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Research article

Extremal graphs and bounds for general Gutman index

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Abstract: In this paper, we solved some open problems on general Gutman index. More precisely, we characterized unicyclic graphs with extremal general Gutman index for some a and b. We presented a sharp bound on general Gutman index of G in terms of order and vertex connectivity of G. Also, we obtained some bounds on general Gutman index in terms of order, general Randić index, diameter, and independence number of graph G. In addition, QSPR analysis on various anticancer drug structures was carried out to relate their physicochemical properties with the general Gutman index of the structure for some a and b.

Keywords: general Gutman index; general Randić index; vertex connectivity; QSPR modeling
Mathematics Subject Classification: 05C09, 05C12, 05C35

1. Introduction

Graphs considered in this paper are simple, undirected and connected. Let $V(G)$ and $E(G)$ be the vertex set and the edge set of a graph G, respectively. The degree $d_G(v)$ of a vertex v in G is the number of vertices adjacent to v. The distance $d_G(u, v)$ between two vertices u and v is the number of edges in a shortest path connecting u and v. A topological index is a numerical quantity derived from the structure of the graph or molecular graph. It is an important tool in the quantitative structure-property relationship (QSPR) analysis of chemical compounds and it is used to predict physicochemical properties of chemical compounds. In recent years, extensive works on topological indices have been carried out (see [11,12,16,18]) and several new topological indices based on degree, distance, both degree and distance, eccentricity, eigenvalues, etc. are introduced; see [1,2,10]. For real constants a and b, the general Gutman index of G is defined as follows:

$$Gut_{a,b}(G) = \sum_{\{u,v\}\subseteq V(G)} [d_G(u)d_G(v)]^a \, [d_G(u, v)]^b .$$

The definition of general Gutman index was put forward by Das and Vetrík in [8]. For $a = 1$ and

$b = 1$, $Gut_{a,b}(G)$ is the Gutman index. For $a = 0$ and $b = 1$, $Gut_{a,b}(G)$ is the classical Wiener index. For $a = 0$ and $b = -1$, $Gut_{a,b}(G)$ is the Harary index. Thus, the general Gutman index generalizes several well-known graph indices so its study would be interesting. Studies on Gutman index can be found in [4,7,9,14]. Das and Vetrík [8] presented sharp bounds on the $Gut_{a,b}(G)$ index for multipartite graphs of given order, graphs of given order and chromatic number, and starlike trees of given order and maximum degree. The authors also stated the following open problems.

Problem 1. Find a tree with the smallest or a tree having the largest $Gut_{a,b}$ index among trees with given order for some a and b.

Problem 2. Find bounds on the $Gut_{a,b}$ index for unicyclic graphs and bicyclic graphs with given order for some a and b.

Problem 3. Find a sharp lower bound or an upper bound on the $Gut_{a,b}$ index for graphs with given order and vertex connectivity for some a and b.

Problem 4. Find bounds on the general Gutman index for graphs with a given order and the number of pendant vertices.

After which, Cheng and Li [6] characterized trees of given order with extreme $Gut_{a,b}$ index.

In QSPR-analysis, computational methods and topological indices are employed to streamline the design of fine chemicals by predicting the relationship between molecular structure and their physicochemical properties. This analysis accelerates drug discovery and reduces the cost and time in developing targeted therapeutic agents. For some recent works on topological indices and QSPR modeling, one can refer [3, 13, 15, 17]. Anticancer drugs are those which are used to cure cancer (malignant disease). The alkalyting agents, hormones, and antimetabolites are some of the anticancer drugs. Recently, QSPR analysis of anticancer drugs with respect to various degree-based indices was carried out; see [17].

Motivated by these works, in Section 3 we characterize n-vertex unicyclic graphs, having minimum general Gutman index and maximum general Gutman index for some values of a and b. In Section 4, we present a sharp bound on the general Gutman index of graphs of given order and vertex connectivity. In Section 5, we obtain some bounds on the general Gutman index in terms of order, general Randić index, diameter, and independence number of graph G. At last, in Section 6, by employing a linear regression model, we relate the physicochemical properties of some anticancer drugs with the general Gutman index for some values of a and b. Also, it is observed that for some specified values of a and b, $Gut_{a,b}(G)$ index is found to correlate well with some physicochemical properties (namely, boiling point, melting point, enthalpy, and molar refractivity) of anticancer drugs.

