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Degree Based Topological Indices on Fuzzy Graph and its Applications

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Abstract:- The degree-based topological indices of fuzzy graphs, emphasizing their mathematical definitions, properties, and potential applications. Topological indices are numerical values that characterize the structure of a graph and are widely applied in chemistry and network analysis. The fuzzy graphs have emerged as powerful tools for developing novel degree-based topological indices, effectively capturing uncertainty and vagueness in real-world systems. In this study explore the relationships with topological indices, and highlight their applicability in modeling complex networks. The work particularly emphasizes fuzzy graphs based on the Hyper-Zagreb index and contributes to the understanding of fuzzy regularization, with a specific focus on antiviral drugs. This research opens new avenues for both theoretical exploration and applied studies in the domain of fuzzy graph theory.

Keywords: degree, molecular structure, drugs, fuzzy graph.

1. Introduction

Topological indices are quantitative descriptors that are obtained from molecular graph structural features and are widely applied in chemical graph theory to estimate physicochemical, biological, and pharmacological activities of chemical compounds. In recent years, fuzzy sets have been incorporated in chemical graph theory to handle uncertainty and vagueness in real chemical systems more effectively. A fuzzy graph permits imprecise or uncertain relations among atoms or molecules to be modeled through degrees of membership. This fuzzy context increases the realism and flexibility of chemical graph models. Zadeh introduced the concept of fuzzy sets in 1965 [1], establishing a framework in which each element possesses a degree of membership within a set. Building upon this, fuzzy graphs emerged as a powerful extension, enabling the modeling of fuzzy relationships between objects. In 1975, Rosenfeld further advanced this idea by exploring fuzzy relations between fuzzy sets and laying the foundation for fuzzy graph structures through analogs of classical graph-theoretic concepts. In 2015, Akram et al. introduced the notion of soft fuzzy graphs [2]. In the realm of chemical graph theory, numerical descriptors derived from molecular graph structures play a pivotal role. Binuet et al. investigated neighborhood indices of fuzzy graphs and their application to human trafficking networks in 2019 [3], and later examined the Wiener index in the context of illegal immigration networks in 2020 [4]. Numerous topological indices have since been developed. In 2024, Biswajit et al. presented various boundaries and structural features [5], while Chen et al. established extremal values for acyclic graphs in 2022 [6], and Das et al. analyzed Zagreb connection indices that same year [7]. Deng et al. studied molecular trees exhibiting extremal Sombor index values in 2022 [8], recognizing molecular trees as fundamental structures in chemical graph theory. Girish et al. analyzed hyper Zagreb indices and their relevance in mathematical chemistry in 2023 [9]. Islam et al. introduced the first Zagreb index in fuzzy graphs and its applications in 2021 [10], later extending this to the second Zagreb index in 2023 [11]. Montal et al. examined the neighborhood Zagreb index in product graphs in 2021 [12], while Milovanović et al. discussed key mathematical properties of the Sombor index that same year [13]. Contributions by Pouliket et al. and Redžepović in 2021 further expanded the understanding of soft fuzzy graphs and the chemical applicability of Sombor indices [14, 15]. The hyper Zagreb index has also been extended within fuzzy graph theory. Jamil et al. explored its behavior under various graph operations in 2017 [16], and Sharmila Devi et al. examined it in the context of composite graphs [17]. In 2024, Sk. Rabiul et al. investigated the hyper Zagreb index in fuzzy environments and its practical applications [18].Fuzzy topological indices hold significant importance in areas such as drug design, molecular stability prediction, and reaction pathway modeling, especially where data uncertainty is prevalent. These indices are particularly valuable in correlation analysis, where they serve as independent variables to determine their relationship with experimental descriptors like boiling point, melting point, biological activity, or toxicity. A strong positive or negative correlation coefficient indicates a substantial linear relationship between a fuzzy topological index and the associated property, offering insights into molecular behavior. Such methods are widely used in quantitative structure–activity relationship (QSAR) and quantitative structure–property relationship (QSPR) studies, making them valuable in drug discovery, environmental research, and material science. The primary objective of this paper is to conduct a comparative analysis of various fuzzy topological indices in fuzzy graphs and hypergraphs. Specifically, the study focuses on indices such as the Hyper Zagreb Index (HZI), the Second Zagreb Index in Fuzzy Graphs, and the Sombor Index on Fuzzy Graphs (SO(G)).

