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Research article

Proof of a conjecture on the geometric-quadratic index of unicyclic graphs and its applications

Abeer M. Albalahi[1], **Kinkar Chandra Das**[2,*], **Sultan Ahmad**[3], **Tariq Alraqad**[1] and **Akbar Ali**[1,*]

[1] Department of Mathematics, College of Science, University of Ha'il, Ha'il 81451, Saudi Arabia
[2] Department of Mathematics, Sungkyunkwan University, Suwon 16419, Republic of Korea
[3] Department of Mathematics, School of Natural Sciences, National University of Sciences and Technology, H-12, Islamabad 44000, Pakistan

* **Correspondence:** Email: kinkardas2003@gmail.com, akbarali.maths@gmail.com.

Abstract: The geometric-quadratic (GQ) index is defined for a graph Γ as $GQ(\Gamma) = \sum_{v_iv_j\in\mathcal{E}(\Gamma)} \sqrt{\frac{2\,d_i\,d_j}{d_i^2+d_j^2}}$, where d_i denotes the degree of the vertex v_i. This degree-based topological index captures structural information by combining both geometric and quadratic contributions of adjacent vertex degrees. Recently, Furtula and Oz [Geometric-quadratic index from a mathematical perspective, *Iranian J. Math. Chem.*, 16 (2025), 85–89] proposed a conjecture concerning the behavior of the GQ index for unicyclic graphs. In the present paper, we rigorously established the validity of this conjecture, thereby contributing to the theoretical understanding of degree-based graph invariants. Furthermore, Kumar and Das [Comparative study of GQ and QG indices as potentially favorable molecular descriptors, *Int. J. Quantum Chem.*, 124 (2024), #27334] suggested that the GQ index may serve as a more effective molecular descriptor in quantitative structure-property relationship (QSPR) analysis, particularly for predicting physicochemical properties of molecular compounds beyond the extensively studied class of alkane isomers. Motivated by these findings, we further investigated the applicability of the GQ index by examining its role in elucidating QSPR in benzene-based hydrocarbons. For octane isomers, we extended this analysis using linear, quadratic, and cubic regression models across sixteen properties. The cubic model proved most effective for several properties, including four that previously failed under linear models alone. This analysis highlights the broader potential of the GQ index as a chemically meaningful descriptor, including its possible relevance in therapeutic and pharmaceutical contexts.

Keywords: molecular descriptor; geometric-quadratic (GQ) index; unicyclic graph; QSPR modeling; chemical graph theory
Mathematics Subject Classification: 05C07, 05C09, 05C92

1. Introduction

Chemical graph theory (CGT) forms a vital bridge between chemistry and mathematics by modeling molecular structures through graph-theoretical concepts. In this representation, atoms and chemical bonds correspond to the vertices and edges of a graph, respectively, allowing molecular properties to be examined using mathematical and computational tools. Among the central notions in CGT are topological indices, which assign a real number to each molecular graph in a way that remains invariant under graph isomorphism. These indices encode structural information such as molecular size, branching, and connectivity, and have been widely employed in quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies to predict physicochemical and biological characteristics of chemical compounds. The simplicity, invariance, and predictive efficiency of topological indices make them indispensable in the study of molecular structure and reactivity. For an overview of current advances and chemical applications of topological indices, we refer to [14, 26].

Throughout the paper, Γ denotes a connected simple graph with vertex set $\mathcal{V}(\Gamma)$ and edge set $\mathcal{E}(\Gamma)$. The cardinality of a set Q is indicated by $|Q|$. The order and size of Γ are defined as $\eta = |\mathcal{V}(\Gamma)|$ and $m = |\mathcal{E}(\Gamma)|$. If $m = \eta$, then Γ is called a unicyclic graph. The notation $v_iv_j \in \mathcal{E}(\Gamma)$ signifies that v_i and v_j share an edge in Γ. If an edge is inserted between two non-adjacent vertices v_i and v_j, the resulting graph is denoted by $\Gamma + v_iv_j$; conversely, removing an existing edge v_iv_j yields the graph $\Gamma - v_iv_j$. For a vertex $v_i \in \mathcal{V}(\Gamma)$, the set of its adjacent vertices is represented by $N_\Gamma(v_i) = \{v_j \in \mathcal{V}(\Gamma) : v_iv_j \in \mathcal{E}(\Gamma)\}$, and the degree of v_i is written as $d_i = |N_\Gamma(v_i)|$. A vertex v_i in Γ with $d_i = 1$ is said to be a pendant vertex, and an edge incident to it is called a pendant edge. Denote by $\Delta(\Gamma) = \max_{1\le i\le\eta} d_i$ and $\delta(\Gamma) = \min_{1\le i\le\eta} d_i$ the maximum and minimum degrees of Γ, respectively. If v_1 is a vertex such that $d_1 = \Delta(\Gamma)$, then the second-largest degree of Γ is termed as $\Delta_2(\Gamma) = \max_{2\le i\le\eta} d_i$. The graphs S_η and C_η represent the star and cycle graphs, respectively, each having η vertices.

A starlike unicyclic graph is a unicyclic graph that has only one vertex with degree greater than two. The graph $C_3S_{\eta-3}$ represents this graph constructed by merging the central vertex of the star $S_{\eta-2}$ with a vertex of degree two in the cycle C_3; see Figure 1.

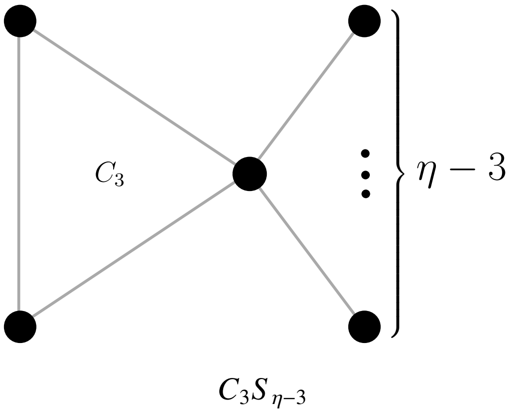

Figure 1. The starlike unicyclic graph $C_3S_{\eta-3}$.

Any undefined terminology and notation in this paper follows those in [5]. Within the diverse families of topological indices, those based on vertex degrees (see, for example, [1–3]) are particularly significant, owing to their ease of computation and their consistently strong correlations with numerous molecular characteristics (see, for example, [20,29,37]).

The primary focus of this study is the geometric-quadratic (GQ) index, introduced by Kulli [23] with the motivation of the geometric–arithmetic index [36]. The GQ index of a graph Γ is formulated as:

$$GQ(\Gamma) = \sum_{v_i v_j \in \mathcal{E}(\Gamma)} \sqrt{\frac{2\, d_i\, d_j}{d_i^2 + d_j^2}}.$$

In a recent study, Furtula and Oz [18] investigated extremal graphs for the GQ index among graphs, trees, and unicyclic graphs. They also established several mathematical relations between the GQ index and other well-known topological indices. In their study, they identified $C_3S_{\eta-3}$ as the unicyclic graph minimizing the GQ index, although a formal proof was not provided. Consequently, they posed it as an open problem and formulated the following conjecture:

Conjecture 1. [18] *Let Γ be a unicyclic graph with $\eta \geq 4$ vertices. Then*

$$GQ(\Gamma) \geq GQ(C_3S_{\eta-3}) = (\eta - 3)\sqrt{\frac{2\,(\eta-1)}{(\eta-1)^2+1}} + 2\sqrt{\frac{4\,(\eta-1)}{(\eta-1)^2+4}} + 1$$

with equality if and only if (iff) $\Gamma \cong C_3S_{\eta-3}$.

This paper addresses Conjecture 1 and provides its complete solution. Furthermore, Kumar and Das [24] suggested exploring the GQ index beyond alkane isomers. Motivated by this suggestion, we investigate the role of the GQ index in elucidating structure–property relationships of benzene hydrocarbon compounds, thereby demonstrating its broader applicability as a molecular descriptor of therapeutic relevance.

The organization of the paper is outlined as follows:

- Section 2 provides the complete solution of Conjecture 1.
- Section 3 examines the role of the GQ index in elucidating structure-property relationships for benzene hydrocarbons and octane isomers, with an emphasis on properties of pharmaceutical relevance.
- Section 4 concludes the paper with final remarks and suggests directions for future research.

2. Proof of Conjecture 1

This section provides a complete solution to Conjecture 1. Before presenting the proof, we state several supporting results that will be used in the derivation.

Lemma 2.1. *Let v_iv_j be any edge in graph Γ such that $b \leq d_j \leq d_i \leq a$. Then*

$$\frac{d_i\, d_j}{d_i^2 + d_j^2} \geq \frac{a\, b}{a^2 + b^2}$$

with equality exactly for $d_i = a$ and $d_j = b$.

Proof. For an edge v_iv_j in Γ with $b \leq d_j \leq d_i \leq a$, we have

$$\frac{d_i}{d_j} \leq \frac{a}{b} \text{ and } \frac{d_j}{d_i} \geq \frac{b}{a}$$

with equality iff $d_i = a$ and $d_j = b$. Thus we have

$$\sqrt{\frac{d_i}{d_j}} - \sqrt{\frac{d_j}{d_i}} \leq \sqrt{\frac{a}{b}} - \sqrt{\frac{b}{a}}$$

with equality iff $d_i = a$ and $d_j = b$. Squaring both sides, we obtain

$$\frac{d_i}{d_j} + \frac{d_j}{d_i} \leq \frac{a}{b} + \frac{b}{a},$$

that is,

$$\frac{d_i\,d_j}{d_i^2 + d_j^2} \geq \frac{a\,b}{a^2 + b^2}$$

with equality exactly for $d_i = a$ and $d_j = b$. □

Choosing $(a, b) \in \left\{(1,\, \eta - 1), (2, \eta - 1), (1, \Delta_2)\right\}$ in Lemma 2.1 yields the following corollaries.