2. Preliminaries

We need the following lemmas to prove our main results.

Lemma 2.1. [6] *Let* $0 < u_1 < u_2$, $v > 0$ *and* $f(u) = u^a$. *Then* $f(u_1 + v) - f(u_1) < f(u_2 + v) - f(u_2)$ *for* $a > 1$ *or* $a < 0$, *and* $f(u_1 + v) - f(u_1) > f(u_2 + v) - f(u_2)$ *for* $0 < a < 1$.

Lemma 2.2. [8] *Let* $a \geq 0$ *and* $b \leq 0$, *where at least one of a and b is nonzero. For a connected graph* G, *where* u_1, u_2 *are any nonadjacent vertices in* G, *we have* $Gut_{a,b}(G + u_1u_2) > Gut_{a,b}(G)$.

Lemma 2.3. [8] *Let G be a connected graph with n vertices. For* $a \leq 0$ *and* $b \geq 0$, *where at least one of a and b is nonzero,* $Gut_{a,b}(G) \geq \frac{n(n-1)^{2a+1}}{2}$. *For* $a \geq 0$ *and* $b \leq 0$, *where at least one of a and b is* *nonzero,* $Gut_{a,b}(G) \leq \frac{n(n-1)^{2a+1}}{2}$*. The equalities hold only if* G *is* K_n*.*

3. General Gutman index of unicyclic graphs

We need the following graph transformations on unicyclic graphs.

Operation 1 on unicyclic graphs: Let G be a unicyclic graph with $p \geq 1$ pendant vertices $v_1, v_2, \ldots, v_p$ which are adjacent to v, and u be a non-pendant vertex which is adjacent to v. We obtain a new graph G_1 by moving the vertices $v_1, v_2, \ldots, v_p$ to u, i.e., $G_1 = G - \left\{vv_1, vv_2, \ldots, vv_p\right\} + \left\{uv_1, uv_2, \ldots, uv_p\right\}$, see Figure 1.

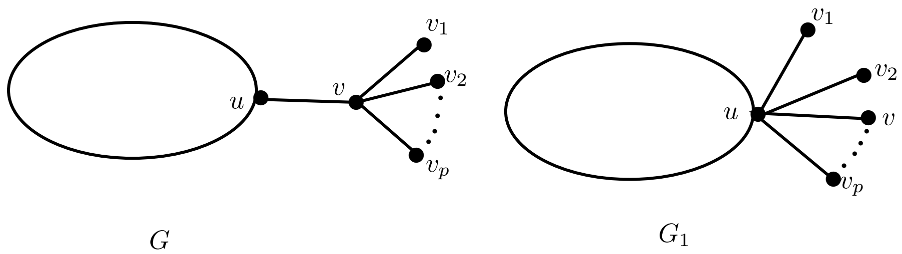

Figure 1. Graph G and resultant graph G_1.

The following results proved in [6] relates the general Gutman index of unicyclic graphs G and G_1.

Theorem 3.1. [6] *Let* $0 \leq a \leq 1$ *and* $b \geq 0$ *such that at least one of a and b is nonzero. Then,* $Gut_{a,b}(G_1) < Gut_{a,b}(G)$*.*

Theorem 3.2. [6] *Let* $a \leq b \leq 0$ *such that at least one of a and b is nonzero. Then,* $Gut_{a,b}(G_1) > Gut_{a,b}(G)$*.*

Operation 2 on unicyclic graphs: Let G be a unicyclic graph obtained by attaching pendant vertices to a cycle. Let u be any non-pendant vertex such that p pendant vertices $u_1, u_2, \ldots, u_p$ are attached to u, and v be another vertex on the cycle such that there are q pendant vertices $v_1, v_2, \ldots, v_q$ attached to it. Define $G' = G - \left\{vv_1, vv_2, \ldots, vv_q\right\} + \left\{uv_1, uv_2, \ldots, uv_q\right\}$ and $G'' = G - \left\{uu_1, uu_2, \ldots, uu_p\right\} + \left\{vu_1, vu_2, \ldots, vu_p\right\}$; see Figure 2.