2. Preliminaries

The Zagreb indices are among the earliest and most extensively studied degree-based topological indices in chemical graph theory, originally introduced by Gutman and Trinajstić in 1972. To address the uncertainty inherent in molecular structures and their relationships, these indices have been extended into the fuzzy graph framework. Notably, Md. Rabiul Islam et al. introduced the First Zagreb Index on fuzzy graphs and explored its applications in 2021 [10], followed by the Second Zagreb Index on fuzzy graphs in 2023 [9]. In these works, the classical definitions were generalized using fuzzy degree functions, wherein both vertices and edges are assigned membership values within the interval [0, 1].

Let G = (v, e) be a connected fuzzy graph. is a pair of functions $(\aleph,\beth)$ where $\aleph : V \longrightarrow [0, 1]$ is a fuzzy subset of a non empty set v and $\beth : \aleph\times \aleph \longrightarrow [0, 1]$ is a symmetric fuzzy relation on $\aleph$ such that for all u and v in $\aleph$ the relation $\beth(u, v) = \beth(uv) \leq \aleph(u) \wedge \aleph(v)$ is satisfied. The first Zagreb index of the graph G defined by $FZI_1(G)= \sum_{uv\in E}[\aleph(\mu)\deg(\mu)]^2$. The second Zagreb index of the graph G defined by $FZI_2(G)= \sum_{uv\in E}[\aleph(\mu)\deg(\mu)\aleph(\rho)\deg(\rho)]$. Let G = (v, e) be a connected fuzzy graph. Then first hyper Zagreb index of the fuzzy graph G is denoted by FHZI(G) and is defined by $FHZI(G)= \sum_{uv\in E}[\aleph(\mu)\deg(\mu) + \aleph(\rho)\deg(\rho)]^2$. The second hyper Zagreb index of the fuzzy graph G is denoted by SHZI(G) and is defined by $SHZI(G)= \sum_{uv\in E}[\aleph(\mu)\deg(\mu)\, \aleph(\rho)\deg(\rho)]$.

3. Main Results

Theorem 3.1 Let $G = (v, \aleph,\beth)$ and $H = (W, \aleph',\beth')$ are a fuzzy graphs. Then $FHM_1(G)=FHM_1(H)$.

Proof: If $G = (v, \aleph,\beth)$ and $H = (W, \aleph',\beth')$ are a fuzzy isomorphic hyper graphs then there exists bijection function $f: v\rightarrow W$ such that for every u in v and $uv\in\beth$, $\aleph(u)=\aleph'(f(u))$ and $\beth(uv)=\aleph'(uv)$. $FHM_1(G)=\sum_{uv\square\beth}[\aleph(u)d_u+\aleph(v)d_v]^2$

$FHM_1(G)=FHM_1(H)$.

Theorem 3.2 Let G = (v, e) be a fuzzy graph. Then $EFI(G)\geq\frac{1}{2}HZI(G)$.

Proof: If any two positive numbers, σ and τ, we have $\sigma^2+\tau^2\geq\frac{1}{2}(\sigma+\tau)^2$

Let $\sigma=\aleph(\mu_i)\beth(\mu_i)$ and $\tau=\aleph(\mu_j)\beth(\mu_j)$, $\left(\aleph(\mu_i)\beth(\mu_i)\right)^2+\left(\aleph(\mu_j)\beth(\mu_j)\right)^2\geq\frac{1}{2}\left[\left(\aleph(\mu_i)\beth(\mu_i)\right)+\left(\aleph(\mu_j)\beth(\mu_j)\right)\right]^2$

$$\sum_{\substack{i\neq j\\ \mu_i\mu_j\epsilon G}}\left(\aleph(\mu_i)\beth(\mu_i)\right)^2+\left(\aleph(\mu_j)\beth(\mu_j)\right)^2\geq\frac{1}{2}\sum_{\substack{i\neq j\\ \mu_i\mu_j\epsilon G}}\left[\left(\aleph(\mu_i)\beth(\mu_i)\right)+\left(\aleph(\mu_j)\beth(\mu_j)\right)\right]^2\quad EFI(G)\geq\frac{1}{2}HZI(G).$$

Theorem 3.3 Let G = (v, e) be a fuzzy graph. Then $[EFI(G)]2\geq\frac{1}{2}FZI_2(G)$.

