Following simplifications and the entry of the values from Table 1 into Equation 1, the resultant expression is as follows:

$$ENT_{\operatorname{Re}ZG_1}(G) = \log(\operatorname{Re}ZG_1) - \frac{1}{\operatorname{Re}ZG_1}\sum_{i=1}^{m}\sum_{r\,s\in G_i}\log\left[\left(\frac{\psi_r+\psi_s}{\psi_r\times\psi_s}\right)\right]^{\left(\frac{\psi_r+\psi_s}{\psi_r\times\psi_s}\right)} \text{———(10)}$$

The second Redefined Zagreb entropy: Following simplifications and the entry of the values from Table 1 into Equation 1, the resultant expression is as follows:

$$ENT_{\operatorname{Re}ZG_2}(G) = \log(\operatorname{Re}ZG_2) - \frac{1}{\operatorname{Re}ZG_2}\sum_{i=1}^{m}\sum_{r\,s\in G_i}\log\left[\left(\frac{\psi_r\times\psi_s}{\psi_r+\psi_s}\right)\right]^{\left(\frac{\psi_r\times\psi_s}{\psi_r+\psi_s}\right)} \text{———(11)}$$

Third Redefined Zagreb Index entropy: The following is the final expression following simplifications and the entry of the values from Table 1 into Equation 1:

$$ENT_{\operatorname{Re}ZG_3}(G) = \log(\operatorname{Re}ZG_3) - \frac{1}{\operatorname{Re}ZG_3}\sum_{i=1}^{m}\sum_{r\,s\in G_i}\log\left[(\psi_r\times\psi_s)\times(\psi_r+\psi_s)\right]^{(\psi_r\times\psi_s)\times(\psi_r+\psi_s)} \text{——(12)}$$

3. Results

Porphyrazine (Pzs) graph:

Porphyrazine is composed of meso-nitrogen atoms or azomethine bridges, which connect its aromatic rings rather than the methine bridges found in porphyrins. Two primary techniques are available to alter the physical properties and chemical attributes of these macro cycles. One technique involves changing the exterior structure with different substituents, whereas the other involves changing the metal captions at the core. The unique optical and electrochemical characteristics of porphyrazine make it useful for both technology and medicine. The three-dimensional structure of porphyrazine is shown on the left side of Figure 1, providing a better understanding of its molecular bonding. With 34 vertices and 41 edges, the two-dimensional unit structure ($n = 1$) is displayed on the right. Figure 1 shows the carbon atoms as gray dots, nitrogen atoms as blue dots, and hydrogen atoms as red dots. In addition, Fig. 2 shows two more detailed representations of the structure: porphyrazine units with 66 vertices and 82 edges joined ($n = 2$). A total of $32n + 2$ vertices and $41n$ edges make up the porphyrazine chemical graph for n. V_1 indicates that there are $5n + 4$ vertices of degree one, V_2 indicates that there are $6n - 2$ vertices of degree two, V_3 indicate that there are $20n$ vertices of degree three, and V_4 indicates that there are n vertices of degree five. Table 3 provides edge partitioning.

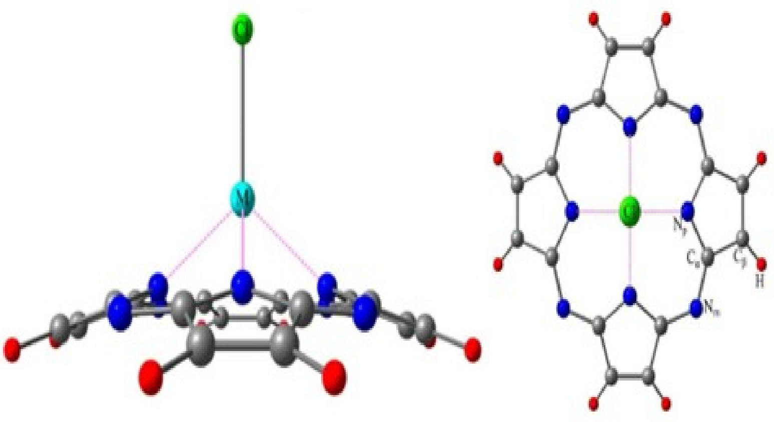

Figure 1: Unit molecular structure of Porphyrazine ($n = 1$)

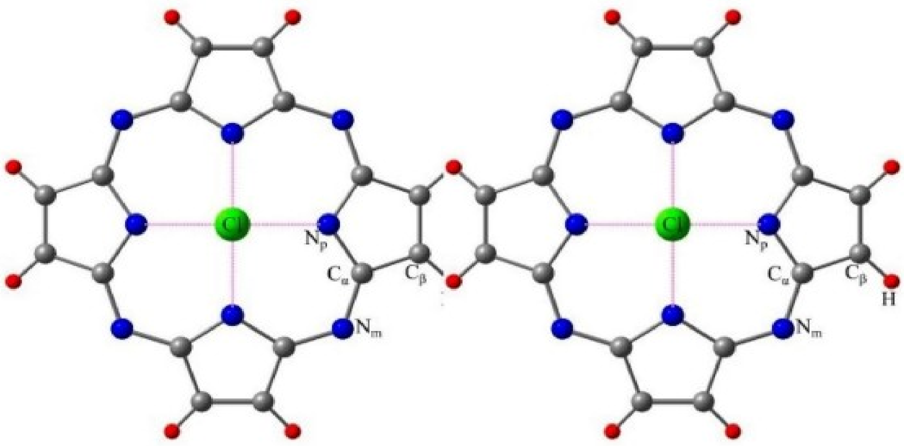

Figure 2: Porphyrazine's double molecular structure ($n = 2$)

Table 2: Edge Partitions of Porphyrazine's

d_r, d_s where $r\,s \in E\,(G)$	$(1,3)$	$(1,5)$	$(2,3)$	$(3,3)$	$(3,5)$
Number of edges	$4n+4$	n	$12n-4$	$20n$	$4n$