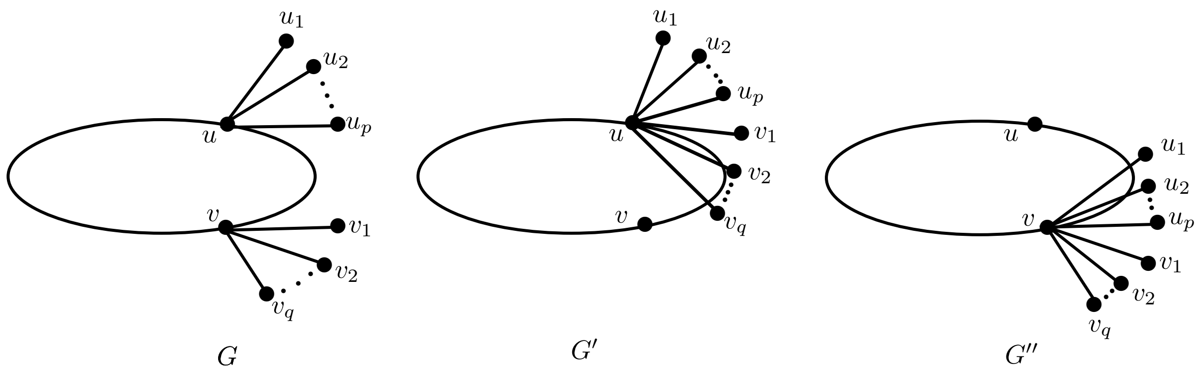

Figure 2. Graph G and resultant graphs G' and G''.

We partition $V(G)$ into sets $V_1 = \{u, v\}$, $V_2 = \left\{u_1, u_2, \ldots, u_p\right\}$, $V_3 = \left\{v_1, v_2, \ldots, v_q\right\}$, and $V_4 = V(G) - V_1 - V_2 - V_3$. For $1 \leq i < j \leq 4$, define

$$E'_i = \sum_{\{w,y\}\subseteq V_i} \left[d_{G'}(w)^a d_{G'}(y)^a d_{G'}(w,y)^b - d_G(w)^a d_G(y)^a d_G(w,y)^b\right];$$
$$E'_{ij} = \sum_{w\in V_i, y\in V_j} \left[d_{G'}(w)^a d_{G'}(y)^a d_{G'}(w,y)^b - d_G(w)^a d_G(y)^a d_G(w,y)^b\right];$$
$$E''_i = \sum_{\{w,y\}\subseteq V_i} \left[d_{G''}(w)^a d_{G''}(y)^a d_{G''}(w,y)^b - d_G(w)^a d_G(y)^a d_G(w,y)^b\right];$$
$$E''_{ij} = \sum_{w\in V_i, y\in V_j} \left[d_{G''}(w)^a d_{G''}(y)^a d_{G''}(w,y)^b - d_G(w)^a d_G(y)^a d_G(w,y)^b\right].$$

Then,

$$Gut_{a,b}(G') - Gut_{a,b}(G) = \sum_{i=1}^{4} E'_i + \sum_{j=2}^{4} E'_{1j} + \sum_{j=3}^{4} E'_{2j} + E'_{34}, \tag{3.1}$$

and

$$Gut_{a,b}(G'') - Gut_{a,b}(G) = \sum_{i=1}^{4} E''_i + \sum_{j=2}^{4} E''_{1j} + \sum_{j=3}^{4} E''_{2j} + E''_{34}. \tag{3.2}$$