Corollary 2.2. *Consider an edge* v_iv_j *in* Γ *such that* $1 \leq d_j \leq d_i \leq \eta - 1$. *Then*

$$\frac{d_i\,d_j}{d_i^2 + d_j^2} \geq \frac{(\eta - 1)}{(\eta - 1)^2 + 1}$$

with equality exactly for $d_i = \eta - 1$ *and* $d_j = 1$.

Corollary 2.3. *Consider an edge* v_iv_j *in* Γ *such that* $2 \leq d_j \leq d_i \leq \eta - 1$. *Then*

$$\frac{d_i\,d_j}{d_i^2 + d_j^2} \geq \frac{2(\eta - 1)}{(\eta - 1)^2 + 4}$$

with equality exactly for $d_i = \eta - 1$ *and* $d_j = 2$.

Corollary 2.4. *Consider an edge* v_iv_j *in* Γ *such that* $1 \leq d_j \leq d_i \leq \Delta_2$, *where* Δ_2 *is the second-maximum degree in* Γ. *Then*

$$\frac{d_i\,d_j}{d_i^2 + d_j^2} \geq \frac{\Delta_2}{\Delta_2^2 + 1}$$

with equality exactly for $d_i = \Delta_2$ *and* $d_j = 1$.

Lemma 2.5. *Let*

$$f(x) = \frac{x}{x - 1} \cdot \sqrt{\frac{2x}{x^2 + 1}} - \frac{1}{x - 1}, \quad x \geq 5.$$

Then the function $f(x)$ *is a strictly decreasing function on* $x \geq 5$.

Proof. We have

$$f(x)=\frac{x}{x-1}\cdot\sqrt{\frac{2x}{x^2+1}}-\frac{1}{x-1},\quad x\geq 5.$$

Then

$$f'(x)=-\frac{1}{(x-1)^2}\cdot\sqrt{\frac{2x}{x^2+1}}-\frac{\sqrt{x}\,(x+1)}{\sqrt{2}\,(x^2+1)^{3/2}}+\frac{1}{(x-1)^2}.$$

Since $x\geq 5$, one can easily check that

$$2x\,(x-1)>\frac{3}{x}+\frac{1}{x^3},$$

that is,

$$x\,(x+1)^2=x\,(x^2+2x+1)>x^3+3x+\frac{3}{x}+\frac{1}{x^3}=\left(x+\frac{1}{x}\right)^3,$$

that is,

$$x^2\,(x+1)>(x^2+1)^{3/2}. \tag{2.1}$$

Since $x\geq 5$, one can easily see that

$$(x-3)^2-4+\frac{1}{x^2}+\left(1-\frac{4}{x}\right)>0,$$

that is,

$$(x-2)^2+\frac{1}{x^2}+2\left(1-\frac{2}{x}\right)>2x,$$

that is,

$$x-2+\frac{1}{x}>\sqrt{2x},$$

that is,

$$(x-1)^2>\sqrt{2}\,x^{3/2}. \tag{2.2}$$

Using (2.1) and (2.2), we obtain

$$f'(x)<-\frac{\sqrt{x}\,(x+1)}{\sqrt{2}\,(x^2+1)^{3/2}}+\frac{1}{(x-1)^2}<-\frac{1}{\sqrt{2}\,x^{3/2}}+\frac{1}{(x-1)^2}<0.$$

Therefore, $f(x)$ is a decreasing function on $x\geq 5$. □

Lemma 2.6. *Let*

$$f(x)=\frac{\sqrt{2x}}{\sqrt{x^2+1}}+\frac{2\sqrt{x}}{(x-2)\sqrt{x^2+4}}-\frac{1}{x-2},\quad x\geq 9.$$

Then the function $f(x)$ strictly decreases on $x\geq 9$.

Proof. Since

$$f(x) = \frac{\sqrt{2x}}{\sqrt{x^2+1}} + \frac{2\sqrt{x}}{(x-2)\sqrt{x^2+4}} - \frac{1}{x-2},$$

we have

$$f'(x) = -\frac{(x^2-1)}{\sqrt{2x}(x^2+1)^{3/2}} - \frac{2\sqrt{x}}{(x-2)^2\sqrt{x^2+4}} - \frac{(x+2)}{\sqrt{x}\,(x^2+4)^{3/2}} + \frac{1}{(x-2)^2}. \tag{2.3}$$

Since $x \geq 9$, one can easily see that

$$\left(\sqrt{x} - \frac{1}{x\sqrt{x}}\right)^2 \left(1 - \frac{2}{x}\right)^4 > 3 > 2\left(1 + \frac{1}{x^2}\right)^3,$$

that is,

$$(x^2-1)^2 (x-2)^4 > 2\,x\,(x^2+1)^3,$$

that is,

$$\frac{(x^2-1)}{\sqrt{2x}\,(x^2+1)^{3/2}} > \frac{1}{(x-2)^2}.$$

Using the above result in (2.3), we obtain $f'(x) < 0$. Thus $f(x)$ is a strictly decreasing function on $x \geq 9$. □

Theorem 2.7. *Let* Γ *be a unicyclic graph of order* η. *Then*

$$GQ(\Gamma) \geq (\eta-3)\sqrt{\frac{2(\eta-1)}{(\eta-1)^2+1}} + 2\sqrt{\frac{4(\eta-1)}{(\eta-1)^2+4}} + 1 \tag{2.4}$$

with equality exactly for $\Gamma \cong C_3S_{\eta-3}$.

Proof. For $\eta \leq 9$, the inequality (2.4) can be easily verified using Sage [35], with equality holding iff $\Gamma \cong C_3S_{\eta-3}$. Hence, we focus on the case $\eta \geq 10$. Let C_k ($k \geq 3$) denote the cycle of length k in Γ. Let v_1 and v_2 denote the vertices of maximum and second-maximum degree, having degrees Δ and Δ_2, respectively. Since Γ is unicyclic, we have $2 \leq \Delta_2 \leq \frac{\eta+1}{2}$. We consider the following cases:

Case 1. $\Delta_2 = 2$. We have $2 \leq \Delta \leq \eta - 1$. For $\Delta = \eta - 1$, we have $\Gamma \cong C_3S_{\eta-3}$ with

$$GQ(\Gamma) = (\eta-3)\sqrt{\frac{2(\eta-1)}{(\eta-1)^2+1}} + 2\sqrt{\frac{4(\eta-1)}{(\eta-1)^2+4}} + 1$$

and hence the equality holds in (2.4). For $\Delta = 2$, we have $\Gamma \cong C_\eta$ and hence

$$GQ(\Gamma) = \eta > (\eta-3)\sqrt{\frac{2(\eta-1)}{(\eta-1)^2+1}} + 2\sqrt{\frac{4(\eta-1)}{(\eta-1)^2+4}} + 1.$$

Then the inequality (2.4) holds strictly.

Otherwise, $3 \leq \Delta \leq \eta - 2$. Since $\Delta_2 = 2$, there is exactly one vertex $v_1 \in \mathcal{V}(C_k)$ whose degree is at least 3, while all other vertices of $\mathcal{V}(C_k)$ have degree 2. Then $d_1 = \Delta$. Let v_1v_2, $v_1v_k \in \mathcal{E}(C_k)$. Since $k \geq 3$, there exists an edge $v_pv_q \in \mathcal{E}(C_k)$ such that $d_p = d_q = 2$. By Lemma 2.1, we obtain

$$\sqrt{\frac{2\,d_pd_q}{d_p^2 + d_q^2}} = 1, \quad \sqrt{\frac{2\,d_1d_2}{d_1^2 + d_2^2}} > \sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}} \text{ and } \sqrt{\frac{2\,d_1d_k}{d_1^2 + d_k^2}} > \sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}}$$

as $\Delta < n - 1$. Thus we have

$$\sum_{v_iv_j \in \mathcal{E}(C_k)} \sqrt{\frac{2\,d_i\,d_j}{d_i^2 + d_j^2}} > 2\,\sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}} + k - 2.$$

Moreover, for any edge $v_iv_j \in \mathcal{E}(\Gamma)$, by Corollary 2.2, we obtain

$$\sqrt{\frac{2\,d_id_j}{d_i^2 + d_j^2}} \geq \sqrt{\frac{2\,(\eta - 1)}{(\eta - 1)^2 + 1}}.$$

Now,

$$\begin{aligned} GQ(\Gamma) &= \sum_{v_iv_j \in \mathcal{E}(\Gamma)} \sqrt{\frac{2\,d_i\,d_j}{d_i^2 + d_j^2}} \\ &= \sum_{v_iv_j \in \mathcal{E}(C_k)} \sqrt{\frac{2\,d_i\,d_j}{d_i^2 + d_j^2}} + \sum_{v_iv_j \in \mathcal{E}(\Gamma) \setminus \mathcal{E}(C_k)} \sqrt{\frac{2\,d_i\,d_j}{d_i^2 + d_j^2}} \\ &> 2\,\sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}} + k - 2 + (\eta - k)\,\sqrt{\frac{2\,(\eta - 1)}{(\eta - 1)^2 + 1}} \\ &\geq (\eta - 3)\,\sqrt{\frac{2\,(\eta - 1)}{(\eta - 1)^2 + 1}} + 2\,\sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}} + 1 \end{aligned}$$

as $k \geq 3$ and

$$\sqrt{\frac{2\,(\eta - 1)}{(\eta - 1)^2 + 1}} < 1.$$

Then the inequality (2.4) holds strictly.