Porphyrazine Drawing Algorithms

You can ensure accuracy by using a step-by-step algorithmic technique when drawing the unit molecular structure of porphyrazine. The structure is composed of a macrocyclic ring with aza bridges and pyrrole-like units that alternate. Here's how to accomplish it:

Step 1: Identify the Fundamental Elements Core Shape: Porphyrazine's macrocycle is made up of four pyrrole units, giving it a square-like symmetry. Foundational Elements: Five-membered rings (C4N) with alternating single and double bonds are known as pyrrole rings.Aza Bridges: The pyrrole rings are joined by nitrogen atoms (N).
Step 2: Sketch the Central Symmetry of the Framework: To begin, draw a square pattern that serves as a guide and shows where the four pyrrole rings are located.Include Bridges for Nitrogen: To serve as the aza bridges, place a nitrogen atom (N) in each corner of the square.
Step 3: Build Pyrrole Units Hook together the Pyrrole Rings: Drawing a pyrrole unit (C 4 N) with the nitrogen atom of the pyrrole attached to the nearby aza bridge is done at each side of the square. Bonding Style: Change the pyrrole ring's single and double bonds. Attach the nitrogens of the aza bridge to the pyrrole's carbon atoms.
Step 4: Give Atoms of Hydrogen Pyrrole Units with Hydrogens: The valency of the outer carbon atoms is completed by the contribution of two hydrogens from each pyrrole unit. Aza Bridges have no hydrogens: Since they are involved in double bonding with the pyrrole units, the aza bridges (N) lack hydrogens.
Step 5: Check for Aromaticness Make sure the structure is aromatic throughout: The conjugated system ought to adhere to Huckel's rule, which states that $4n + 2$-electrons
Step 6: Atom Labeling Label the important atoms for clarity: The pyrrole units and aza bridges include nitrogen atoms. The pyrrole rings contain carbon atoms.
Step 7: Complete the Symmetry of the Drawing: Given that porphyrazine is a highly symmetric chemical, make sure the structure retains full symmetry. Indicators of Aroma: Delocalized electrons can optionally be indicated with dashed or curved arrows.

Table 3: Numerical comparison of topological indices

Index [m]	[1]	[2]	[3]	[4]	[5]	[6]	[7]	[8]	[9]	[10]
$R_1(G)$	317	646	975	1304	1633	1962	2291	2620	2949	3278
$R_{-1}(G)$	6.6	12.7	18.7	24.7	30.7	36.8	42.2	48.8	54.8	60.8
$R_{\frac{1}{2}}(G)$	111.1	225.2	339.2	453.3	567.3	681.4	795.4	909.5	1023.5	1137.6
$R_{-\frac{1}{2}}(G)$	16.0	31.3	46.7	62.0	77.4	92.8	108.1	123.5	138.8	154.2
$ABC(G)$	39.2	78.7	118.3	157.8	197.3	236.9	276.4	315.9	355.5	395.0
$GA(G)$	39.3	79.2	119.0	158.9	198.7	238.5	278.4	318.2	358.1	397.9
$M_1(G)$	230	464	698	932	1166	1400	1634	1868	2102	2336
$M_2(G)$	317	646	975	1304	1633	1962	2291	2620	2949	3278
$M_3(G)$	36	68	100	132	164	196	228	260	292	324
$HM(G)$	1340	2716	4092	5468	6844	8220	9596	10972	12348	13724
$FG(G)$	706	1424	2142	2860	3578	4296	5014	5732	6450	7168
$\mathrm{Re}\,ZG_1(G)$	34	66	98	130	162	194	226	258	290	322
$\mathrm{Re}\,ZG_2(G)$	53.9	109.6	165.4	221.1	276.8	332.6	388.3	444.0	499.8	555.5
$\mathrm{Re}\,ZG_3(G)$	1926	3924	5922	7920	9918	11916	13914	15912	17910	19908