Let $d_G(u, v) = l$. For $\{w, y\} \subseteq V_i$, $i = 2, 3, 4$,
$d_G(w)^a d_G(y)^a d_G(w, y)^b = d_{G'}(w)^a d_{G'}(y)^a d_{G'}(w, y)^b = d_{G''}(w)^a d_{G''}(y)^a d_{G''}(w, y)^b$ as the degrees and distance between w and y does not change in G' and G''. Hence,

$$E'_2 = E'_3 = E'_4 = E''_2 = E''_3 = E''_4 = 0.$$

Note that for any $y \in V_4$, $d_{G'}(y) = d_{G''}(y) = d_G(y)$, $d_{G'}(u, y) = d_{G''}(u, y) = d_G(u, y)$ and $d_{G'}(v, y) = d_{G''}(v, y) = d_G(v, y)$. Also, $d_G(u) = p + 2$, $d_G(v) = q + 2$, $d_{G'}(u) = p + q + 2$, $d_{G'}(v) = 2$, $d_{G''}(u) = 2$, and $d_{G''}(v) = p + q + 2$. Thus,

$E'_1 = (p + q + 2)^a 2^a l^b - (p + 2)^a (q + 2)^a l^b;$

$E'_{12} = p\left[\left[(p + q + 2)^a - (p + 2)^a\right] + (l + 1)^b \left[2^a - (q + 2)^a\right]\right];$

$E'_{13} = q\left[\left[(p + q + 2)^a - (q + 2)^a\right] + (l + 1)^b \left[2^a - (p + 2)^a\right]\right];$

$E'_{14} = [(p+q+2)^a - (p+2)^a] \sum_{y\in V_4} d_G(y)^a d_G(u,y)^b - [(q+2)^a - 2^a] \sum_{y\in V_4} d_G(y)^a d_G(v,y)^b$;

$E'_{23} = pq\left[2^b - (l+2)^b\right]$;

$E'_{24} = \sum_{w\in V_2,,y\in V_4} d_{G'}(y)^a \left[d_{G'}(y,u)+1\right]^b - \sum_{w\in V_2,y\in V_4} d_G(y)^a \left[d_G(y,u)+1\right]^b = 0$;

$E'_{34} = q\left[\sum_{y\in V_4} d_G(y)^a \left(d_G(u,y)+1\right)^b - \sum_{y\in V_4} d_G(y)^a \left(d_G(v,y)+1\right)^b\right]$.

Similarly, $E'_1 = E''_1$, $E'_{12} = E''_{12}$, $E'_{13} = E''_{13}$ and $E'_{23} = E''_{23}$ and $E''_{34} = 0$;

$E''_{14} = [(p+q+2)^a - (q+2)^a] \sum_{y\in V_4} d_G(y)^a d_G(v,y)^b - [(p+2)^a - 2^a] \sum_{y\in V_4} d_G(y)^a d_G(u,y)^b$;

$E''_{24} = p\left[\sum_{y\in V_4} d_G(y)^a \left(d_G(v,y)+1\right)^b - \sum_{y\in V_4} d_G(y)^a \left(d_G(u,y)+1\right)^b\right]$.

The following theorem gives the relations between $Gut_{a,b}(G)$, $Gut_{a,b}(G')$, and $Gut_{a,b}(G'')$ for some values of a and b.

Theorem 3.3. *Let G be a unicyclic graph of girth k and let $0 \le a \le 1$. Then, $Gut_{a,b}(G) > Gut_{a,b}(G')$ or $Gut_{a,b}(G) > Gut_{a,b}(G'')$ for $b = 0$ or $b = 1$. Furthermore, if $k = 3$, then $Gut_{a,b}(G) > Gut_{a,b}(G')$ or $Gut_{a,b}(G) > Gut_{a,b}(G'')$ for $b \ge 0$ and at least one of a and b is nonzero.*

Proof. For $0 \le a \le 1$ and $b \ge 0$, $E'_1 = (p+q+2)^a 2^a l^b - (p+2)^a (q+2)^a l^b \le 0$. By Lemma 2.1, we get $\left[(p+q+2)^a - (p+2)^a\right] + (l+1)^b \left[2^a - (q+2)^a\right] \le 0$ and $\left[(p+q+2)^a - (q+2)^a\right] + (l+1)^b \left[2^a - (p+2)^a\right] \le 0$. Thus, $E'_{12} \le 0$ and $E'_{13} \le 0$. Also, since $b \ge 0$, $E'_{23} = pq\left[2^b - (l+2)^b\right] \le 0$.

