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Exploring Novel Topological Descriptors: Geometric-Harmonic and Harmonic-Geometric Descriptors for HAC and HAP Conjugates

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Abstract: In this investigation, the exact formulas for geometric-harmonic (GH), neighborhood geometric-harmonic (NGH), harmonic-geometric (HG), and neighborhood harmonic-geometric (NHG) indices were systematically evaluated for hyaluronic acid-curcumin (HAC) and hyaluronic acid-paclitaxel (HAP) conjugates. Through this evaluation, a comprehensive quantitative assessment was conducted to elucidate the structural characteristics of these conjugates, highlighting the intricate geometric and harmonic relationships present within their molecular graphs. The study leveraged these indices to illuminate the complex interplay between geometric and harmonic properties, providing a novel perspective on the molecular architecture of HAC and HAP conjugates. This analytical approach not only sheds light on the structural nuances of these compounds but also offers a unique lens through which their potential in drug delivery applications can be assessed. Graphical analyses of the results further enhance the understanding of these molecular properties, presenting a detailed visualization that complements the quantitative findings. The integration of these topological descriptors into the study of HAC and HAP conjugates represents a significant advance in the field of medicinal chemistry, offering valuable insights for researchers engaged in the development of innovative drug delivery systems. The findings underscore the utility of these descriptors in characterizing the molecular topology of complex conjugates, setting the stage for further exploration of their applications in therapeutic contexts.

Keywords: Topological descriptor; Connected graphs; Harmonic index; Geometric index; Molecular graph; Drug delivery; Medicinal chemistry

1 Introduction

In this era of exponential technological advancement, the fields of pharmaceutical and chemical technologies have undergone rapid growth. Graph theory plays a pivotal role in guiding chemical investigations. Chemists commonly employ quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) methodologies [1–4] to streamline the evaluation of the biological, physical, and chemical properties of myriad newly developed nanomaterials, crystalline substances, and drugs. Topological indices (TIs), or numerical invariants, constitute a crucial tool within QSPR and QSAR analyses [5–9]. These indices are usually described as numbers that are linked to the chemical structure. They make it easier to connect the shape of a chemical with its different properties [10–14]. Topological indices (TIs), which are numeric invariants describing the properties of specific molecular systems, play a pivotal role as an essential tool in both QSPR and QSAR.

The exploration of topological indices dates back several decades, with seminal contributions by Randic [15], Wiener [16], and Balaban [17]. Randic's work laid the foundation for understanding molecular branching, while Wiener introduced the concept of a distance-based index. Balaban's contributions expanded the scope of topological indices, paving the way for subsequent developments. The literature on topological indices has witnessed a surge in recent years, driven by advancements in computational methods and an increased understanding of molecular properties. Notable recent contributions include studies by Taherpour and Shafiei [18], exploring novel topological indices for improved drug design, and Chen et al. [19], who applied machine learning techniques to enhance the predictive power of topological indices. Recent advances in topological indices include the development of

indices tailored for specific applications, such as predicting toxicity [20] and assessing environmental impact [21]. Researchers have also looked into how to combine topological indices with other molecular descriptors to make hybrid models that give a fuller picture of how molecules behave [22]. Beyond their role in drug design, isomer discrimination, chemical documentation, and biological characterization, TIs find special applications in mathematical chemistry [23–26]. This diverse range of applications underscores the versatility and importance of TIs in understanding and manipulating molecular structures, making them indispensable tools in various scientific and industrial pursuits. As researchers delve into the nuanced behaviors of TIs, it not only enhances our understanding of molecular systems but also contributes to the ongoing advancements in the interdisciplinary fields of chemistry and computational sciences [27, 28].