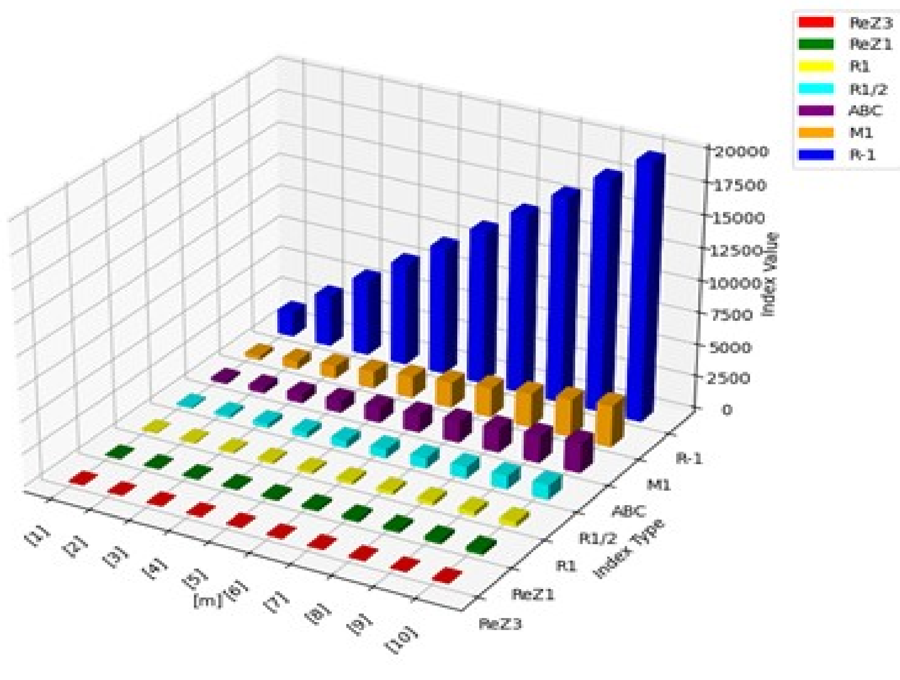

Figure 3: A visual comparison of several topological indices

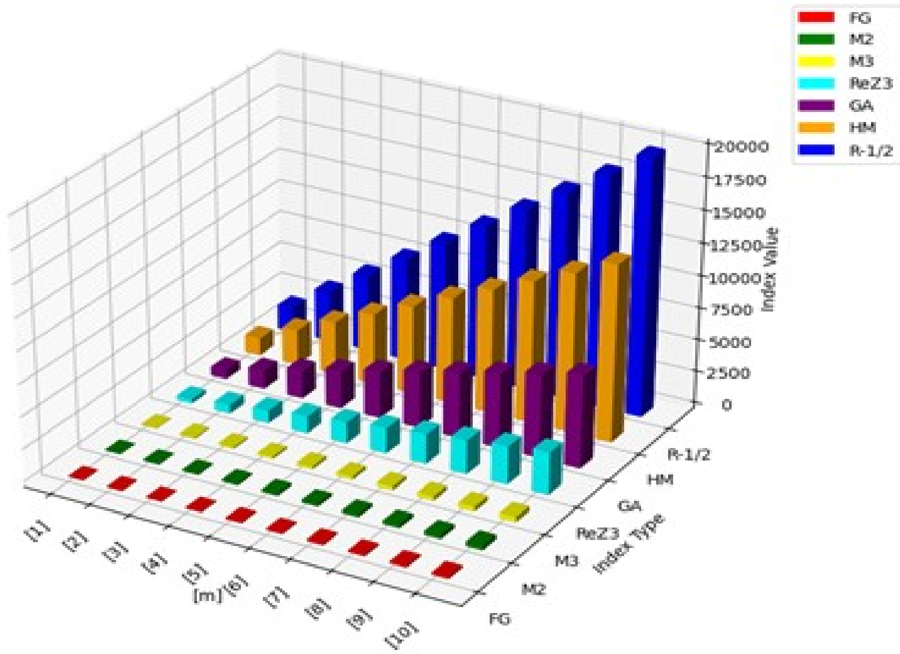

Figure 4: A visual comparison of several topological indices

It is clear from Table 3 and [Figure 4] that the Randi index increases noticeably faster than the other indices as m and n rise. Likewise, we can see in (Figure 5). Observe that the Third Redefined Zagreb Index shows a more noticeable growth rate than the other indices when m and n increase. Our work primarily focused on utilizing a range of topological indices to calculate the entropy measure. With this method, we can use the topological features of a system to quantify its complexity or information content.

Randic entropy of Porphyrazine (Pzs):

We may determine the Randic index for $\alpha = 1$ by using Table 2 and Equation 2.

$$ENT_{R_1}(Pzs) = \log(R_1) - \frac{1}{R_1}\sum_{i=1}^{m}\sum_{r\, s\in G_i} \log\left[\psi_r \times \psi_s\right]^{\psi_r \times \psi_s}$$

$$ENT_{R_1}(P_{zs}) = \log(329n-12) - \frac{(4n+4)\log(3^3)}{329n-12} - \frac{n\log(5^5)}{329n-12} - \frac{(12n-4)\log(6^6)}{329n-12} - \frac{20n\log(9^9)}{329n-12} - \frac{4n\log(15^{15})}{329n-12} \tag{3.1}$$

We may determine the Randic index for $\alpha = -1$ by using Table 2 and Equation 2.

$$\begin{aligned} ENT_{R_{-1}}(P_{zs}) = \log(6.0222n + 0.6666) &- \frac{(4n+4)\,\log\left(\left(\frac{1}{3}\right)^{1/3}\right)}{6.0222n+0.6666} + \frac{n\,\log\left(\left(\frac{1}{5}\right)^{1/5}\right)}{6.0222n+0.6666} \\ &+ \frac{(12n-4)\,\log\left(\left(\frac{1}{6}\right)^{1/6}\right)}{6.0222n+0.6666} + \frac{20n\,\log\left(\left(\frac{1}{9}\right)^{1/9}\right)}{6.0222n+0.6666} + \frac{4n\,\log\left(\left(\frac{1}{15}\right)^{1/15}\right)}{6.0222n+0.6666} \end{aligned} \tag{3.2}$$

We may determine the Randic index for $\alpha = \frac{1}{2}$ by using Table 2 and Equation 2.

$$ENT_{R_{\frac{1}{2}}}(P_{zs}) = \log(114.05n - 4.6018) - \frac{(4n+4)\,\log\Big((\sqrt{3})^{\sqrt{3}}\Big)}{114.05n - 4.6018} + \frac{n\,\log\Big((\sqrt{5})^{\sqrt{5}}\Big)}{114.05n - 4.6018} + \frac{(12n-4)\,\log\Big((\sqrt{6})^{\sqrt{6}}\Big)}{114.05n - 4.6018} + \frac{20n\,\log\Big((\sqrt{9})^{\sqrt{9}}\Big)}{114.05n - 4.6018} + \frac{4n\,\log\Big((\sqrt{15})^{\sqrt{15}}\Big)}{114.05n - 4.6018} \quad (3.3)$$

We may determine the Randic index for $\alpha = -\frac{1}{2}$ by using Table 2 and Equation 2.

$$ENT_{ABC}(P_{zs}) = \log(19.9555n - 0.6666) - \frac{(4n+4)\,\log\left((\sqrt{\frac{2}{3}})^{\sqrt{\frac{2}{3}}}\right)}{19.9555n - 0.6666} + \frac{n\,\log\left((\sqrt{\frac{4}{5}})^{\sqrt{\frac{4}{5}}}\right)}{19.9555n - 0.6666} + \frac{(12n-4)\,\log\left((\sqrt{\frac{1}{2}})^{\sqrt{\frac{1}{2}}}\right)}{19.9555n - 0.6666} + \frac{20n\,\log\left((\sqrt{\frac{4}{9}})^{\sqrt{\frac{4}{9}}}\right)}{19.9555n - 0.6666} + \frac{4n\,\log\left((\sqrt{\frac{6}{15}})^{\sqrt{\frac{6}{15}}}\right)}{19.9555n - 0.6666} \quad (3.4)$$

A comparison of the Randic entropies numerically is displayed in Table 4.