Proof: If any two positive numbers, σ and τ, we have $\frac{\sigma^2+\tau^2}{2}\geq\sqrt{\sigma\tau}$, $\sigma^2+\tau^2\geq2\sqrt{\sigma\tau}$

Let $\sigma=\aleph(\mu_i)\beth(\mu_i)$ and $\tau=\aleph(\mu_j)\beth(\mu_j)$, $\left(\aleph(\mu_i)\beth(\mu_i)\right)^2+\left(\aleph(\mu_j)\beth(\mu_j)\right)^2\geq2\left(\aleph(\mu_i)\beth(\mu_i)\right)\left(\aleph(\mu_j)\beth(\mu_j)\right)$

$$\sum_{\substack{i\neq j\\ \mu_i\mu_j\epsilon G}} \left(\aleph(\mu_i)\beth(\mu_i)\right)^2+\left(\aleph(\mu_j)\beth(\mu_j)\right)^2 \geq 2\sum_{\substack{i\neq j\\ \mu_i\mu_j\epsilon G}} \left(\aleph(\mu_i)\beth(\mu_i)\right)\left(\aleph(\mu_j)\beth(\mu_j)\right)$$

$[EFI(G)]2\geq\frac{1}{2}FZI_2(G)$.

Theorem 3.4 Let G = (v, e) be a fuzzy graph. Then $SO(F(G))\leq\frac{1}{2}EFI(G)$.

Proof: If any two positive numbers, σ and τ, we have $\sqrt{\sigma^2+\tau^2}\leq\sigma^2+\tau^2$

Let $\sigma=\aleph(\mu_i)\beth(\mu_i)$ and $\tau=\aleph(\mu_j)\beth(\mu_j)$ we get $\sqrt{\left(\aleph(\mu_i)\beth(\mu_i)\right)^2+\left(\aleph(\mu_j)\beth(\mu_j)\right)^2}\leq\left(\aleph(\mu_i)\beth(\mu_i)\right)^2+\left(\aleph(\mu_j)\beth(\mu_j)\right)^2$

$$\sum_{\substack{i\neq j\\ \mu_i\mu_j\epsilon G}} \sqrt{\left(\aleph(\mu_i)\beth(\mu_i)\right)^2+\left(\aleph(\mu_j)\beth(\mu_j)\right)^2}\leq\sum_{\substack{i\neq j\\ \mu_i\mu_j\epsilon G}} \left(\aleph(\mu_i)\beth(\mu_i)\right)^2+\left(\aleph(\mu_j)\beth(\mu_j)\right)^2$$

Hence $SO(F(G))\leq\frac{1}{2}EFI(G)$.

Theorem 3.5 Let G = (v, e) be a fuzzy graph. Then $EFI(G)\leq HZI(G)$.

Proof: If any two positive numbers, σ and τ, we have $\sigma^2+\tau^2\leq(\sigma^2+\tau^2)^2$

Let $\sigma=\aleph(\mu_i)\beth(\mu_i)$ and $\tau=\aleph(\mu_j)\beth(\mu_j)$ we get $\left(\aleph(\mu_i)\beth(\mu_i)\right)^2+\left(\aleph(\mu_j)\beth(\mu_j)\right)^2\leq\left(\left(\aleph(\mu_i)\beth(\mu_i)\right)^2+\left(\aleph(\mu_j)\beth(\mu_j)\right)^2\right)^2$

$$\sum_{\substack{i\neq j\\ \mu_i\mu_j\epsilon G}} \left(\aleph(\mu_i)\beth(\mu_i)\right)^2+\left(\aleph(\mu_j)\beth(\mu_j)\right)^2\leq\sum_{\substack{i\neq j\\ \mu_i\mu_j\epsilon G}} \left(\left(\aleph(\mu_i)\beth(\mu_i)\right)^2+\left(\aleph(\mu_j)\beth(\mu_j)\right)^2\right)^2$$

$EFI(G)\leq HZI(G)$.

Theorem 3.6 Let G = (v, e) be a fuzzy graph. Then $FHZI(G) = EFI(G) + 2\,FZI_2(G)$.