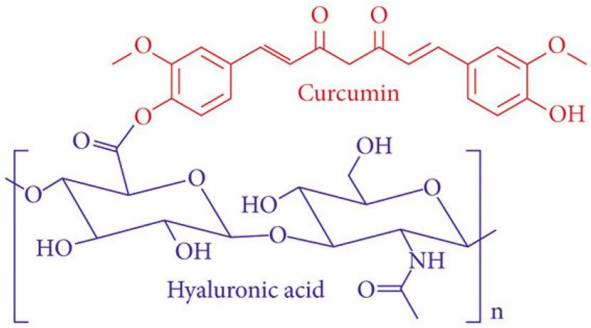

Figure 1. The molecular structure of HAC

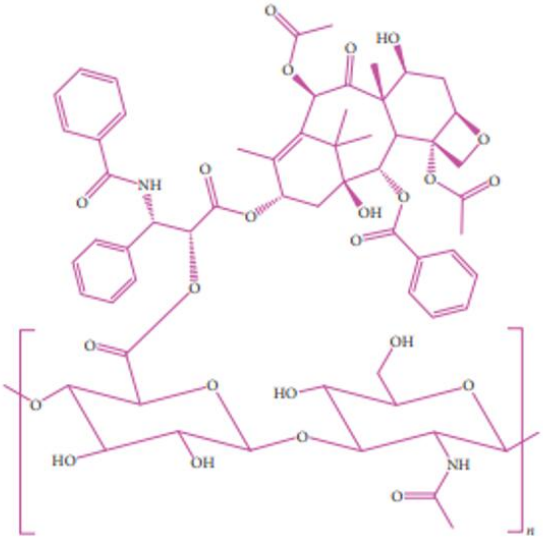

Figure 2. The molecular structure of HAP

Hyaluronic acid (HA) conjugates, such as HAC and HAP conjugates represented in Figures 1 and 2, have emerged as promising platforms for drug delivery owing to their unique properties. HA, a natural biopolymer, exhibits excellent biocompatibility and biodegradability. The anti-inflammatory and antioxidant properties of curcumin are combined with the targeted drug delivery potential of HA in HAC. This creates a more effective way to fight diseases. Adding HA to curcumin not only makes it more stable and easy to dissolve, but it also makes it easier for cells that have lots of HA receptors to get the curcumin. In the same way, HAP uses the chemotherapy drug paclitaxel to deliver drugs specifically to cancer cells by increasing the number of HA receptors. These HA conjugates have shown promising results in preclinical studies, demonstrating improved therapeutic efficacy and reduced side effects compared to conventional drug formulations. Recent research has focused on optimizing the synthesis methods of HAC and HAP to enhance their drug-loading capacities and stability during circulation. According to Lee et al. [29], they looked into new ways to efficiently couple curcumin to HA. Zhu et al. [30], on the other hand, studied the therapeutic potential of HAC in living animals. Additionally, the work of Saravanakumar et al. [31] highlights advancements in the development of HAP, showcasing its targeted delivery and enhanced antitumor effects. The utilization of

HA conjugates in drug delivery continues to be an active area of research, with ongoing efforts to translate these innovative formulations into clinically viable therapies.

The concept of neighborhood degrees, initially proposed by Chellali et al. [32], has been elaborated in numerous articles [33–35]. Recently, Usha et al. [36] introduced the geometric-harmonic ($\mathcal{GHI}$) index , combining geometric and harmonic indices, inspired by the work of Vukicevic and Furtula [37] in designing the $\mathcal{GHI}$ index.

$$\mathcal{GHI}(G) = \sum \frac{(d_u + d_v)\sqrt{d_u.d_v}}{2}$$

Shanmukha et al. [38] introduced three degree and neighborhood degree based novel indices, namely, harmonic-geometric ($\mathcal{HGI}$), neighborhood harmonic-geometric ($\mathcal{NHGI}$) and neighborhood geometric-harmonic ($\mathcal{NGHI}$) indices motivated by the above work. They are defined as follows:

$$\mathcal{HGI}(G) = \sum \frac{2}{(d_u + d_v)\sqrt{d_u.d_v}}$$

$$\mathcal{NGHI}(G) = \sum \frac{(\lambda_u + \lambda_v)\sqrt{\lambda_u.\lambda_v}}{2}$$

$$\mathcal{NHGI}(G) = \sum \frac{2}{(\lambda_u + \lambda_v)\sqrt{\lambda_u.\lambda_v}}$$

2 Methodology

Table 1 illustrates the various types of edges within the molecular graph of hyaluronic acid-curcumin conjugates, categorized by their vertex degrees and corresponding frequencies. Each edge set underwent the application of the $\mathcal{GHI}$ formula, and the resultant value was determined by multiplying it with the respective frequency. For the computation of the extensive summations, Maple was employed. In Table 2, edges are classified based on the neighborhood degrees of the corresponding vertices. The $\mathcal{NGHI}$ formula, integrating both neighborhood degrees and the edge count for each edge set, was utilized to calculate precise index values. Likewise, $\mathcal{HGI}$ and $\mathcal{NHGI}$ were computed using a similar methodology. Employing a consistent format, identical calculations were conducted for hyaluronic acid-paclitaxel conjugates. Section 4 presents all results in an explanatory manner, while in Section 3, results are depicted in a concise format due to their similarity. The evaluation of results is graphically represented in Section 5 to scrutinize the behavior of the newly introduced indices.