Table 4: Numerical comparison of randic entropies

Entropy [m]	[1]	[2]	[3]	[4]	[5]	[6]	[7]	[8]	[9]	[10]
$R_1(G)$	2.30	2.61	2.79	2.92	3.02	3.10	3.17	3.22	3.28	3.32
$R_{-1}(G)$	1.55	1.86	2.04	2.16	2.26	2.34	2.41	2.47	2.52	2.56
$R_{\frac{1}{2}}(G)$	1.58	1.89	2.07	2.20	2.30	2.37	2.44	2.50	2.55	2.60
$R_{-\frac{1}{2}}(G)$	1.38	1.69	1.87	2.00	2.09	2.19	2.23	2.30	2.35	2.40

The atom bond connectivity entropy of Pzs
The following results can be obtained by using the data in Table 2 and Equation 3:

$$ENT_{ABC}(P_{zs}) = \log(19.9555n - 0.6666) - \frac{(4n+4)\,\log\left((\sqrt{\frac{2}{3}})^{\sqrt{\frac{2}{3}}}\right)}{19.9555n - 0.6666} + \frac{n\,\log\left((\sqrt{\frac{4}{5}})^{\sqrt{\frac{4}{5}}}\right)}{19.9555n - 0.6666} + \frac{(12n-4)\,\log\left((\sqrt{\frac{1}{2}})^{\sqrt{\frac{1}{2}}}\right)}{19.9555n - 0.6666} + \frac{20n\,\log\left((\sqrt{\frac{4}{9}})^{\sqrt{\frac{4}{9}}}\right)}{19.9555n - 0.6666} + \frac{4n\,\log\left((\sqrt{\frac{6}{15}})^{\sqrt{\frac{6}{15}}}\right)}{19.9555n - 0.6666} \quad (3.5)$$

The Geometric arithmetic entropy of Pzs
The following results can be obtained by using the data in Table 2 and Equation 4:

$$ENT_{GA}(P_{zs}) = \log(39.8399n - 0.4550) - \frac{(4n+4)\,\log\left(\left(\frac{\sqrt{3}}{2}\right)^{\frac{\sqrt{3}}{2}}\right)}{39.8399n - 0.4550} + \frac{n\,\log\left(\left(\frac{\sqrt{5}}{3}\right)^{\frac{\sqrt{5}}{3}}\right)}{39.8399n - 0.4550} + \frac{(12n-4)\,\log\left(\left(\frac{2\sqrt{6}}{5}\right)^{\frac{2\sqrt{6}}{5}}\right)}{39.8399n - 0.4550} + \frac{20n\,\log(1^1)}{39.8399n - 0.4550} + \frac{4n\,\log\left(\left(\frac{\sqrt{15}}{4}\right)^{\frac{\sqrt{15}}{4}}\right)}{39.8399n - 0.4550} \quad (3.6)$$

First Zagreb entropy of Pzs
The following results can be obtained by using the data in Table 2 and Equation 5:

$$ENT_{M_1}(P_{zs}) = \log(39.8399n - 0.4550) - \frac{(4n+4)\,\log\left(\left(\frac{\sqrt{3}}{2}\right)^{\frac{\sqrt{3}}{2}}\right)}{39.8399n - 0.4550} + \frac{n\,\log\left(\left(\frac{\sqrt{5}}{3}\right)^{\frac{\sqrt{5}}{3}}\right)}{39.8399n - 0.4550} + \frac{(12n-4)\,\log\left(\left(\frac{2\sqrt{6}}{5}\right)^{\frac{2\sqrt{6}}{5}}\right)}{39.8399n - 0.4550} + \frac{20n\,\log(1^1)}{39.8399n - 0.4550} + \frac{4n\,\log\left(\left(\frac{\sqrt{15}}{4}\right)^{\frac{\sqrt{15}}{4}}\right)}{39.8399n - 0.4550} \tag{3.7}$$

Second Zagreb entropy of Pzs
The following results can be obtained by using the data in Table 2 and Equation 6:

$$ENT_{M_2}(P_{zs}) = \log(329n - 12) - \frac{(4n+4)\,\log(3^3)}{329n - 12} + \frac{n\,\log(5^5)}{329n - 12} + \frac{(12n-4)\,\log(6^6)}{329n - 12} + \frac{20n\,\log(9^9)}{329n - 12} + \frac{4n\,\log(15^{15})}{329n - 12} \tag{3.8}$$

Numerical comparison between $ABC\,(G)$;$GA\,(G)$; $M_1\,(G)$ and $M_2\,(G)$ entropies is shown in Table 5.