Proof: If any two positive numbers, σ and τ, we have $(\sigma+\tau)^2=\sigma^2+\tau^2+2\sigma\tau$

Let $\sigma=\aleph(\mu_i)\beth(\mu_i)$ and $\tau=\aleph(\mu_j)\beth(\mu_j)$ we get

$$\left(\left(\aleph(\mu_i)\beth(\mu_i)\right)+\left(\aleph(\mu_j)\beth(\mu_j)\right)\right)^2=\left(\aleph(\mu_i)\beth(\mu_i)\right)^2+\left(\aleph(\mu_j)\beth(\mu_j)\right)^2+2\left(\aleph(\mu_i)\beth(\mu_i)\right)\left(\aleph(\mu_j)\beth(\mu_j)\right)$$

$$\sum_{\substack{i\neq j\\ \mu_i\mu_j\epsilon G}} \left(\left(\aleph(\mu_i)\beth(\mu_i)\right)+\left(\aleph(\mu_j)\beth(\mu_j)\right)\right)^2=\sum_{\substack{i\neq j\\ \mu_i\mu_j\epsilon G}} \left(\aleph(\mu_i)\beth(\mu_i)\right)^2+\left(\aleph(\mu_j)\beth(\mu_j)\right)^2+2\sum_{\substack{i\neq j\\ \mu_i\mu_j\epsilon G}} \left(\aleph(\mu_i)\beth(\mu_i)\right)\left(\aleph(\mu_j)\beth(\mu_j)\right)$$

$FHZI(G) = EFI(G) + 2\,FZI_2(G)$.

Theorem 3.7 Let G = (v, e) be a fuzzy graph. Then HFHZI(G) ≥ 4FZI2(G).

Proof: If any two positive numbers, σ and τ, we have $\frac{\sigma+\tau}{2}=\sqrt{\sigma\tau}$, $\left(\frac{\sigma+\tau}{2}\right)^2\geq\sigma\tau$

Let $\sigma=\aleph(\mu_i)\beth(\mu_i)$ and $\tau=\aleph(\mu_j)\beth(\mu_j)$ we get

$$\left[\frac{\left(\aleph(\mu_i)\beth(\mu_i)\right)+\left(\aleph(\mu_j)\beth(\mu_j)\right)}{2}\right]^2\geq\left(\aleph(\mu_i)\beth(\mu_i)\right)\left(\aleph(\mu_j)\beth(\mu_j)\right)$$

$$\left[\left(\aleph(\mu_i)\beth(\mu_i)\right)\left(\aleph(\mu_j)\beth(\mu_j)\right)\right]^2\geq4\left(\aleph(\mu_i)\beth(\mu_i)\right)\left(\aleph(\mu_j)\beth(\mu_j)\right)$$

$$\sum_{\substack{i\neq j\\ \mu_i\mu_j\epsilon G}}\left[\left(\aleph(\mu_i)\beth(\mu_i)\right)+\left(\aleph(\mu_j)\beth(\mu_j)\right)\right]^2\geq 4\sum_{\substack{i\neq j\\ \mu_i\mu_j\epsilon G}}\left(\aleph(\mu_i)\beth(\mu_i)\right)\left(\aleph(\mu_j)\beth(\mu_j)\right)$$

$\mathrm{FHZI}(G) \geq 4\mathrm{FZI2}(G)$.

4. Antiviral drugs on Hyper Zagreb index

The integration of topological indices and fuzzy graph theory in antiviral research can lead to more effective strategies for drug development, potentially improving outcomes in the treatment of viral infections. This section follows fuzzy antiviral drugs, which assign a membership values which attains the fuzzy hyper zagreb index.