3 Results for HAC

Utilizing edges partition strategies, degree and ev-degree based frequencies of different edges for two dimensional molecular structure of HAC are analyzed in Tables 1 and 2. Whereas, Figure 3 describes unit molecular cell and SiC_3-III[3,1] having 1 row and 3 unit molecules in each row.

Table 1. Degree based partition of edges of HAC

$(d(u), d(v))$	**Edge Frequency**
$(1, 2)$	$3n + 1$
$(1, 3)$	$13n + 1$
$(2, 2)$	$13n + 1$
$(2, 3)$	$29n - 1$
$(3, 3)$	$11n - 1$

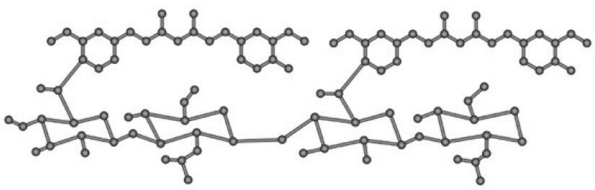

Figure 3. The unit cell and HAC[3,1], respectively

Table 2. Neighborhood degree based partition of edges of HAC

$((\lambda_u), (\lambda_v))$	**Edge Frequency**
$(2,4)$	$3n+1$
$(3,5)(3,6)(3,4)$	$2n$
$(3,7)(4,7)$	$3n$
$(5,5)$	$6n+1$
$(4,8)$	1
$(6,7)$	$9n-2$
$(6,8)$	$5n-2$
$(5,7)$	$n+2$
$(4,6)$	n
$(6,6)(7,8)$	$3n$
$(5,6)$	$7n$
$(8,8)$	$2n-1$
$(7,7)$	$4n$

By using the definition of EV-degree based geometric harmonic index, harmonic geometric index, and edges frequency of HAC given in Table 1, we compute following outcomes:

$$\begin{aligned}
\mathcal{GHI}^d(HAC) &= \sum_{e\in E(HAC\,conjugates)} \frac{(d_u+d_v)\sqrt{d_u.d_v}}{2} \\
&= (3n+1)\times\frac{(1+2)\sqrt{1\times 2}}{2} + (13n+1)\times\frac{(1+3)\sqrt{1\times 3}}{2} \\
&+(13n+1)\times\frac{(2+2)\sqrt{2\times 2}}{2} + (29n-1)\times\frac{(2+3)\sqrt{2\times 3}}{2} \\
&+ (11n-1)\times\frac{(3+3)\sqrt{3\times 3}}{2} \\
&= (3n+1)\times\frac{3\sqrt{2}}{2} + (13n+1)\times\frac{4\sqrt{3}}{2} + (13n+1)\times\frac{4\sqrt{4}}{2} \\
&+ (29n-1)\times\frac{5\sqrt{6}}{2} + (11n-1)\times\frac{6\sqrt{9}}{2} \\
&= 380.03n - 1.5
\end{aligned}$$

$$\begin{aligned}
\mathcal{HGI}^d(HAC) &= \sum_{e\in E(HAC\,conjugates)} \frac{2}{(d_u+d_v)\sqrt{d_u.d_v}} \\
&= (3n+1)\times\frac{2}{(1+2)\sqrt{1\times 2}} + (13n+1)\times\frac{2}{(1+3)\sqrt{1\times 3}} \\
&+(13n+1)\times\frac{2}{(2+2)\sqrt{2\times 2}} + (29n-1)\times\frac{2}{(2+3)\sqrt{2\times 3}} \\
&+(11n-1)\times\frac{2}{(3+3)\sqrt{3\times 3}} \\
&= (3n+1)\times\frac{2}{3\sqrt{2}} + (13n+1)\times\frac{2}{4\sqrt{3}} + (13n+1)\times\frac{2}{\sqrt{4}} \\
&+ (29n-1)\times\frac{2}{5\sqrt{6}} + (11n-1)\times\frac{2}{6\sqrt{9}} \\
&= 43.91n + 1.5
\end{aligned}$$