Case 2. $3 \leq \Delta_2 \leq \frac{\eta+1}{2}$. Let

$$h(\Delta_2) = \frac{\Delta_2}{\Delta_2 - 1} \cdot \sqrt{\frac{2\,\Delta_2}{\Delta_2^2 + 1}} - \frac{1}{\Delta_2 - 1}.$$

One can easily see that $h(3) > h(4) > h(5)$. By Lemma 2.5,

$$h(x) = \frac{x}{x - 1} \cdot \sqrt{\frac{2x}{x^2 + 1}} - \frac{1}{x - 1}$$

is a strictly decreasing function on $5 \leq x \leq \frac{\eta+1}{2}$. Thus we have

$$h(5) > h(6) > \cdots > h\left(\frac{\eta+1}{2}\right).$$

Since $3 \leq \Delta_2 \leq \frac{\eta+1}{2}$, from the above results, we obtain

$$\frac{\Delta_2}{\Delta_2-1} \cdot \sqrt{\frac{2\,\Delta_2}{\Delta_2^2+1}} - \frac{1}{\Delta_2-1} = h(\Delta_2) \geq h\Big(\frac{\eta+1}{2}\Big) = \frac{\eta+1}{\eta-1} \cdot \sqrt{\frac{4\,(\eta+1)}{(\eta+1)^2+4}} - \frac{2}{\eta-1}. \tag{2.5}$$

We now prove the following claim:

Claim 1.

$$\frac{\eta+1}{\eta-1} \cdot \sqrt{\frac{4\,(\eta+1)}{(\eta+1)^2+4}} - \frac{2}{\eta-1} > \sqrt{\frac{2}{\eta-1}}. \tag{2.6}$$

Proof of Claim 1. For $10 \leq \eta \leq 12$, the inequality (2.6) can be verified directly. Hence, it suffices to consider $\eta \geq 13$. Observed that

$$1 + \frac{4}{\eta-1} + \frac{4}{(\eta-1)^2} > 1 + \frac{2}{\eta-1} + \frac{4}{\eta^2-1},$$

which implies

$$\frac{\eta+1}{\eta-1} = 1 + \frac{2}{\eta-1} > \sqrt{1 + \frac{2}{\eta-1} + \frac{4}{\eta^2-1}} = \sqrt{\frac{(\eta+1)^2+4}{\eta^2-1}}.$$

Consequently,

$$\frac{\eta+1}{\eta-1} \cdot \sqrt{\frac{4\,(\eta+1)}{(\eta+1)^2+4}} > \sqrt{\frac{4}{\eta-1}},$$

that is,

$$\frac{\eta+1}{\eta-1} \cdot \sqrt{\frac{4\,(\eta+1)}{(\eta+1)^2+4}} - \frac{2}{\eta-1} > \sqrt{\frac{4}{\eta-1}} - \frac{2}{\eta-1}. \tag{2.7}$$

We have to prove that

$$\sqrt{\frac{4}{\eta-1}} - \frac{2}{\eta-1} > \sqrt{\frac{2}{\eta-1}}, \tag{2.8}$$

that is,

$$2 - \sqrt{2} > \frac{2}{\sqrt{\eta-1}},$$

that is,

$$\eta > 1 + \left(\frac{2}{2-\sqrt{2}}\right)^2,$$

which is true for $\eta \geq 13$. Combining (2.7) and (2.8), the proof of Claim 1 is now complete.

Using Claim 1 in (2.5), we obtain

$$\frac{\Delta_2}{\Delta_2 - 1} \cdot \sqrt{\frac{2\Delta_2}{\Delta_2^2 + 1}} - \frac{1}{\Delta_2 - 1} > \sqrt{\frac{2}{\eta - 1}},$$

that is,

$$\Delta_2 \sqrt{\frac{2\Delta_2}{\Delta_2^2 + 1}} > 1 + (\Delta_2 - 1) \sqrt{\frac{2}{\eta - 1}}. \tag{2.9}$$

Let

$$S_1 = \left\{v_1 v_i \in \mathcal{E}(\Gamma) \mid v_i \in N_\Gamma(v_1)\right\} \quad \text{and} \quad S_2 = \left\{v_2 v_i \in \mathcal{E}(\Gamma) \mid v_i \in N_\Gamma(v_2)\right\}.$$

Then we have $|S_1| = \Delta$ and $|S_2| = \Delta_2$. Also let $S = S_1 \cup S_2$. We have $S \subseteq \mathcal{E}(\Gamma)$ and hence $|S| \leq |\mathcal{E}(\Gamma)|$. We take into account the following two cases:

Case 2.1. $|S| < |\mathcal{E}(\Gamma)|$. We have

$$\begin{aligned} GQ(\Gamma) &= \sum_{v_i v_j \in \mathcal{E}(\Gamma)} \sqrt{\frac{2\, d_i\, d_j}{d_i^2 + d_j^2}} \\ &= \sum_{v_i v_j \in S_2} \sqrt{\frac{2\, d_i\, d_j}{d_i^2 + d_j^2}} + \sum_{v_i v_j \in \mathcal{E}(\Gamma) \setminus S_2} \sqrt{\frac{2\, d_i\, d_j}{d_i^2 + d_j^2}}. \end{aligned} \tag{2.10}$$

We further proceed by examining two distinct cases:

Case 2.1.1. $v_1 v_2 \notin \mathcal{E}(\Gamma)$. Let $v_i v_j \in S_2$ be an edge in Γ. Then $1 \leq d_j \leq d_i \leq \Delta_2$ and by Corollary 2.4, we obtain

$$\sum_{v_i v_j \in S_2} \sqrt{\frac{2 d_i\, d_j}{d_i^2 + d_j^2}} \geq \Delta_2 \cdot \sqrt{\frac{2\, \Delta_2}{\Delta_2^2 + 1}}.$$

Since Γ is unicyclic and $v_1 v_2 \notin \mathcal{E}(\Gamma)$, it follows that Γ contains at least one non-pendant edge, say $v_1 v_y$, such that $2 \leq d_y \leq d_1 = \Delta < \eta - 1$. By Corollary 2.3, we obtain

$$\sqrt{\frac{2 d_1\, d_y}{d_1^2 + d_y^2}} > \sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}}.$$

Since Γ is connected unicyclic with $v_1 v_2 \notin \mathcal{E}(\Gamma)$ and $|S| < |\mathcal{E}(\Gamma)|$, then there exists an edge $v_p v_q \in \mathcal{E}(\Gamma)$ such that $v_p v_q \notin S$, where $1 \leq d_q \leq d_p \leq \frac{\eta - 1}{2}$. Applying Lemma 2.1, we obtain

$$\sqrt{\frac{2\, d_p\, d_q}{d_p^2 + d_q^2}} \geq \sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}}.$$

Let $S_3 = S_2 \cup \{v_1 v_y,\ v_p v_q\}$. Using the above results with (2.9) and Corollary 2.2 in (2.10), we obtain

$$\begin{aligned} GQ(\Gamma) &= \sum_{v_i v_j \in S_2} \sqrt{\frac{2\,d_i\,d_j}{d_i^2 + d_j^2}} + \sqrt{\frac{2d_1\,d_y}{d_1^2 + d_y^2}} + \sqrt{\frac{2d_p\,d_q}{d_p^2 + d_q^2}} + \sum_{v_i v_j \in \mathcal{E}(\Gamma)\setminus S_3} \sqrt{\frac{2\,d_i\,d_j}{d_i^2 + d_j^2}} \\ &> \Delta_2 \cdot \sqrt{\frac{2\,\Delta_2}{\Delta_2^2 + 1}} + 2\,\sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}} + (\eta - \Delta_2 - 2)\,\sqrt{\frac{2\,(\eta - 1)}{(\eta - 1)^2 + 1}} \\ &> 1 + (\Delta_2 - 1)\,\sqrt{\frac{2}{\eta - 1}} + 2\,\sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}} + (\eta - \Delta_2 - 2)\,\sqrt{\frac{2\,(\eta - 1)}{(\eta - 1)^2 + 1}} \\ &> (\eta - 3)\,\sqrt{\frac{2\,(\eta - 1)}{(\eta - 1)^2 + 1}} + 2\,\sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}} + 1 \end{aligned}$$

as

$$\sqrt{\frac{2}{\eta - 1}} > \sqrt{\frac{2\,(\eta - 1)}{(\eta - 1)^2 + 1}}.$$

Inequality (2.4) strictly holds.

Case 2.1.2. $v_1 v_2 \in \mathcal{E}(\Gamma)$. Since Γ is connected unicyclic and $|S| < |\mathcal{E}(\Gamma)|$, then there exists an edge $v_p v_q \in \mathcal{E}(\Gamma)$ such that $v_p v_q \notin S$, where $1 \le d_q \le d_p \le \Delta_2$. Applying Corollary 2.4, we obtain

$$\sqrt{\frac{2\,d_p\,d_q}{d_p^2 + d_q^2}} \ge \sqrt{\frac{2\,\Delta_2}{\Delta_2^2 + 1}}. \tag{2.11}$$

For $v_i v_j \in S_2 \setminus \{v_1 v_2\}$, we have $1 \le d_j \le d_i \le \Delta_2$. Again applying Corollary 2.4, we obtain

$$\sum_{v_i v_j \in S_2 \setminus \{v_1 v_2\}} \sqrt{\frac{2\,d_i\,d_j}{d_i^2 + d_j^2}} + \sqrt{\frac{2\,d_p\,d_q}{d_p^2 + d_q^2}} \ge (\Delta_2 - 1) \cdot \sqrt{\frac{2\,\Delta_2}{\Delta_2^2 + 1}} + \sqrt{\frac{2\,\Delta_2}{\Delta_2^2 + 1}} = \Delta_2 \cdot \sqrt{\frac{2\,\Delta_2}{\Delta_2^2 + 1}}.$$