Case 1. Suppose $\sum_{y\in V_4} d_G(y)^a d_G(u,y)^b \le \sum_{y\in V_4} d_G(y)^a d_G(v,y)^b$. By Lemma 2.1, $(q+2)^a - 2^a \ge (p+q+2)^a - (p+2)^a$. Thus, $E'_{14} \le 0$. If $b = 0$ or 1, then $E'_{34} \le 0$. Further, if G is of girth 3, then $E'_{34} = 0$. Hence, from Eq (3.1), we get $Gut_{a,b}(G') \le Gut_{a,b}(G)$, and the equality holds only if both a and b are zero.

Case 2. Suppose $\sum_{y\in V_4} d_G(y)^a d_G(u,y)^b > \sum_{y\in V_4} d_G(y)^a d_G(v,y)^b$. By Lemma 2.1, $\left[(p+2)^a - 2^a\right] \ge \left[(p+q+2)^a - (q+2)^a\right]$. Thus, $E''_{14} \le 0$. If $b = 0$ or 1, then $E''_{24} \le 0$. Further, if G is of girth 3, then $E''_{24} = 0$. Hence, from Eq (3.2), we get $Gut_{a,b}(G'') \le Gut_{a,b}(G)$, and the equality holds only if both a and b are zero. □

The proof of the following theorem is similar to that of Theorem 3.3.

Theorem 3.4. *Let G be a unicyclic graph of girth k. Then, $Gut_{a,b}(G) < Gut_{a,b}(G')$ or $Gut_{a,b}(G) < Gut_{a,b}(G'')$ for $a < 0$ and $b = 0$. Furthermore, if $k = 3$, then $Gut_{a,b}(G) < Gut_{a,b}(G')$ or $Gut_{a,b}(G) < Gut_{a,b}(G'')$ for $a \le b \le 0$ and at least one of a and b is nonzero.*

We denote by $H_{n,k}$- the graph obtained from the cycle C_k by attaching $n-k$ pendant vertices to a vertex of C_k. The following theorems give the extremal graphs for the general Gutman index of unicyclic graphs.

Theorem 3.5. *Let G be a unicyclic graph of order n with girth k. Then, $Gut_{a,b}(G) \ge Gut_{a,b}(H_{n,k})$ for*

$0 \le a \le 1$ and $b = 0$ or $b = 1$. Further, if $k = 3$, then $Gut_{a,b}(G) \ge Gut_{a,b}(H_{n,3})$ for $0 \le a \le 1$ and $b \ge 0$ such that at least one of a and b is nonzero. The equality holds if, and only if, $G \cong H_{n,k}$.

Proof. By Theorems 3.1 and 3.3, we get the desired result. □

Theorem 3.6. *Let G be a unicyclic graph of order n with girth k. Then, $Gut_{a,b}(G) \le Gut_{a,b}(H_{n,k})$ for $a < 0$ and $b = 0$. Further, if $k = 3$, then $Gut_{a,b}(G) \le Gut_{a,b}(H_{n,3})$ for $a \le b \le 0$, and at least one of a and b is nonzero. The equality holds if, and only if, $G \cong H_{n,k}$.*

Proof. By Theorems 3.2 and 3.4, we get the desired result. □

4. General Gutman index of graphs of given order and vertex connectivity

The union of two graphs G_1 and G_2 is the graph with vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2)$. It is denoted by $G_1 \cup G_2$. The join of two graphs G_1 and G_2 is obtained from G_1 and G_2 by joining each vertex of G_1 with every vertex in G_2. It is denoted by $G_1 + G_2$. As usual, we denote by K_n- the complete graph on n vertices. $\overline{K_n}$ denotes the complement graph of K_n. The vertex connectivity of G is the minimum number of vertices whose removal disconnects the graph G.