(i) Pinocembrin

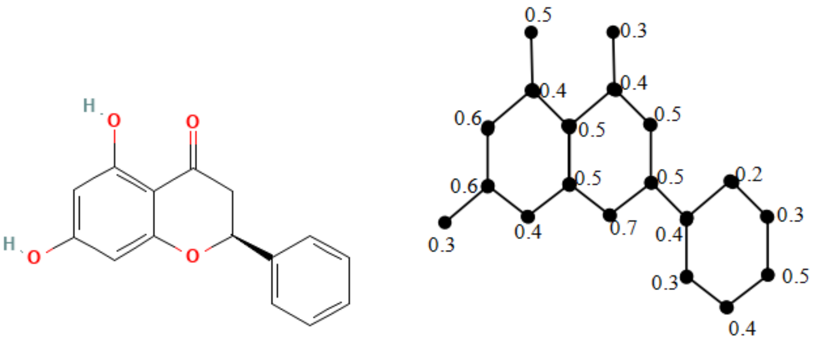


Figure 1. The molecular and graphical representation of Pincembrin

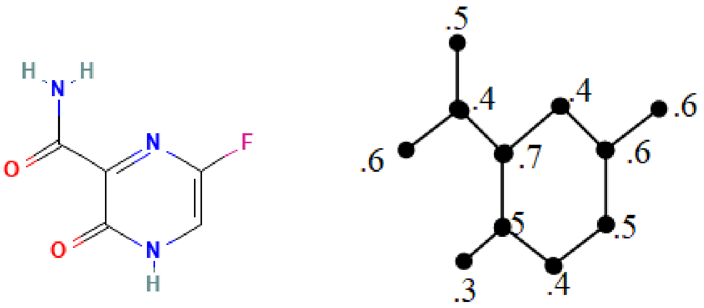
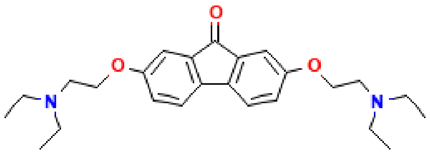