Since Γ is unicyclic, there exists an edge $v_x v_y \in \mathcal{E}(C_k)$ such that $v_x \ne v_2 \ne v_y$. Let $S_4 = S_2 - \{v_1 v_2\} + \{v_p v_q,\ v_x v_y\}$. We have $2 \le \Delta_2 \le \Delta < \eta - 1$ and $2 \le d_x \le d_y < \eta - 1$. By Corollary 2.3, we obtain

$$\sqrt{\frac{2\Delta\,\Delta_2}{\Delta^2 + \Delta_2^2}} > \sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}} \quad \text{and} \quad \sqrt{\frac{2d_y\,d_x}{d_y^2 + d_x^2}} > \sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}}.$$

Applying the above results together with Corollary 2.2 in (2.10), we obtain

$$\begin{aligned} GQ(\Gamma) = &\sum_{v_i v_j \in S_2 \setminus \{v_1 v_2\}} \sqrt{\frac{2\,d_i\,d_j}{d_i^2 + d_j^2}} + \sqrt{\frac{2\Delta\,\Delta_2}{\Delta^2 + \Delta_2^2}} + \sqrt{\frac{2d_p\,d_q}{d_p^2 + d_q^2}} + \sqrt{\frac{2d_y\,d_x}{d_y^2 + d_x^2}} \\ &+ \sum_{v_i v_j \in \mathcal{E}(\Gamma)\setminus S_4} \sqrt{\frac{2\,d_i\,d_j}{d_i^2 + d_j^2}} \end{aligned}$$

$$> \Delta_2 \cdot \sqrt{\frac{2\,\Delta_2}{\Delta_2^2+1}} + 2\,\sqrt{\frac{4\,(\eta-1)}{(\eta-1)^2+4}} + (\eta-\Delta_2-2)\,\sqrt{\frac{2\,(\eta-1)}{(\eta-1)^2+1}}$$

$$> 1 + (\Delta_2-1)\,\sqrt{\frac{2}{\eta-1}} + 2\,\sqrt{\frac{4\,(\eta-1)}{(\eta-1)^2+4}} + (\eta-\Delta_2-2)\,\sqrt{\frac{2\,(\eta-1)}{(\eta-1)^2+1}}$$

$$> (\eta-3)\,\sqrt{\frac{2\,(\eta-1)}{(\eta-1)^2+1}} + 2\,\sqrt{\frac{4\,(\eta-1)}{(\eta-1)^2+4}} + 1$$

as

$$\sqrt{\frac{2}{\eta-1}} > \sqrt{\frac{2\,(\eta-1)}{(\eta-1)^2+1}}.$$

Inequality (2.4) strictly holds.

Case 2.2. $|S| = |\mathcal{E}(\Gamma)|$. Let

$$M(\Delta_2) = \sqrt{\frac{2\,\Delta_2}{\Delta_2^2+1}} + \frac{2}{\Delta_2-2}\cdot\sqrt{\frac{\Delta_2}{\Delta_2^2+4}} - \frac{1}{\Delta_2-2}.$$

By Sage [35], one can easily check that

$$M(3) > M(4) > M(5) > M(6) > M(7) > M(8) > M(9).$$

For $9 \le \Delta_2 \le \frac{\eta+1}{2}$, by Lemma 2.6, we obtain

$$M(\Delta_2) \ge M\left(\frac{\eta+1}{2}\right) = \sqrt{\frac{4\,(\eta+1)}{(\eta+1)^2+4}} + \frac{4}{\eta-3}\cdot\sqrt{\frac{2\,(\eta+1)}{(\eta+1)^2+16}} - \frac{2}{\eta-3}.$$

Since $3 \le \Delta_2 \le \frac{\eta+1}{2}$, using the above results, we conclude that

$$M(\Delta_2) \ge \sqrt{\frac{4\,(\eta+1)}{(\eta+1)^2+4}} + \frac{4}{\eta-3}\cdot\sqrt{\frac{2\,(\eta+1)}{(\eta+1)^2+16}} - \frac{2}{\eta-3}. \tag{2.12}$$

Claim 2.

$$\sqrt{\frac{4\,(\eta+1)}{(\eta+1)^2+4}} + \frac{4}{\eta-3}\cdot\sqrt{\frac{2\,(\eta+1)}{(\eta+1)^2+16}} - \frac{2}{\eta-3} > \sqrt{\frac{2\,(\eta-1)}{(\eta-1)^2+1}}. \tag{2.13}$$

Proof of Claim 2. For $10 \le \eta \le 21$, by Sage [35], the validity of (2.13) can be easily confirmed. Otherwise, $\eta \ge 22$. Using this, one can easily check that

$$4\,(\eta-1) > 3.61\,(\eta+1.2), \quad \text{that is,} \quad \frac{2}{\sqrt{\eta+1.2}} > \frac{1.9}{\sqrt{\eta-1}}.$$

Since $\eta \geq 22$, using the above result, we obtain

$$\begin{aligned}
&\sqrt{\frac{4(\eta+1)}{(\eta+1)^2+4}}+\frac{4}{\eta-3}\cdot\sqrt{\frac{2(\eta+1)}{(\eta+1)^2+16}}-\frac{2}{\eta-3}\\
&>\sqrt{\frac{4(\eta+1)}{(\eta+1)^2+4}}-\frac{2}{\eta-3}\\
&>\frac{2}{\sqrt{\eta+1.2}}-\frac{2}{\eta-3}\\
&>\frac{1.9}{\sqrt{\eta-1}}-\frac{2}{\eta-3}. \qquad (2.14)
\end{aligned}$$

We have to prove that

$$\frac{1.9}{\sqrt{\eta-1}}-\frac{2}{\eta-3}>\frac{\sqrt{2}}{\sqrt{\eta-1}}, \text{ that is, } \frac{1.9-\sqrt{2}}{\sqrt{\eta-1}}>\frac{2}{\eta-3},$$

that is,

$$(\eta-3)^2>16.95(\eta-1), \text{ that is, } \eta(\eta-22.95)+25.95>0,$$

which is true always as $\eta \geq 22$. Thus we have

$$\frac{1.9}{\sqrt{\eta-1}}-\frac{2}{\eta-3}>\frac{\sqrt{2}}{\sqrt{\eta-1}}>\sqrt{\frac{2(\eta-1)}{(\eta-1)^2+1}}.$$

Using the above result in (2.14), we obtain

$$\sqrt{\frac{4(\eta+1)}{(\eta+1)^2+4}}+\frac{4}{\eta-3}\cdot\sqrt{\frac{2(\eta+1)}{(\eta+1)^2+16}}-\frac{2}{\eta-3}>\sqrt{\frac{2(\eta-1)}{(\eta-1)^2+1}}.$$

This proves the Claim 2.

Using Claim 2 in (2.12), we obtain

$$M(\Delta_2)>\sqrt{\frac{2(\eta-1)}{(\eta-1)^2+1}},$$

that is,

$$\sqrt{\frac{2\Delta_2}{\Delta_2^2+1}}+\frac{2}{\Delta_2-2}\cdot\sqrt{\frac{\Delta_2}{\Delta_2^2+4}}-\frac{1}{\Delta_2-2}>\sqrt{\frac{2(\eta-1)}{(\eta-1)^2+1}},$$

that is,

$$(\Delta_2-2)\sqrt{\frac{2\Delta_2}{\Delta_2^2+1}}+\sqrt{\frac{4\Delta_2}{\Delta_2^2+4}}>1+(\Delta_2-2)\sqrt{\frac{2(\eta-1)}{(\eta-1)^2+1}}. \qquad (2.15)$$

If $k \geq 5$, then one can easily see that there exists an edge $v_x v_y \in \mathcal{E}(C_k)$ such that $v_x v_y \notin S$, which leads to a contradiction as $|S| = |\mathcal{E}(\Gamma)|$. Hence we must have $3 \leq k \leq 4$. Since Γ is unicyclic and $|S| = |\mathcal{E}(\Gamma)$, it follows that $v_1 v_2 \in \mathcal{E}(\Gamma)$ when $k = 3$; therefore $\Gamma \cong H_1$ (see Figure 2).

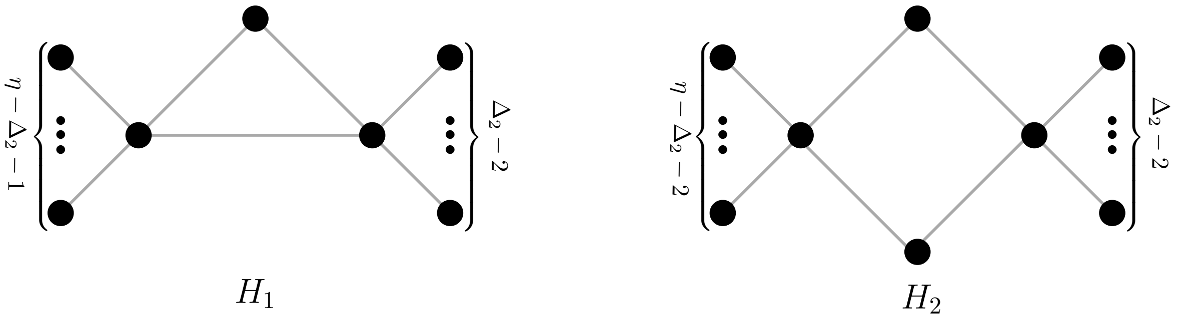

Figure 2. Two unicyclic graphs H_1 and H_2.