By using the definition of EV-degree based geometric harmonic index, harmonic geometric index, and edges frequency of HAC given in Table 2, we compute following outcomes:

$$\mathcal{NGHI}^{ev}(HAC) = \sum_{e\in E(HAC\,conjugates)} \frac{(\lambda_u+\lambda_v)\sqrt{\lambda_u.\lambda_v}}{2}$$
$$= (3n+1)\times\frac{(2+4)\sqrt{2\times4}}{2} + (2n)\times\frac{(4+3)\sqrt{4\times3}}{2}$$
$$+(2n)\times\frac{(3+5)\sqrt{3\times5}}{2} + (2n)\times\frac{(3+6)\sqrt{3\times8}}{2}$$
$$+(3n)\times\frac{(3+7)\sqrt{3\times7}}{2} + (6n+1)\times\frac{(5+5)\sqrt{5\times5}}{2}$$
$$+\frac{(4+8)\sqrt{4\times8}}{2} + (9n-2)\times\frac{6+7\sqrt{6\times7}}{2} + (5n-2)\times\frac{6+8\sqrt{6\times8}}{2}$$
$$+(3n)\times\frac{(7+8)\sqrt{7\times8}}{2} + (n+2)\times\frac{(5+7)\sqrt{5\times7}}{2} + n\times\frac{6+6\sqrt{6\times6}}{2}$$
$$= (3n+1)\times\frac{6\sqrt{8}}{2} + (2n)\times\frac{7\sqrt{12}}{2} + (2n)\times\frac{8\sqrt{15}}{2} + (2n)\times\frac{9\sqrt{18}}{2}$$
$$+ (3n)\times\frac{10\sqrt{21}}{2} + (6n+1)\times\frac{10\sqrt{25}}{2} + \frac{12\sqrt{32}}{2} + (9n-2)\times\frac{13\sqrt{42}}{2}$$
$$+ (5n-2)\times\frac{14\sqrt{48}}{2} + (3n)\times\frac{11\sqrt{28}}{2}$$
$$+ (n+2)\times\frac{12\sqrt{35}}{2} + (n)\times\frac{12\sqrt{36}}{2}$$
$$= 1845.8n - 106.8$$

$$\mathcal{NHGI}^{ev}(HAC) = \sum_{e\in E(HAC\,conjugates)} \frac{2}{(\lambda_u+\lambda_v)\sqrt{\lambda_u.\lambda_v}}$$
$$= (3n+1)\times\frac{2}{(2+4)\sqrt{2\times4}} + (2n)\times\frac{2}{(4+3)\sqrt{4\times3}}$$
$$+(2n)\times\frac{2}{(3+5)\sqrt{3\times5}} + (2n)\times\frac{2}{(3+6)\sqrt{3\times8}}$$
$$+(3n)\times\frac{2}{(3+7)\sqrt{3\times7}} + (6n+1)\times\frac{2}{(5+5)\sqrt{5\times5}}$$
$$+\frac{2}{(4+8)\sqrt{4\times8}} + (9n-2)\times\frac{2}{6+7\sqrt{6\times7}} + (5n-2)\times\frac{2}{6+8\sqrt{6\times8}}$$
$$+(3n)\times\frac{2}{(7+8)\sqrt{7\times8}} + (n+2)\times\frac{2}{(5+7)\sqrt{5\times7}} + n\times\frac{2}{6+6\sqrt{6\times6}}$$
$$= (3n+1)\times\frac{2}{6\sqrt{8}} + (2n)\times\frac{2}{7\sqrt{12}} + (2n)\times\frac{2}{8\sqrt{15}} + (2n)\times\frac{2}{9\sqrt{18}}$$
$$+ (3n)\times\frac{2}{10\sqrt{21}} + (6n+1)\times\frac{2}{10\sqrt{25}} + \frac{2}{12\sqrt{32}} + (9n-2)\times\frac{2}{13\sqrt{42}}$$
$$+ (5n-2)\times\frac{2}{14\sqrt{48}} + (3n)\times\frac{2}{11\sqrt{28}}$$
$$+ (n+2)\times\frac{2}{12\sqrt{35}} + (n)\times\frac{2}{12\sqrt{36}}$$
$$= 2.01n + 0.14$$

4 Results for HAP

Utilizing edges partition strategies, degree and ev-degree based frequencies of different edges for two dimensional molecular structure of HAC are analyzed in Tables 3 and 4. Whereas, Figure 3 describes unit molecular cell and HAC having 1 row and 3 unit molecules in each row.