Table 5: Numerical comparison of $ABC\,(G)$;$GA\,(G)$; $M_1\,(G)$ and $M_2\,(G)$ entropies

Entropy [m]	[1]	[2]	[3]	[4]	[5]	[6]	[7]	[8]	[9]	[10]
$ABC\,(G)$	1.385	1.69	1.88	2.00	2.09	2.17	2.23	2.30	2.35	2.40
$GA\,(G)$	-0.13	-0.14	-0.14	-0.15	-0.15	0.15	-0.16	-0.16	-0.16	-0.16
$M_1\,(G)$ -0.13	-0.14	-0.14	-0.15	-0.15	0.15	-0.16	-0.16	-0.16	-0.16	
$M_2\,(G)$	12.32	13.88	14.78	15.41	15.90	16.30	16.64	16.93	17.18	17.41

Third Zagreb entropy of Pzs
The following results can be obtained by using the data in Table 2 and Equation 9:
$ENT_{M_3}\,(Pzs) = \log\,(32n+4) - \frac{(4n+4)\,\log\,(2)^2}{32n+4} + \frac{(n)\,\log\,(4)^4}{32n+4} + \frac{(12n-4)\,\log\,(1)^1}{32n+4} + \frac{(4n)\,\log\,(2)^2}{32n+4}$

Hyper Zagreb entropy of Pzs
Equation 7 and the data in Table 2 allow us to obtain the following results:

$$ENT_{HM}(P_{zs}) = \log(3013n - 108) - \frac{(4n+4)\,\log(9^9)}{3013n - 108} + \frac{n\,\log(25^{25})}{3013n - 108} + \frac{(12n-4)\,\log(36^{36})}{3013n - 108} + \frac{20n\,\log(81^{81})}{3013n - 108} + \frac{4n\,\log(225^{225})}{3013n - 108} \tag{3.9}$$

Forgotten entropy of Pzs
Equation 8 and the data in Table 2 allow us to obtain the following results:

$$ENT_F(P_{zs}) = \log(718n - 12) - \frac{(4n+4)\,\log(10^{10})}{718n - 12} + \frac{n\,\log(26^{26})}{718n - 12} + \frac{(12n-4)\,\log(13^{13})}{718n - 12} + \frac{20n\,\log(18^{18})}{718n - 12} + \frac{4n\,\log(34^{34})}{718n - 12} \tag{3.10}$$

First Redefined Zagreb entropy of Pzs
Equation 10 and the data in Table 2 allow us to obtain the following results:

$$ENT_{\operatorname{Re}ZG_1}(P_{zs}) = \log(32n+2) - \frac{(4n+4)\,\log\left[\left(\frac{4}{3}\right)^{\frac{4}{3}}\right]}{32n+2} + \frac{n\,\log\left[\left(\frac{6}{5}\right)^{\frac{6}{5}}\right]}{32n+2} + \frac{(12n-4)\,\log\left[\left(\frac{5}{6}\right)^{\frac{5}{6}}\right]}{32n+2} + \frac{20n\,\log\left[\left(\frac{2}{3}\right)^{\frac{2}{3}}\right]}{32n+2} + \frac{4n\,\log\left[\left(\frac{8}{15}\right)^{\frac{8}{15}}\right]}{32n+2} \tag{3.11}$$

Numerical comparison between $M_3\,(G)$;$HM\,(G)$; $FG\,(G)$ and $\operatorname{Re}ZG_1\,(G)$ entropies is shown in Table 6.

Table 6: Numerical comparison of $M_3\,(G)$;$HM\,(G)$; $FG\,(G)$ and $\operatorname{Re}ZG_1\,(G)$ entropies

Entropy [m]	[1]	[2]	[3]	[4]	[5]	[6]	[7]	[8]	[9]	[10]
$M_3\,(G)$	1.28	1.58	1.75	1.88	1.97	2.05	2.12	2.18	2.23	2.28
$HM\,(G)$	1.48	1.79	1.97	2.10	2.19	2.27	2.34	2.40	2.45	2.50
$FG\,(G)$	1.58	1.88	2.06	2.18	2.28	2.36	2.43	2.49	2.54	2.58
$\operatorname{Re}ZG_1\,(G)$	1.59	1.89	2.07	2.19	2.29	2.37	2.44	2.49	2.55	2.59

Second Redefined Zagreb entropy of Pzs
Equation 11 and the data in Table 2 allow us to obtain the following results:

$$ENT_{\operatorname{Re}ZG_2}(P_{zs}) = \log(58.0666\,n-1.8) - \frac{(4n+4)\,\log\left[\left(\frac{3}{4}\right)^{\frac{3}{4}}\right]}{58.0666\,n-1.8} + \frac{n\,\log\left[\left(\frac{5}{6}\right)^{\frac{5}{6}}\right]}{58.0666\,n-1.8} + \frac{(12n-4)\,\log\left[\left(\frac{6}{5}\right)^{\frac{6}{5}}\right]}{58.0666\,n-1.8} + \frac{20n\,\log\left[\left(\frac{3}{2}\right)^{\frac{3}{2}}\right]}{58.0666\,n-1.8} + \frac{4n\,\log\left[\left(\frac{15}{8}\right)^{\frac{15}{8}}\right]}{58.0666\,n-1.8} \tag{3.12}$$

Third Redefined Zagreb entropy of Pzs
Equation 12 and the data in Table 2 allow us to obtain the following results:

$$ENT_{\operatorname{Re}ZG_3}(P_{zs}) = \log(1998n-72) - \frac{(4n+4)\,\log\left[(12)^{12}\right]}{1998n-72} + \frac{n\,\log\left[(30)^{30}\right]}{1998n-72} + \frac{(12n-4)\,\log\left[(30)^{30}\right]}{1998n-72} + \frac{20n\,\log\left[(54)^{54}\right]}{1998n-72} + \frac{4n\,\log\left[(120)^{120}\right]}{1998n-72} \tag{3.13}$$

Numerical comparison between $operatornameReZG_2\,(G)$ and $operatornameReZG_2\,(G)$ entropies is shown in Table 7.