On the other hand, if $k = 4$, then $v_1 v_2 \notin \mathcal{E}(\Gamma)$ and consequently $\Gamma \cong H_2$ (see Figure 2). So we have the following two cases:

Case 2.2.1. $\Gamma \cong H_1$. We have

$$GQ(\Gamma) = (\Delta_2 - 2)\sqrt{\frac{2\,\Delta_2}{\Delta_2^2 + 1}} + \sqrt{\frac{4\,\Delta_2}{\Delta_2^2 + 4}} + (\eta - \Delta_2 - 1)\sqrt{\frac{2\,(\eta - \Delta_2 + 1)}{(\eta - \Delta_2 + 1)^2 + 1}}$$

$$+ \sqrt{\frac{2\,\Delta_2\,(\eta - \Delta_2 + 1)}{(\eta - \Delta_2 + 1)^2 + \Delta_2^2}} + \sqrt{\frac{4\,(\eta - \Delta_2 + 1)}{(\eta - \Delta_2 + 1)^2 + 1}}. \tag{2.16}$$

Since $3 \leq \Delta_2 \leq \frac{\eta+1}{2}$, one can easily see that

$$\sqrt{\frac{2\,(\eta - \Delta_2 + 1)}{(\eta - \Delta_2 + 1)^2 + 1}} > \sqrt{\frac{2\,(\eta - 1)}{(\eta - 1)^2 + 1}} \text{ and } \sqrt{\frac{4\,(\eta - \Delta_2 + 1)}{(\eta - \Delta_2 + 1)^2 + 1}} > \sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}}.$$

Again since $3 \leq \Delta_2 \leq \frac{\eta+1}{2}$, by Corollary 2.3, we obtain

$$\sqrt{\frac{2\,\Delta_2\,(\eta - \Delta_2 + 1)}{(\eta - \Delta_2 + 1)^2 + \Delta_2^2}} > \sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}}.$$

Using the above results with (2.15) in (2.16), we obtain

$$GQ(\Gamma) > 1 + (\Delta_2 - 2)\sqrt{\frac{2\,(\eta - 1)}{(\eta - 1)^2 + 1}} + (\eta - \Delta_2 - 1)\sqrt{\frac{2\,(\eta - 1)}{(\eta - 1)^2 + 1}} + 2\sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}}$$

$$= (\eta - 3)\sqrt{\frac{2\,(\eta - 1)}{(\eta - 1)^2 + 1}} + 2\sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}} + 1.$$

Inequality (2.4) strictly holds.

Case 2.2.2. $\Gamma \cong H_2$. We have

$$GQ(\Gamma) = (\Delta_2 - 2)\sqrt{\frac{2\,\Delta_2}{\Delta_2^2 + 1}} + 2\sqrt{\frac{4\,\Delta_2}{\Delta_2^2 + 4}} + (\eta - \Delta_2 - 2)\sqrt{\frac{2\,(\eta - \Delta_2)}{(\eta - \Delta_2)^2 + 1}}$$

$$+ 2\sqrt{\frac{4\,(\eta - \Delta_2)}{(\eta - \Delta_2)^2 + 4}}. \tag{2.17}$$

Since $3 \leq \Delta_2 \leq \frac{\eta+1}{2}$, one can easily see that

$$\sqrt{\frac{4\,\Delta_2}{\Delta_2^2 + 4}} > \sqrt{\frac{2\,(\eta - 1)}{(\eta - 1)^2 + 1}},$$

$$\sqrt{\frac{2\,(\eta - \Delta_2)}{(\eta - \Delta_2)^2 + 1}} > \sqrt{\frac{2\,(\eta - 1)}{(\eta - 1)^2 + 1}},$$

and

$$\sqrt{\frac{4\,(\eta - \Delta_2)}{(\eta - \Delta_2)^2 + 4}} > \sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}}.$$

Using the above results with (2.15) in (2.17), we obtain

$$GQ(\Gamma) > 1 + (\Delta_2 - 2)\sqrt{\frac{2\,(\eta - 1)}{(\eta - 1)^2 + 1}} + (\eta - \Delta_2 - 1)\sqrt{\frac{2\,(\eta - 1)}{(\eta - 1)^2 + 1}} + 2\sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}}$$

$$= (\eta - 3)\sqrt{\frac{2\,(\eta - 1)}{(\eta - 1)^2 + 1}} + 2\sqrt{\frac{4\,(\eta - 1)}{(\eta - 1)^2 + 4}} + 1.$$

Inequality (2.4) holds strictly, thereby completing the proof. □

3. Potential chemical attributes

The assessment of chemical applicability is a fundamental component of research in CGT, where topological indices are examined for their ability to predict physicochemical and biological properties of molecular structures. One of the principal tools in this direction is the QSPR, which evaluates how well a given index correlates with experimentally measured molecular attributes. Randić and Trinajstić [30] were among the first to propose using octane isomers as benchmark data for testing newly introduced indices. Gutman and Tošović [21] observed that topological indices with absolute correlation coefficients below 0.8 are generally ineffective as QSPR descriptors.

The geometric–arithmetic index [6, 27, 28] and its variants [8, 10], including the arithmetic-geometric index [9,11], have been extensively investigated in the literature. A recent comparative study by Kumar and Das [24] demonstrated the effectiveness of the GQ index using benchmark datasets of alkane isomers, such as octanes, nonanes, and decanes; see also [25] for the case of octanes and [13] for other compounds. The authors showed that for octane isomers, the physicochemical properties such as boiling point (BP), acentric factor (AcentFac), entropy (S), enthalpy of formation (HFORM), enthalpy of vaporization (HVAP), and standard enthalpy of vaporization (DHVAP) are correlated with the GQ index using a linear regression model. In the same work, the authors highlighted a potential research direction, suggesting that the GQ index should be examined for molecular families beyond alkanes, particularly in the prediction of a broader range of physicochemical properties.

Motivated by this suggestion and by the increasing interest in molecular descriptors with strong predictive capability, we investigate the applicability of the GQ index to 22 benzenoid hydrocarbons (BHs). Although benzene hydrocarbons were partially studied in [12], that work considered only a limited subset of molecular properties. In contrast, several important physicochemical attributes remain unexplored despite their relevance in chemical, pharmacological, and industrial contexts. The QSPR analysis of degree-based topological indices with respect to various physicochemical properties of polycyclic aromatic hydrocarbons was investigated in [7, 22, 38]. Kumar and Das [24] demonstrated that six physicochemical properties of octane isomers exhibit good correlation with the GQ index. However, several properties remain to be examined. Therefore, we collected data on sixteen physicochemical properties of octane isomers, including boiling point (BP), melting point (MP), heat capacity at constant temperature, heat capacity at constant pressure, entropy (S), density (DENS), enthalpy of vaporization (HVAP), standard enthalpy of vaporization (DHVAP), enthalpy of formation (HFORM), standard enthalpy of formation, motor octane number (MON), molar refraction (MR), acentric factor (AcentFac), total surface area, octanol-water partition coefficient, and molar volume (MV). We examine these properties using linear, quadratic, and cubic regression models and present a comparative study.

To evaluate the predictive capabilities of the indices, we analyze the following regression models: Linear model:

$$P = m_1 \cdot TI + x_1.$$

Quadratic model:

$$P = m_2 \cdot TI^2 + n_2 \cdot TI + x_2.$$

Cubic model:

$$P = m_3 \cdot TI^3 + n_3 \cdot TI^2 + p_3 \cdot TI + x_3.$$

Here P represents the physical property, TI is the topological index, m_i, n_i and p_i are the regression coefficients, and x_i is the intercept for each respective model, where $i \in \{1, 2, 3\}$. For benzene derivatives, only the linear model was applied, while for octane properties, all three models (linear, quadratic, and cubic) were employed to capture potential nonlinear correlations with the GQ index. Here, $|R|$ denotes the absolute correlation coefficient. We consider structural properties only if they satisfy $|R| \geq 0.94$ for benzene and $R \geq 0.8$ for any regression model for octanes. To compute correlation values, correlation graphs, and index values, we use the Python programming language.

3.1. Comparative analysis using benzene hydrocarbons

In this section, we extend the existing literature by conducting a comprehensive QSPR analysis of 22 benzenoid hydrocarbons using six key physicochemical properties: boiling point (BP), π-electron energy (π-ele), molecular weight (MW), polarizability (PO), molar refractivity (MR), and molar volume (MV), where all experimental data are taken from [32]. The molecular graphs of these 22 hydrocarbons are illustrated in Figure 3. Our study includes only those molecular properties for which the correlation coefficient with the GQ index exceeds 0.94, ensuring statistical robustness and practical relevance. Table 1 provides both the theoretical GQ values and the experimental data for BHs [32]. Our analysis compares the predictive efficiency of the GQ index with several other eminent degree-based indices. Through graphical comparisons, statistical evaluation, and computational tests, we demonstrate the dominating predictive nature of the GQ index across the considered physicochemical properties. The values of the GQ index of the considered BHs are given in Table 1, whereas $|R|$ values are given Tables 2 and 3, and correlation graphs are depicted in Figures 4–11.

Table 1. Experimental properties (BP in °C, π-electron energy in β units, MW in g/mol, PO in 10^{-24} cm^3, MV in cm^3, and MR in cm^3) of benzenoid hydrocarbons (see (A)–(V) in Figure 3), together with the corresponding values of the GQ index.