Table 3. Degree based partition of edges of HAP

$(d(u), d(v))$	**Edge Frequency**
$(1,2)$	$\mathrm{n}+1$
$(1,3)$	$29\mathrm{n}+1$
$(2,2)$	$29\mathrm{n}+1$
$(1,4)$	$36\mathrm{n}-1$
$(2,3)$	$36\mathrm{n}-1$
$(2,4)$	$22\mathrm{n}-1$
$(3,3)$	$22\mathrm{n}-1$
$(3,4)$	$7\mathrm{n}$
$(4,4)$	n

Table 4. Neighborhood degree based partition of edges of HAP

$((\lambda_u), (\lambda_v))$	**Edge Frequency**
$(2,4)$	$\mathrm{n}+1$
$(3,4)$	$6\mathrm{n}$
$(3,6)(6,6)$	$4\mathrm{n}$
$(3,7)$	$5\mathrm{n}$
$(3,8)(5,6)$	n
$(4,4)$	$6\mathrm{n}$
$(4,5)$	$6\mathrm{n}$
$(4,6)(4,7)$	$2\mathrm{n}$
$(4,8)$	1
$(4,9)(4,10)$	$2\mathrm{n}$
$(5,5)$	1
$(5,7)$	$6\mathrm{n}+2$
$(5,8)(9,11)$	n
$(6,7)$	$9\mathrm{n}-2$
$(6,8)$	$10\mathrm{n}-2$
$(6,9)(6,10)$	n
$(7,7)$	$5\mathrm{n}$
$(7,8)(7,10)$	$4\mathrm{n}$
$(8,8)$	$4\mathrm{n}-1$
$(8,10)(9,10)$	$3\mathrm{n}$
$(10,11)$	$2\mathrm{n}$

Using the definition of EV-degree based geometric harmonic index, harmonic geometric index, and edges frequency of HAC given in Table 3, we compute following outcomes:

$$\begin{aligned}
\mathcal{GHI}^d(HAP) &= \sum_{e\in E(HAP\,conjugates)} \frac{(d_u+d_v)\sqrt{d_u.d_v}}{2} \\
&= (n+1)\times\frac{3\sqrt{2}}{2} + (29n+1)\times\frac{4\sqrt{3}}{2} \\
&+ (29n+1)\times\frac{4\sqrt{4}}{2} + (36n-1)\times\frac{5\sqrt{4}}{2} \\
&+ (36n-1)\times\frac{5\sqrt{6}}{2} + (22n-1)\times\frac{6\sqrt{9}}{2} \\
&+ 7n\times\frac{7\sqrt{12}}{2} + (n)\times\frac{8\sqrt{49}}{2} \\
&= 1104.63n-2
\end{aligned}$$

$$\begin{aligned}\mathcal{HGI}^{d}(HAP) &= \sum_{e\in E(HAP\,conjugates)} \frac{2}{(d_u+d_v)\sqrt{d_u.d_v}} \\ &= (n+1)\times\frac{2}{3\sqrt{2}} + (29n+1)\times\frac{2}{4\sqrt{3}} + (29n+1)\times\frac{2}{4\sqrt{4}} \\ &+ (36n-1)\frac{2}{5\sqrt{4}} + (36n-1)\times\frac{2}{5\sqrt{6}} + (22n-1)\times\frac{2}{6\sqrt{9}} \\ &+ 7n\times\frac{2}{7\sqrt{12}} + (n)\times\frac{2}{8\sqrt{49}} \\ &= 34.81n - 0.42\end{aligned}$$