Table 7: Numerical comparison of $\operatorname{Re}ZG_2\,(G)$ and $\operatorname{Re}ZG_2\,(G)$ entropies

Entropy [m]	[1]	[2]	[3]	[4]	[5]	[6]	[7]	[8]	[9]	[10]
$\operatorname{Re}ZG_2\,(G)$	1.62	1.92	2.10	2.22	2.32	2.40	2.47	2.52	2.57	2.62
$\operatorname{Re}ZG_3\,(G)$	1.53	1.84	2.02	2.14	2.24	2.32	2.39	2.45	2.50	2.54

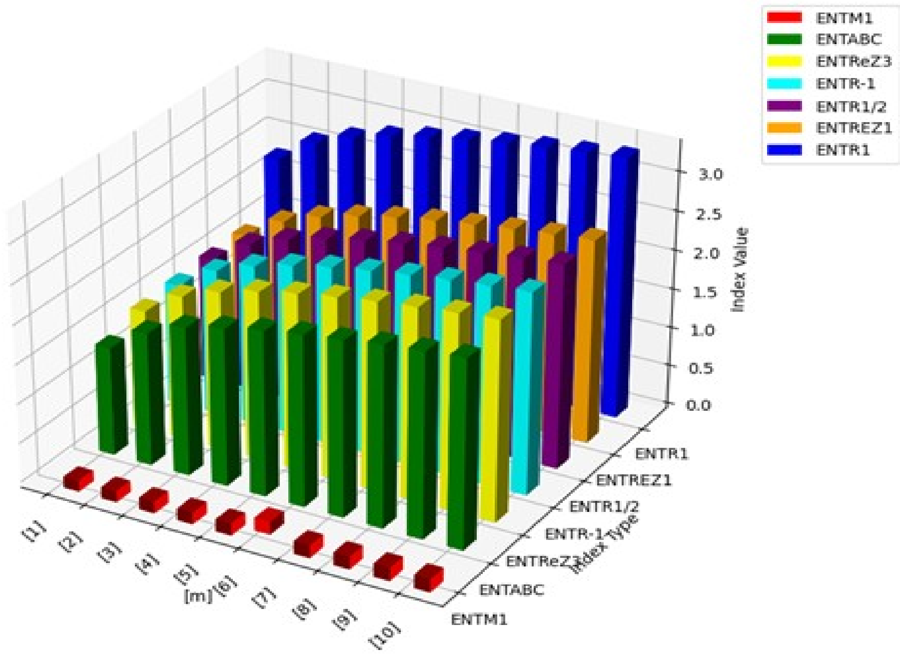

Figure 5: A visual comparison of several entropies

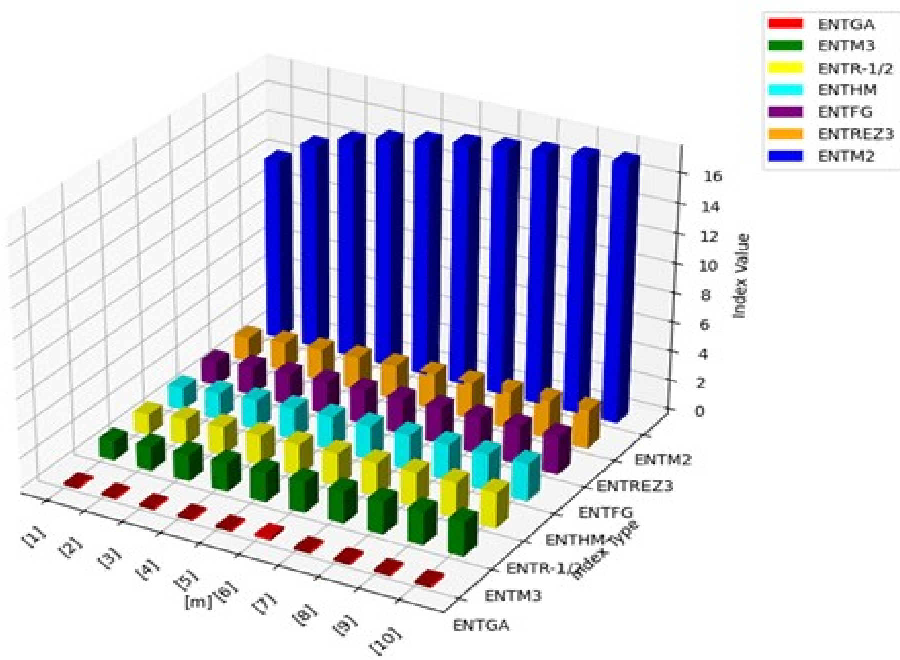

Figure 6: A visual comparison of several entropies

Linear Regression Mode
Pearson correlation coefficient: The Pearson correlation coefficient, commonly expressed as r, is a sta-

tistical measure that evaluates the strength and directionality of the linear relationship between two continuous variables. A perfect positive correlation is indicated by $r = 1$, while $r = -1$ represents a perfect negative correlation. An r value of 0 suggests that there is no linear relationship present. The coefficient itself ranges from -1 to 1.

$$r = \frac{\sum(X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum(X_i - \bar{X})^2 \sum(Y_i - \bar{Y})^2}}$$

Here, the symbols X_i and Y_i refer to individual observations, with $X$and Y representing the mean values of the respective variables. The summation is performed across all observations. The numerator of the equation detrmines the covariance between the two variables, and the denominator normalizes this covariance by the product of their standard deviations, producing a value that lies within the interval of -1 to1.

In this analysis, the Pearson correlation coefficient is utilized to explore the relationship between indices and entropy, particularly in terms of their correlation. A high positive r value indicates that an increase in the index corresponds with an increase in entropy, and the opposite is also true. Conversely, a significant negative r value suggests that one variable tends to decrease as the other increases.