BHs	BP	π-ele	MW	PO	MV	MR	GQ
(A)	78.8	8	78.11	10.4	89.4	26.3	6.000
(B)	221.5	13.683	128.17	17.5	123.5	44.1	10.843
(C)	337.4	19.448	178.23	24.6	157.7	61.9	15.764
(D)	337.4	19.314	178.23	24.6	157.7	61.9	15.686
(E)	448	25.192	228.3	31.6	191.8	79.8	20.686
(F)	436.7	25.101	228.3	31.6	191.8	79.8	20.607
(G)	425	25.275	228.3	31.6	191.8	79.8	20.764
(H)	436.7	25.188	228.3	31.6	191.8	79.8	20.529
(I)	495	28.222	252.3	35.8	196.1	90.3	23.607
(J)	467.5	28.336	252.3	35.8	196.1	90.3	23.725
(K)	467.5	28.245	252.3	35.8	196.1	90.3	23.686
(L)	497.1	31.253	276.3	40	200.4	100.8	26.568
(M)	501	31.425	276.3	40	200.4	100.8	26.646
(N)	518	30.942	278.3	38.7	225.9	97.6	25.607
(O)	524.7	30.881	278.3	38.7	225.9	97.6	25.529
(P)	524.7	30.88	278.3	38.7	225.9	97.6	25.607
(Q)	519	30.943	278.3	38.7	225.9	97.6	25.607
(R)	525.6	34.572	300.4	44.1	204.7	111.4	29.607
(S)	552.3	33.928	302.4	42.9	230.2	108.1	28.529
(T)	552.3	33.954	302.4	42.9	230.2	108.1	28.568
(U)	552.3	34.031	302.4	42.9	230.2	108.1	28.607
(V)	404	22.506	202.25	28.7	162	72.5	18.686

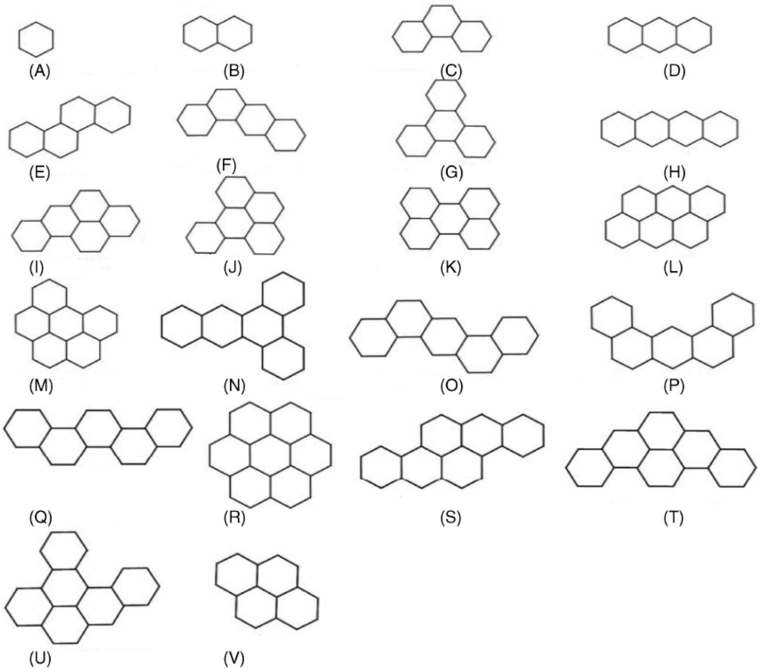

Figure 3. (A) Benzene, (B) Naphthalene, (C) Phenanthrene, (D) Anthracene, (E) Chrysene, (F) Benzo[a]anthracene, (G) Triphenylene, (H) Tetracene, (I) Benzo[a]pyrene, (J) Benzo[e]pyrene, (K) Perylene, (L) Anthanthrene, (M) Benzo[ghi]perylene, (N) Dibenz[a,c]anthracene, (O) Dibenz[a,h]anthracene, (P) Dibenz[a,j]anthracene, (Q) Picene, (R) Coronene, (S) Dibenzo[a,h]pyrene, (T) Dibenzo[a,i]pyrene, (U) Dibenzo[a,l]pyrene, (V) Pyrene.

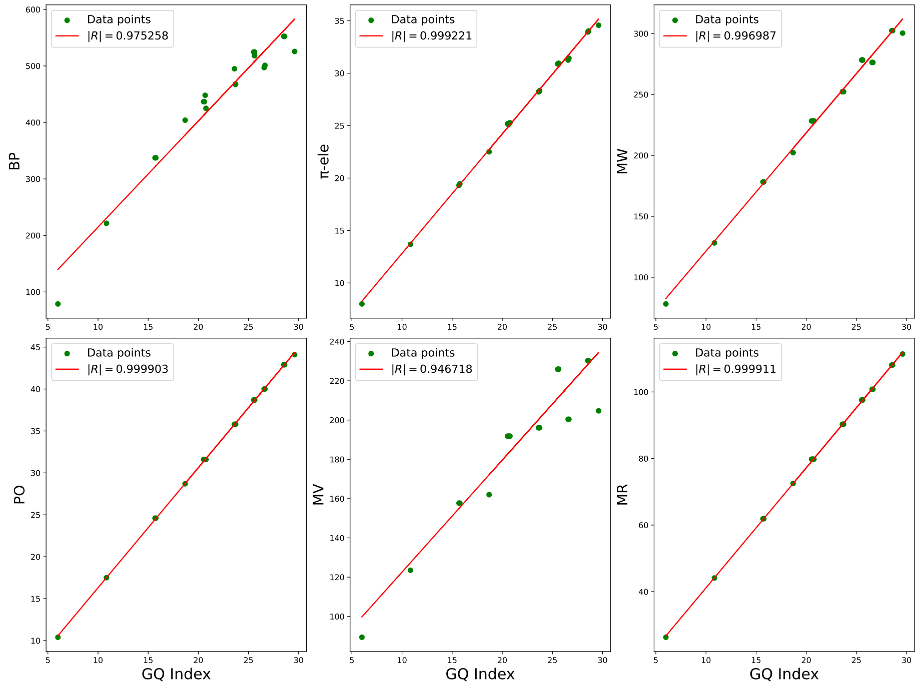

Figure 4. Linear fittings of the GQ index with BP, π-ele, MW, PO, MV, and MR for benzene hydrocarbons.

Comparative analysis

This section evaluates the performance of the GQ index through a comparative study with several classical degree–based topological indices, namely, the first Zagreb index (M_1), second Zagreb index (M_2) [20], forgotten index (F) [17], Randić index (R) [29], harmonic index (H) [15], inverse sum (indeg) index (ISI) [37], augmented Zagreb index (AZI) [16], first hyper Zagreb index (HM) [34], arithmetic–geometric index (AG) [33], and Sombor index (SO) [4, 19]. The comparison is based on the absolute Pearson correlation coefficients ($|R|$) obtained from linear regression models relating each index to six physicochemical properties of benzene hydrocarbons. The corresponding correlation plots are displayed in Figures 5–10.

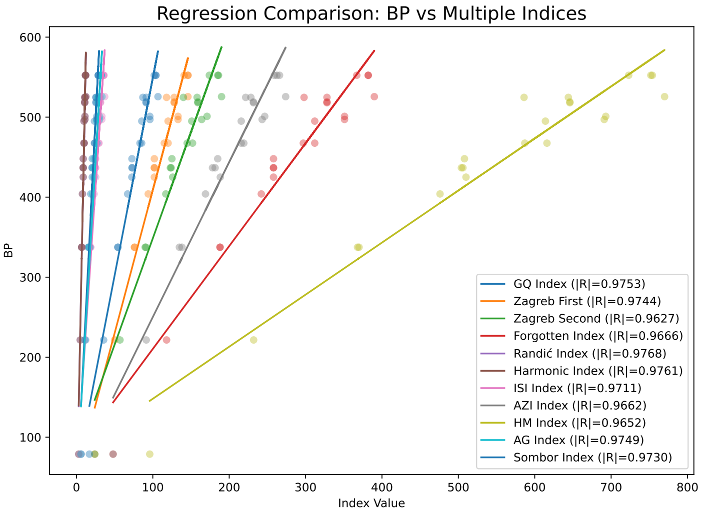

Figure 5. Regression analysis of boiling point (BP) against the considered topological indices.

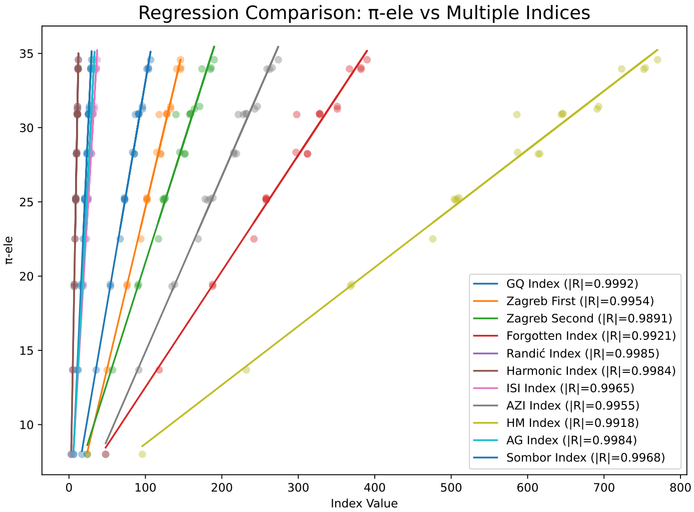

Figure 6. Regression analysis of π-electron energy (π-ele) against the considered topological indices.

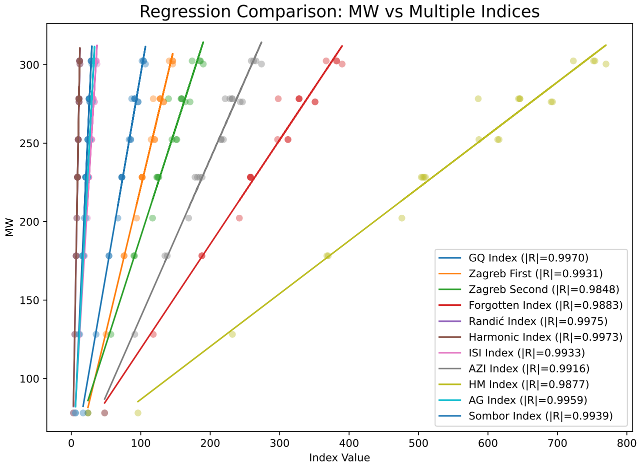

Figure 7. Regression analysis of molecular weight (MW) against the considered topological indices.