Using the definition of EV-degree based geometric harmonic index, harmonic geometric index, and edges frequency of HAC given in Table 4, we compute following results:

$$\begin{aligned}\mathcal{NGHI}^{ev}(HAP) &= \sum_{e\in E(HAP\,conjugates)} \frac{(\lambda_u+\lambda_v)\sqrt{\lambda_u.\lambda_v}}{2} \\ &= (n+1)\times\frac{6\sqrt{8}}{2} + 6n\times\frac{7\sqrt{12}}{2} + 4n\times\frac{9\sqrt{18}}{2} + 5n\times\frac{10\sqrt{21}}{2} + n\times\frac{11\sqrt{24}}{2} \\ &+ 6n\times\frac{32}{2} + 6n\times\frac{9\sqrt{20}}{20} + 2n\times\frac{10\sqrt{244}}{2} + 2n\times\frac{11\sqrt{28}}{2} \\ &+ \frac{12\sqrt{32}}{2} + 2n\times\frac{13\sqrt{36}}{2} + 2n\times\frac{14\sqrt{40}}{2} + \frac{10\sqrt{25}}{2} \\ &+ n\times\frac{11\sqrt{30}}{2} + (6n+2)\times\frac{12\sqrt{35}}{2} + n\times\frac{13\sqrt{40}}{2} + 4n\times\frac{12\sqrt{36}}{2} \\ &+ (9n-2)\times\frac{13\sqrt{42}}{2} + (10n-2)\times\frac{14\sqrt{48}}{2} + n\times\frac{15\sqrt{54}}{2} + n\times\frac{16\sqrt{60}}{2} \\ &+ 5n\times\frac{14\sqrt{49}}{2} + 4n\times\frac{15\sqrt{56}}{2} + 4n\times\frac{17\sqrt{70}}{2} + (4n-1)\times\frac{16\sqrt{64}}{2} \\ &+ 3n\times\frac{18\sqrt{80}}{2} + 3n\times\frac{19\sqrt{90}}{2} + n\times\frac{20\sqrt{99}}{2} + 2n\times\frac{21\sqrt{110}}{2} \\ &= (4040.63n - 106.82)\end{aligned}$$

$$\begin{aligned}\mathcal{NHGI}^{ev}(HAP) &= \sum_{e\in E(HAP\,conjugates)} \frac{2}{(\lambda_u+\lambda_v)\sqrt{\lambda_u.\lambda_v}} \\ &= (n+1)\times\frac{2}{6\sqrt{8}} + 6n\times\frac{2}{7\sqrt{12}} + 4n\times\frac{2}{9\sqrt{18}} + 5n\times\frac{2}{10\sqrt{21}} + n\times\frac{2}{11\sqrt{24}} \\ &+ 6n\times\frac{2}{32} + 6n\times\frac{20}{9\sqrt{20}} + 2n\times\frac{2}{10\sqrt{244}} + 2n\times\frac{2}{11\sqrt{28}} + \frac{2}{12\sqrt{32}} \\ &+ 2n\times\frac{2}{13\sqrt{36}} + 2n\times\frac{2}{14\sqrt{40}} + \frac{2}{10\sqrt{25}} + n\times\frac{2}{11\sqrt{30}} + (6n+2)\times\frac{2}{12\sqrt{35}} \\ &+ n\times\frac{2}{13\sqrt{40}} + 4n\times\frac{2}{12\sqrt{36}} + (9n-2)\times\frac{2}{13\sqrt{42}} + (10n-2)\times\frac{2}{14\sqrt{48}} \\ &+ n\times\frac{2}{15\sqrt{54}} + n\times\frac{2}{16\sqrt{60}} + 5n\times\frac{2}{14\sqrt{49}} + 4n\times\frac{2}{15\sqrt{56}} \\ &+ 4n\times\frac{2}{17\sqrt{70}} + (4n-1)\times\frac{2}{16\sqrt{64}} + 3n\times\frac{2}{18\sqrt{80}} \\ &+ 3n\times\frac{2}{19\sqrt{90}} + n\times\frac{2}{20\sqrt{99}} + 2n\times\frac{2}{21\sqrt{110}} \\ &= (3.11n - 0.22)\end{aligned}$$

5 Discussion and Graphical Analysis

In addition to providing a visual understanding of the computed formulas for various indices through graphical representations in Figures 4 and 5, the insights derived from this section hold particular significance in the realm of drug design. The correlation observed between these indices and intricate molecular structures serves as a valuable guide for designing more effective and targeted pharmaceutical compounds. The nuanced interpretation of the impact of molecular-scale variations on the calculated indices contributes to the rational design of molecules with optimized pharmacological properties. The fact that the index values go up proportionally as the number of molecules we look at goes up shows that these results can be applied to a larger scale. This opens up exciting possibilities for making new drugs that work better and more specifically. Thus, the applications of these insights extend beyond theoretical understanding, playing a pivotal role in shaping the future landscape of drug discovery and design.