To enhance our comprehension of the strength and direction of the relationships between entropy and various indices, we developed a heat map based on the Pearson correlation coefficient, as shown in Figure 5. This heat map visually conveys the correlation coefficients, enabling us to determine whether the variables exhibit a positive or negative association. This knowledge is vital for grasping the complex interactions between entropy and the indices, as it indicates how changes in entropy may be linked to variations in the indices. Consequently, this understanding bolsters our ability to analyze complex systems and make more informed decisions. However, additional research is frequently required to uncover the underlying mechanisms that contribute to these observed relationships.
The findings of our study indicated strong correlations between entropy assessments and specific topological indices, illustrating the relationship between the structural attributes and complexity of Pzs. Such relationships provide critical insights into the material's potential role as a conductor for Nano electronic devices. Through the application of the Pearson correlation coefficient, we quantified the relationship between the entropic and topological properties of the material, thereby enriching our understanding of its suitability for innovative technological applications.

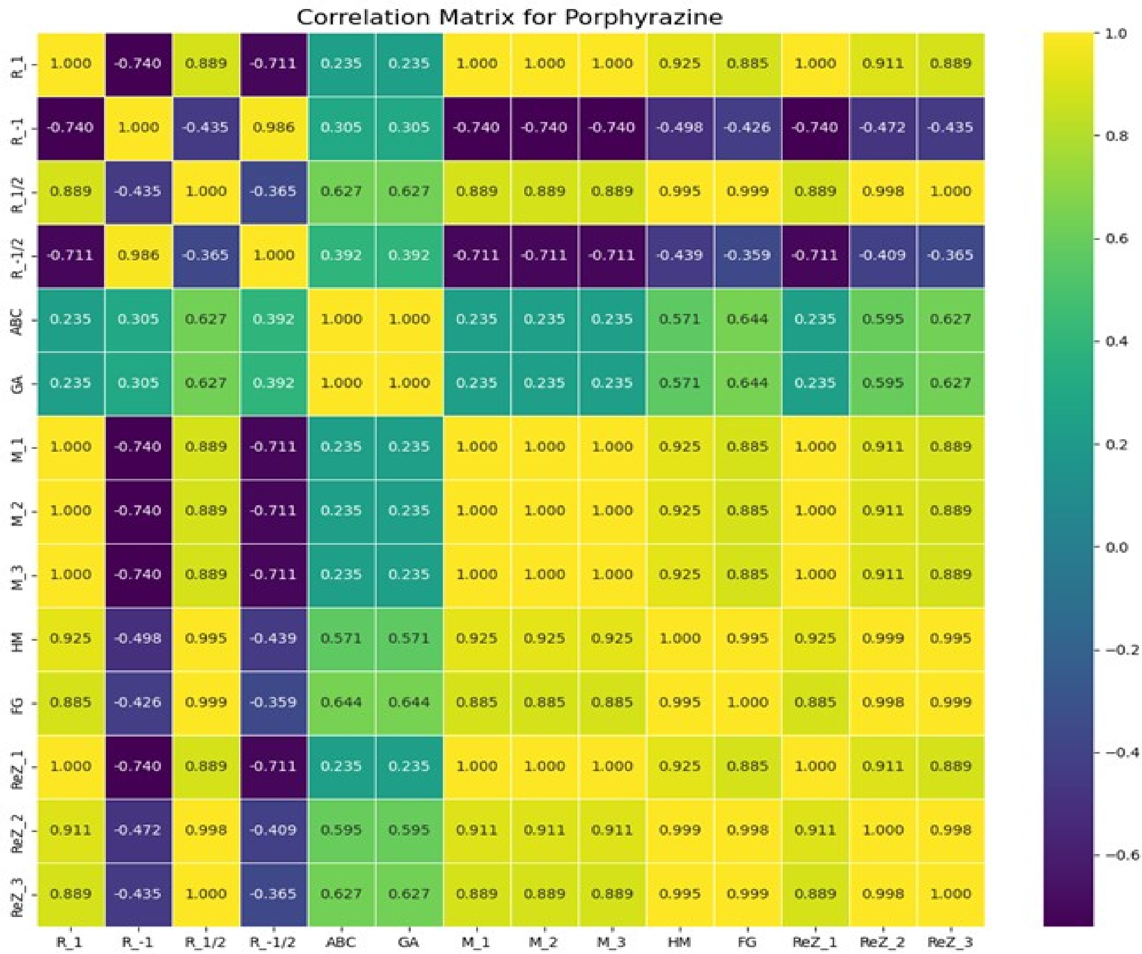

Figure 7: Correlation matrix for porphyrazine

Figure 8: Entropy Correlation matrix for porphyrazine

The R-squared approach was used to calculate the proportion of the dependent variable's variance (entropy), which can be explained by the independent variable or variables (indices). Between 0 and 1, where 1 represents perfect fit. The variables were more strongly correlated when the R-squared values were higher than a certain threshold. The standard error is the mean difference between the expected and observed values of the dependent variable in the statistical model. The degree to which the sample mean deviated from the average expected population mean was measured. This statistical measure assesses the precision and reliability of estimates derived from the sample data, which is useful for inferential statistics and hypothesis testing. It shows the accuracy of the model's future predictions. A better match between the model predictions and actual data points is shown by a reduced standard error. F-statistic was used to determine the overall significance of the linear regression model. It assesses and ascertains the statistical significance of the linear relationship between independent and dependent variables. A stronger correlation is indicated by a higher F-statistic.

To determine which linear regression model is better, we can compare the R-squared values, standard errors, and F-statistics of the different models. A greater R-squared often indicates a better fit, a lower standard error indicates a more accurate prediction, and a higher F-statistic indicates a more significant link. Considering various values of m and n, we examined the entropies related to the Pz configuration. The linear fitting between the indices and entropy measure is shown in Figures 6–12. By altering the underlying parameters through curve-fitting techniques, a linear curve-fitting strategy was employed to ascertain the relationship between entropy and other indices. The correlation coefficient values for each index with respect to the entropy are listed in Table 8.