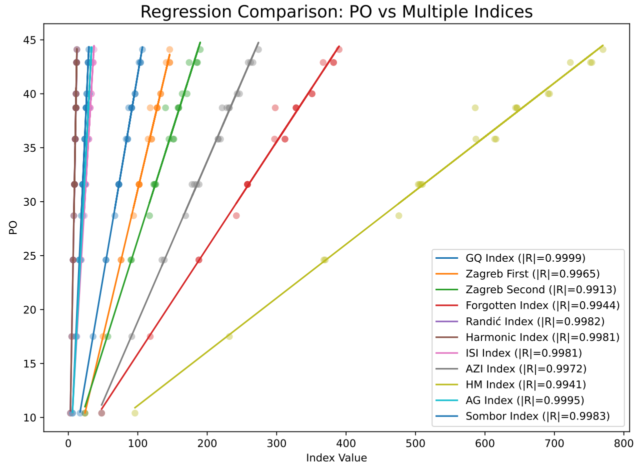

Figure 8. Regression analysis of polarizability (PO) against the considered topological indices.

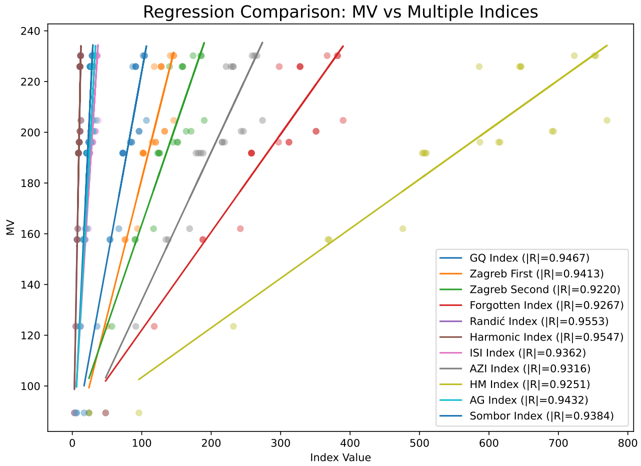

Figure 9. Regression analysis of molar volume (MV) against the considered topological indices.

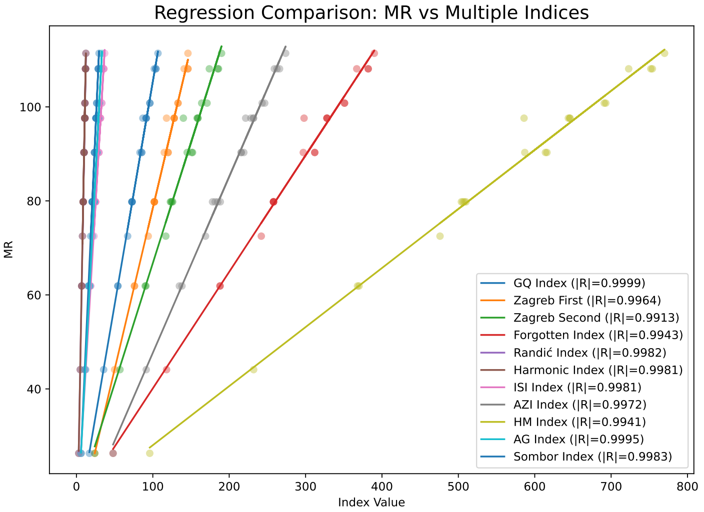

Figure 10. Regression analysis of molar refractivity (MR) against the 11 topological indices.

A consolidated overview of the comparative performance of all considered indices is provided in Table 2. For each property, the highest correlation coefficient among all indices is highlighted in bold. As can be observed, the GQ index consistently exhibits very strong predictive capability and outperforms the other descriptors for several key physicochemical attributes.

Table 2. Ranking table (absolute correlations).

	Absolute correlations $\lvert R\rvert$					
TI	BP	π-ele	MW	PO	MV	MR
AG	0.974946	0.998420	0.995898	0.999483	0.943220	0.999486
AZI	0.966196	0.995487	0.991605	0.997212	0.931636	0.997219
F	0.966608	0.992130	0.988268	0.994357	0.926683	0.994349
GQ	0.975258	**0.999221**	0.996987	**0.999903**	0.946718	**0.999911**
HM	0.965238	0.991800	0.987732	0.994105	0.925116	0.994099
H	0.976124	0.998417	0.997291	0.998125	0.954669	0.998141
ISI	0.971096	0.996539	0.993298	0.998108	0.936212	0.998108
R	**0.976810**	0.998516	**0.997489**	0.998199	**0.955321**	0.998214
SO	0.973041	0.996827	0.993900	0.998285	0.938364	0.998283
M_1	0.974377	0.995403	0.993073	0.996463	0.941268	0.996441
M_2	0.962730	0.989149	0.984834	0.991250	0.922044	0.991287

Based on the computed correlation coefficients, the topological indices satisfy the following ordering relations with respect to each physicochemical property:

(i) Boiling Point (BP):

$$R > H > GQ > AG > M_1 > SO > ISI > F > AZI > HM > M_2,$$

(*ii*) π-Electron Energy (π-ele):

$$GQ > R > AG > H > SO > ISI > AZI > M_1 > F > HM > M_2,$$

(*iii*) Molecular Weight (MW):

$$R > H > GQ > AG > SO > ISI > M_1 > AZI > F > HM > M_2,$$

(*iv*) Polarizability (PO):

$$GQ > AG > SO > R > H > ISI > AZI > M_1 > F > HM > M_2,$$

(*v*) Molar Volume (MV):

$$R > H > GQ > AG > M_1 > SO > ISI > AZI > F > HM > M_2,$$

(*vi*) Molar Refractivity (MR):

$$GQ > AG > SO > R > H > ISI > AZI > M_1 > F > HM > M_2.$$

The ordering relations in (*i*)–(*vi*), together with the correlation plots in Figures 5–10 and the numerical values in Table 2, allow us to draw the following observations:

(*i*) The GQ index exhibits exceptionally high correlations with π-ele, PO, and MR of benzenoid hydrocarbons, with correlation coefficients 0.999221, 0.999903, and 0.999911, respectively. For the remaining physicochemical properties, the GQ index consistently attains the third-highest correlation among all considered indices.

(*ii*) The Randić index (R) achieves the highest correlations with BP, MW, and MV, with correlation coefficients 0.976810, 0.997489, and 0.955321, respectively.

In light of these results, it is evident that among all the examined degree–based topological indices, the newly introduced GQ index demonstrates superior predictive power for a majority of the studied physicochemical properties of benzene hydrocarbons. This establishes the GQ index as a competitive and dominant descriptor within the family of degree–based molecular invariants.

Correlation analysis of the GQ index with other degree-based indices

To examine the relationship between the GQ index and several classical degree-based topological indices, we computed their pairwise Pearson correlation coefficients over a dataset consisting of 22 benzene hydrocarbons. The corresponding results are illustrated in Figure 11. In this figure, each vertex represents a particular topological index. Two vertices are joined by an edge whenever the Pearson correlation coefficient between the corresponding indices is greater than 0.98. The thickness of each edge reflects the strength of the correlation, where thicker edges indicate stronger associations.

From Figure 11, it is observed that the vertex corresponding to the GQ index has a degree equal to 10, which indicates that the GQ index exhibits very strong correlations with five other degree-based invariants under consideration. The relatively large thickness of the incident edges further confirms that the GQ index maintains an especially high level of correlation with all the examined indices.

Table 3 presents the complete correlation matrix. For clarity, the highest correlation values for each pair of indices are highlighted in bold. The GQ index exhibits notably high correlation coefficients with all other considered indices. This suggests that a significant portion of the structural information captured by the GQ index is also reflected in these other indices. Based solely on these observations, one might conclude that the introduction of the GQ index as an additional topological descriptor could be questioned.

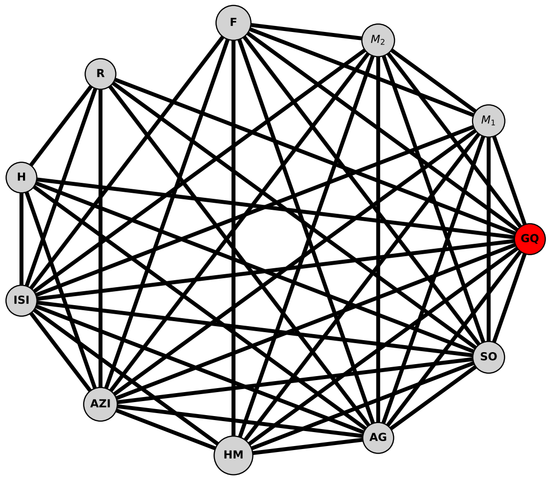

Figure 11. Correlation network of the considered degree-based topological indices, with the vertex corresponding to the GQ index highlighted in red.

Table 3. Correlation matrix of the 11 considered degree-based topological indices.

	GQ	M_1	M_2	F	R	H	ISI	AZI	HM	AG	SO
GQ	1.000000	0.996369	0.991810	0.994647	0.998045	0.998037	0.998377	0.997910	0.994512	**0.999529**	0.998369
M_1	0.996369	1.000000	0.997797	0.999162	0.989749	0.989591	0.999127	0.997607	0.998952	0.998355	**0.999323**
M_2	0.991810	0.997797	1.000000	0.999000	0.982192	0.982198	0.997173	0.996707	**0.999170**	0.994727	0.996802
F	0.994647	**0.999162**	0.999000	1.000000	0.986340	0.986246	0.998893	0.997782	0.999958	0.997226	0.998844
R	0.998045	0.989749	0.982192	0.986340	1.000000	**0.999986**	0.992877	0.992421	0.986053	0.995849	0.993051
H	0.998037	0.989591	0.982198	0.986246	**0.999986**	1.000000	0.992849	0.992586	0.986007	0.995771	0.992946
ISI	0.998377	0.999127	0.997173	0.998893	0.992877	0.992849	1.000000	0.999364	0.998856	0.999534	**0.999893**
AZI	0.997910	0.997607	0.996707	0.997782	0.992421	0.992586	**0.999364**	1.000000	0.998061	0.998585	0.998745
HM	0.994512	0.998952	**0.999170**	0.999958	0.986053	0.986007	0.998856	0.998061	1.000000	0.997040	0.998674
AG	0.999529	0.998355	0.994727	0.997226	0.995849	0.995771	0.999534	0.998585	0.997040	1.000000	**0.999639**
SO	0.998369	0.999323	0.996802	0.998844	0.993051	0.992946	**0.999893**	0.998745	0.998674	0.999639	1.000000

3.2. Comparative analysis using octane isomers

This section focuses on the chemical applicability of the GQ index in framing linear, quadratic, and cubic regression models for sixteen physicochemical properties of octane isomers.