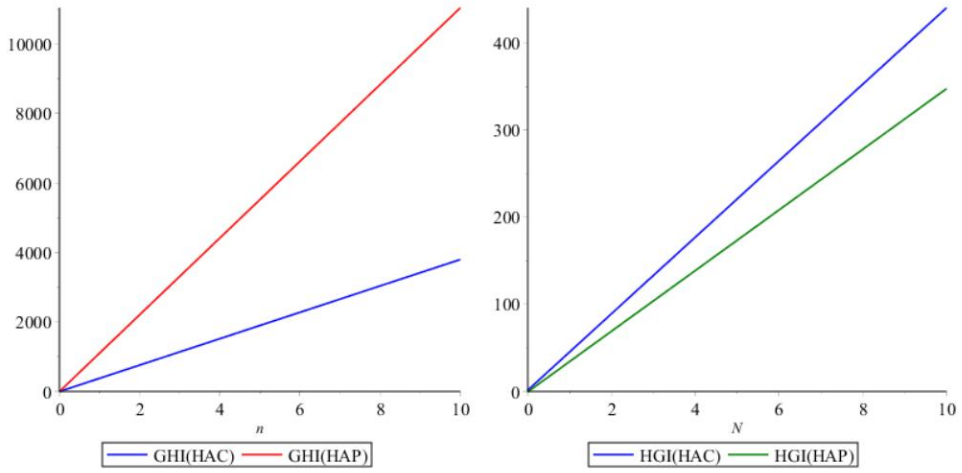

Figure 4. Variations of $\mathcal{GHI}$ and $\mathcal{HGI}$ for HAC and HAP

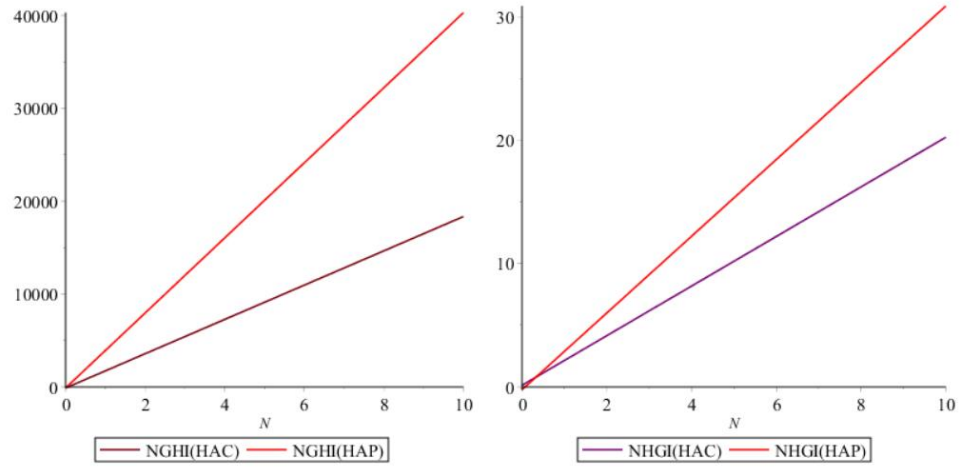

Figure 5. Variations of $\mathcal{NGHI}$ and $\mathcal{NHGI}$ for HAC and HAP

6 Conclusions

A contemporary trend in the field of mathematical and computational chemistry revolves around the assessment of diverse properties in molecular structures using numerical graph descriptors. These mathematical invariants have proven to be invaluable in various applications, such as QSAR and QSPR studies, contributing significantly to advancements in molecular design, drug discovery, and the hazard assessment of chemicals. We present a new set of indices, the geometric-harmonic index, the harmonic-geometric index, the neighborhood geometric-harmonic index, and the neighborhood harmonic-geometric index. These indices were specifically designed for the molecular graphs of hyaluronic acid-curcumin and paclitaxel conjugates and are based on numbers. Our numerical findings

are visually presented, highlighting the potential correlation of the evaluated results with the structural aspects of the mentioned molecular structures.

Data Availability

Not applicable.

Conflicts of Interest

The authors declare no conflict of interest.

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