Figure 2. The molecular and graphical representation of Favipiravir



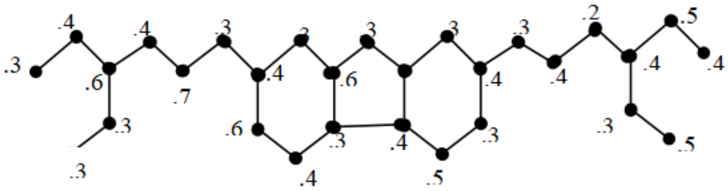


Figure 3. The molecular and graphical representation of Tolorone

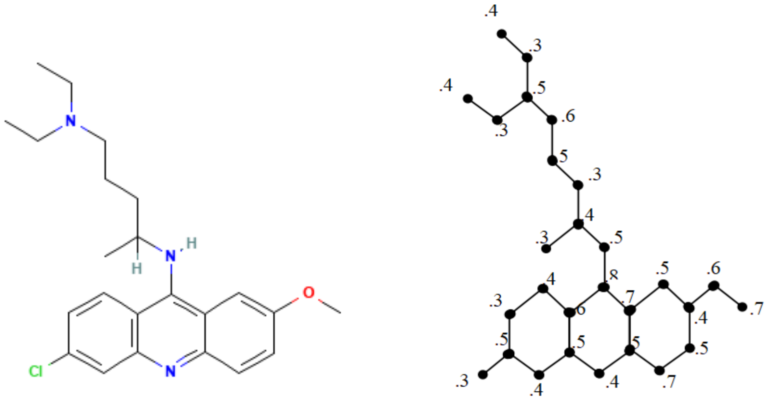


Figure 4. The molecular and graphical representation of Quinacrine

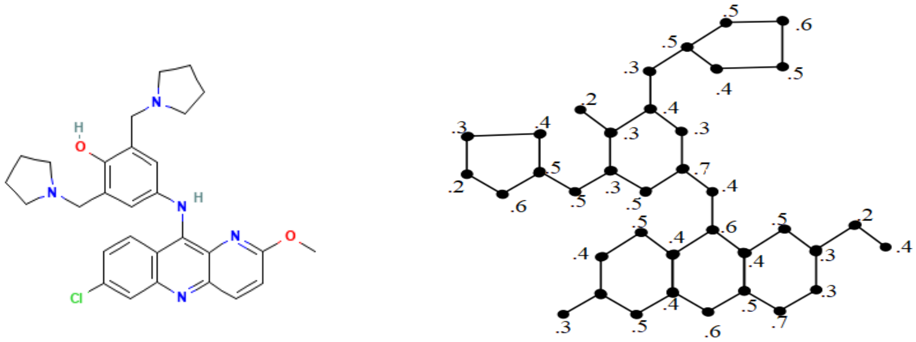


Figure 5. The molecular and graphical representation of Pyronaridine

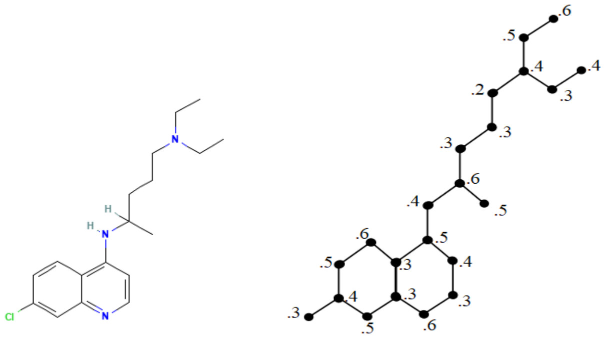


Figure 6. The molecular and graphical representation of chloroquine

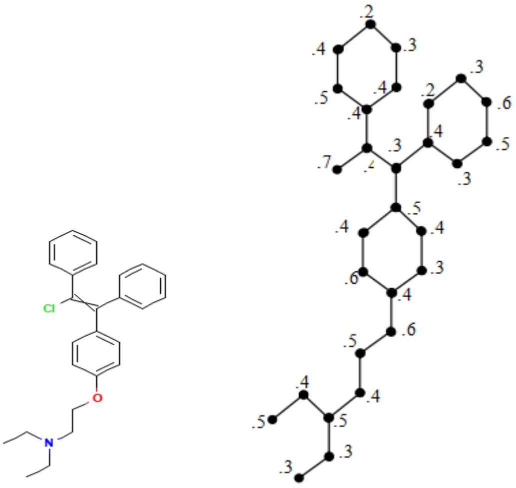


Figure 7. The molecular and graphical representation of clomiphene

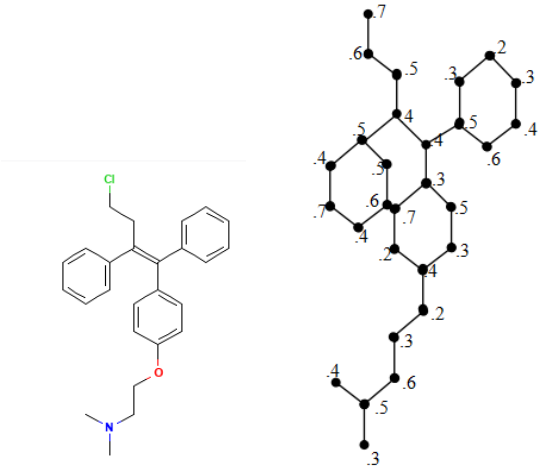


Figure 8. The molecular and graphical representation of Toremifene

5. Methodology

The antiviral drugs Pinocembrin, Favipiravir, Tilorone, Quinacrine, Pyronaridine, Chloroquine, Clomiphene, and Toremifene are shown in Figures 1 to 8. The molecular structures of these drugs were obtained from the PubChem database.

Table 1: Physico chemical properties of antiviral drugs

Drugs	**Hyper Zagreb Index**	**XlogP**	**Density**	**Index of refraction**
Pinocembrin	17.4903	3093	1.4	1.66
Favipiravir	9.7851	0.98	1.6	1.6
Tilorone	18.8561	5.25	1.11	1.5
Quinacrine	36.185	5.5	1.2962	1.63
Pyronaridine	27.215	4.8	1.4	1.72
Chloroquine	10.0104	4.69	1.1	1.52

Clomiphene	14.9426	8.01	1.1	1.598
Toremifene	16.2108	7.2	1.104	2.2

Table 1. presents the physicochemical properties of the antiviral drugs, along with their corresponding fuzzy Hyper-Zagreb indices, based on the molecular structures shown in Figures 1 to 8. A regression analysis was used to assess the relationship between the fuzzy Hyper-Zagreb index and certain physicochemical properties of antiviral drugs. The association of the fuzzy Hyper-Zagreb index with XLogP yielded a correlation coefficient (R) of 0.092, and as implied, even less linear association than before. Density was associated with the fuzzy Hyper-Zagreb index with an R value of 0.828, and similarly the refractive index provided a strong correlation coefficient of 0.857. These structures, in combination with the fuzzy Hyper-Zagreb index, suggests that the fuzzy Hyper-Zagreb index is better associated with density and refractive index than with lipophilicity (XLogP) suggesting that the fuzzy Hyper-Zagreb index has potential in capturing structural properties associated with molecular compactness, such as electronic, various intermolecular forces, etc.

6. Conclusion

The research demonstrates that degree-based topological indices, within the framework of fuzzy graphs, offer powerful mathematical representations of structural uncertainty and fuzziness in complex systems. Focusing on the fuzzy Hyper-Zagreb index, the study establishes its relevance to key physicochemical properties of antiviral drugs, thereby confirming the utility of fuzzy topological indices in drug activity prediction and design. Thus, the contribution of the fuzzy Hyper-Zagreb index serves both as a significant theoretical advancement in fuzzy graph theory and as a foundational tool for future applications in cheminformatics, network modeling, and data-driven decision-making under uncertainty.

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