The study in [24] focused on only six properties and considered only the linear model. Here, we reconsider and present a comparative study by considering three different models to determine which model performs best. All data regarding physicochemical properties were obtained from the database: `https://web.archive.org/web/20180912171255if_/http://www.moleculardescriptors.eu/index.htm`, and index values can be found in [24]. Our study includes only those properties of octane for which the correlation coefficient with the GQ index exceeds 0.8 for at least one model. For correlation graphs, see Figure 12, and for R values, see Table 4.

Table 4. Correlation performance (R) between the GQ index and octane properties for linear, quadratic, and cubic models. Best correlation values for each property are in bold.

	Correlation R		
Property	Linear	Quadratic	Cubic
BP	0.826914	0.839400	**0.839596**
S	0.911572	0.915108	**0.920986**
DENS	0.538143	0.756523	**0.873813**
HVAP	0.948451	0.960901	**0.962319**
DHVAP	0.972569	0.976891	**0.977123**
HFORM	0.855586	0.860373	**0.860435**
MON	0.060687	0.885662	**0.887709**
MR	0.565522	0.861714	**0.965964**
AcentFac	0.919681	0.919687	**0.922619**
MV	0.524952	0.731399	**0.850143**

A complete correlation comparison analysis is presented in Table 4, which shows that the cubic model is more effective than the linear and quadratic models. Moreover, by considering the quadratic and cubic models, four additional properties (namely, DENS, MON, MR, and MV) fulfill our criteria ($R \geq 0.8$), whereas these properties were excluded from the study in [24] because they did not meet the criteria under the linear model alone. It is worth noting for the property MON that the linear correlation R is very low (see Table 4), but under the quadratic or cubic models, this property improves substantially.

Based on the computed correlation study presented in Table 4, the three models satisfy the following ordering relations with respect to each property. The properties are written in descending order with respect to the correlation value.

(i) Standard Enthalpy of Vaporization (DHVAP): Cubic > Quadratic > Linear,
(ii) Molar Refraction (MR): Cubic > Quadratic > Linear,
(iii) Enthalpy of Vaporization (HVAP): Cubic > Quadratic > Linear,
(iv) Acentric Factor (AcentFac): Cubic > Quadratic > Linear,
(v) Entropy (S): Cubic > Quadratic > Linear,
(vi) Motor Octane Number (MON): Cubic > Quadratic > Linear,
(vii) Density (DENS): Cubic > Quadratic > Linear,
(viii) Enthalpy of Formation (HFORM): Cubic > Quadratic > Linear,
(ix) Molar Volume (MV): Cubic > Quadratic > Linear,

(x) Boiling Point (BP): Cubic > Quadratic > Linear.

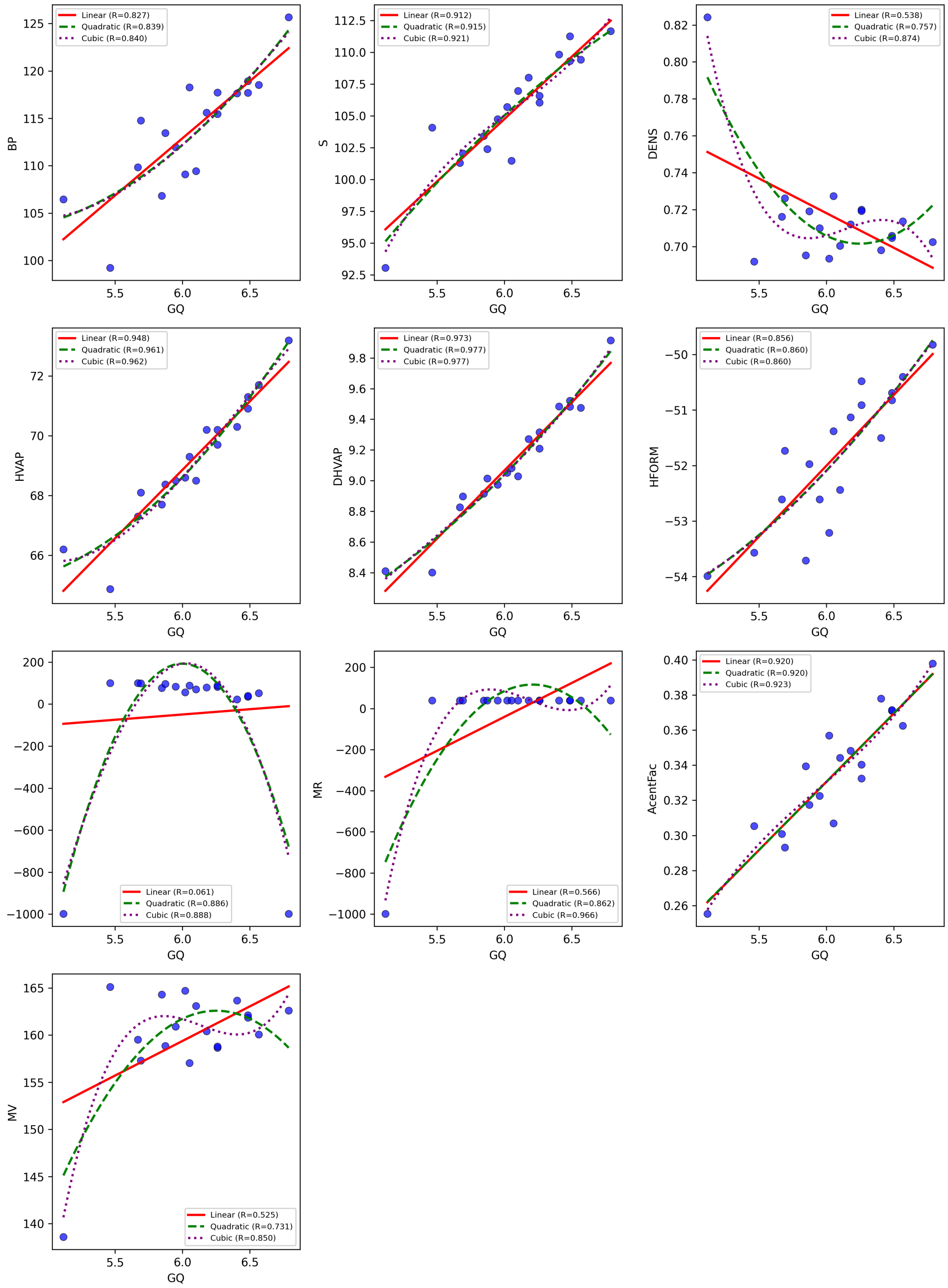

Figure 12. Correlation performance of linear, quadratic, and cubic fittings between the GQ index and octane properties (BP, S, DENS, HVAP, DHVAP, HFORM, MON, MR, AcentFac, and MV) that hold $R \geq 0.8$ for any model.

4. Conclusions

In this paper, we have addressed and completely resolved Conjecture 1 proposed by Furtula and Oz [18] concerning the characterization of the unicyclic graph with the minimum GQ index. Our proof confirms that among all unicyclic graphs on η vertices, the graph $C_3S_{\eta-3}$ uniquely attains the minimum value of the GQ index, thereby closing an open problem that previously remained unverified.

Motivated by the suggestion of Kumar and Das [24] to study the GQ index beyond alkane isomers, we investigated its predictive capability for benzene hydrocarbons by examining its correlation with six key physicochemical properties. A comparative analysis with several classical degree-based indices was also carried out. The results show that the GQ index exhibits particularly strong correlations with π-electron energy, polarizability, and molar refractivity, while maintaining competitive performance for the remaining properties. These findings demonstrate that the GQ index captures essential structural information and serves as an effective molecular descriptor. Extending this investigation to octane isomers, we employed linear, quadratic, and cubic regression models to correlate the GQ index with sixteen physicochemical properties. The cubic model consistently outperformed both linear and quadratic models, achieving correlation coefficients $R \geq 0.8$ for all qualifying properties. Notably, four properties: density (DENS), motor octane number (MON), molar refraction (MR), and molar volume (MV) satisfied this criterion only under quadratic or cubic models, having been excluded from prior linear-only studies. The property MON exhibited a particularly dramatic improvement, rising from a very low linear correlation to strong quadratic and cubic correlations. The ordering Cubic > Quadratic > Linear held uniformly across all properties, demonstrating the enhanced predictive capability of higher-order models.

Beyond resolving the underlying extremal problem, this study underscores the practical relevance of the GQ index in QSPR modeling and supports its broader applicability to chemical datasets, including both benzene and octane systems. As a direction for future research, we also suggest re-examining the correlations between physico-chemical characteristics and anticancer drugs reported in [31], as those results appear to merit further verification.

Author contributions

Conceptualization, A.M.A., K.C.D., and S.A.; Validation, K.C.D., S.A., and A.A.; Formal analysis, K.C.D. and S.A.; Investigation, A.M.A., K.C.D., and S.A.; Writing – original draft, A.M.A. and K.C.D.; Writing – review and editing, K.C.D., S.A., T.A., and A.A.; Supervision, K.C.D. All authors have read and approved the final version of the manuscript for publication.

Use of Generative-AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The authors declare no conflicts of interest.

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