For $ENTR_{\frac{1}{2}}(G)$, we find that the values of R and R-squared are the highest of all the indices, showing a substantial association with the entropy measure, according to the data in Table 8 and Figure 6a. Furthermore, the SE has the lowest value among the indices, suggesting that the forecasts are more accurate. Among the indices taken into consideration, these results imply that $ENTR_{\frac{1}{2}}(G)$ is the most accurate predictor.
Due to the volume of calculations, I will provide the results in a tabular form, assuming standard linear regression computations for each row against the index [1,2,3,... 10].

Table 8: Numerical comparison of $\mathrm{Re}\, ZG_2(G)$ and $\mathrm{Re}\, ZG_2(G)$ entropies

Entropy [m]	[R]	[R-squ]	[SSR]	[SSE]	[MSR]	[MSE]	[F-stat]	[Sig F]
$ENTR_1(G)$	0.9993	0.9986	1.25	0.001	1.25	0.0002	5920	< 0.0001
$ENTR_{-1}(G)$	0.99	0.99	1.83	0.01	1.83	0.001	1430.8	< 0.0001
$ENTR_{\frac{1}{2}}(G)$	0.99	0.99	1.6372	0.002	1.63	0.00033	4961.2	< 0.0001
$ENTR_{-\frac{1}{2}}(G)$	0.99	0.99	3.65	0.007	3.65	0.0009	3883.8	< 0.0001
$ENTABC(G)$	0.99	0.99	3.65	0.007	3.65	0.0009	3883.8	< 0.0001
$ENTGA(G)$	0.99	0.99	4.88	0.03	4.88	0.004	1202.3	< 0.0001
$ENTM_1(G)$	0.99	0.99	4.88	0.03	4.88	0.004	1202.3	< 0.0001
$ENTM_2(G)$	0.99	0.99	2.05	0.0016	2.052	0.0002	10263	< 0.0001
$ENTM_3(G)$	0.99	0.99	2.50	0.0030	2.50	0.00037	6778.6	< 0.0001
$ENTHM(G)$	0.96	0.92	3.44	0.26	3.44	0.033	102.4	< 0.0001
$ENTFG(G)$	0.99	0.99	5.37	0.005	5.37	0.0006	8028.2	< 0.0001
$ENT\,\mathrm{Re}\, ZG_1(G)$	0.99	0.998	4.39	0.008	4.39	0.00111	3963	< 0.0001
$ENT\,\mathrm{Re}\, ZG_2(G)$	0.01	0.0002	0.0012	6.8920	0.0012	0.86	0.001	0.97
$ENT\,\mathrm{Re}\, ZG_3(G)$	0.012	0.0001	0.0009	7.97	0.0009	0.99	0.0009	0.97

The linear regression models developed for each index and its connection with entropy are listed below:
$ENTR_1(G) = 2.3761 + 0.1118\,[R_1]$
$ENTR_{-1}(G) = 0.0519 + 0.1384\,[R_{-1}]$
$ENTR_{\frac{1}{2}}(G) = 1.4880 + 0.1481\,[R_{\frac{1}{2}}]$
$ENTR_{-\frac{1}{2}}(G) = 2.1156 + 0.2606\,[R_{-\frac{1}{2}}]$
$ENTABC(G) = 2.1156 + 0.2606\,[ABC]$
$ENTGA(G) = 3.7383 + 0.2526\,[GA]$
$ENTM_1(G) = 3.7383 + 0.2526\,[M_1]$
$ENTM_2(G) = 7.5818 + 0.2602[M_2]$
$ENTM_3(G) = 3.4975 + 0.2464[M_3]$
$ENTHM(G) = 12.5939 + 0.2115[HM]$
$ENTFG(G) = 8.7846 + 0.2872[FG]$
$ENT\,\mathrm{Re}\, ZG_1(G) = 3.3283 + 0.2429[\mathrm{Re}\, ZG_1]$
$ENT\,\mathrm{Re}\, ZG_2(G) = 5.5684 + 0.0076[\mathrm{Re}\, ZG_2]$
$ENT\,\mathrm{Re}\, ZG_3(G) = 12.6375 + 0.0062[\mathrm{Re}\, ZG_3]$

Based on the information provided in Table 8 and Figure 6(b), we observe that for $ENTR_{\frac{1}{2}}(G)$, the values of R and R2 are the highest among all the indices, indicating a strong correlation with the entropy measure. Furthermore, the value of SE is the lowest compared to the other indices, implying superior forecast accuracy. These findings suggest that $ENTR_{\frac{1}{2}}(G)$serves as the best predictor among the indices considered.

4. Conclusion

This study examined the relationship between entropy and several topological indices as well as the best predictor of entropy. Redefined Zagreb indices, $HM(G)$, $M_1(G)$, $M_2(G)$, atom bond connection entropy, and Randic entropy were among the indices that were studied. Owing to its largest link with entropy, the study concluded that the $ENTR_{\frac{1}{2}}(G)$ index was the best predictor. This suggests that $ENTR_{\frac{1}{2}}(G)$ is a reliable signal for predicting the entropy measure in the current scenario. The results demonstrate that the structural features represented by the $ENTR_{\frac{1}{2}}(G)$ index have a considerable impact on the system's entropy. The results of this study have important implications for understanding how entropy and topological indices relate to one another in the field of chemistry. Researchers can estimate and examine the entropy values of various chemical systems by using the $ENTR_{\frac{1}{2}}(G)$ index, which is a reliable predictor. This information can be used to predict the physicochemical properties, stability, and complexity of molecules. Based on both theoretical and empirical data, our results indicate a linear relationship between entropy and topological indices. We were able to approximate this relationship and discover important topological factors that affect entropy in subdivided cage networks.
Data Availability
The text contains references to the sources utilized in this study.

Conflicts of interest
According to the authors, there are no conflicts of interest.

Author's Contributions
Each author made an equal contribution to this research.

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