In this section, we show that for graphs with given vertex connectivity, $Gut_{a,b}(G)$ ($a > 1$ and $b \le 0$) is extreme for the graph $(K_{n-\kappa-1} \cup K_1) + K_\kappa$.

The following lemma gives the general Gutman index of $(K_{n-\kappa-1} \cup K_1) + K_\kappa$. We omit the proof as it is direct.

Lemma 4.1. *Let $G \cong (K_{n-\kappa-1} \cup K_1) + K_\kappa$. Then*
$Gut_{a,b}(G) = (n-\kappa-1)(n-2)^a \left[\frac{n-\kappa-2}{2}(n-2)^a + \kappa(n-1)^a + \kappa^a 2^b\right] + \kappa(n-1)^a \left[\frac{(\kappa-1)}{2}(n-1)^a + \kappa^a\right]$.

Theorem 4.2. *Let G be a graph of order n and vertex connectivity κ, where $1 \le \kappa \le n-2$. Then, for $a > 1$, $b \le 0$, and $|b| \le \frac{\log \frac{4\kappa}{(n-\kappa-1)^2}}{\log 2}$,*

$$\begin{aligned} Gut_{a,b}(G) \le{} & (n-\kappa-1)(n-2)^a \left[\frac{n-\kappa-2}{2}(n-2)^a + \kappa(n-1)^a + \kappa^a 2^b\right] \\ & + \kappa(n-1)^a \left[\frac{(\kappa-1)}{2}(n-1)^a + \kappa^a\right], \end{aligned}$$

with equality holding only if $G \cong (K_{n-\kappa-1} \cup K_1) + K_\kappa$.

Proof. Let Γ be a graph with the maximum $Gut_{a,b}$ with respect to order n and vertex connectivity κ. Let $V_0 \subseteq V(\Gamma)$ such that $|V_0| = \kappa$ and the graph $\Gamma \backslash V_0$ is disconnected.

We assert that- $\Gamma \backslash V_0$ has exactly two components. On the contrary, suppose that $\Gamma \backslash V_0$ consists of at least three components. Let Γ_1 and Γ_2 be two components of $\Gamma \backslash V_0$, then for any $u_1 \in V(\Gamma_1)$ and $u_2 \in V(\Gamma_2)$, as $\Gamma \backslash V_0$ consists of at least three components, the graph $\Gamma + u_1u_2$ has vertex connectivity κ. Then, by Lemma 2.2, $Gut_{a,b}(\Gamma + u_1u_2) > Gut_{a,b}(\Gamma)$, a contradiction. Thus, $\Gamma \backslash V_0$ has exactly two components.

Let V_1 and V_2 be the vertex sets of the two components of $\Gamma \backslash V_0$. By Lemma 2.2, any two vertices of V_1 and any two vertices of V_2 are adjacent and $d_\Gamma(x) = n-1$ for all $x \in V_0$. Let $|V_1| = n_1$, $|V_2| = n_2$ with $n_1 \ge n_2 \ge 1$. Then, $n = n_1 + n_2 + \kappa$ and $\Gamma \cong (K_{n_1} \cup K_{n_2}) + K_\kappa$.

Claim: $n_2 = 1$. Assume that $n_1 \ge n_2 \ge 2$. We now compare the $Gut_{a,b}$ indices of $\Gamma = (K_{n_1} \cup K_{n_2}) + K_\kappa$ and $\Gamma' = (K_{n_1+1} \cup K_{n_2-1}) + K_\kappa$.

Let $V'_0 = V_0 = \{w_1, w_2, \dots, w_\kappa\}$, $V'_1 = V_1 = \{v_1, v_2, \dots, v_{n_1}\}$, and $V_2 = V'_2 \cup V'_3$, where $V'_2 = \{u_2, u_3, \dots, u_{n_2}\}$ and $V'_3 = \{u_1\}$. Now, in the graph Γ', we can assume that $V(K_\kappa) = V'_0$, $V(K_{n_1+1}) = V'_1 \cup V'_3$ and $V(K_{n_2-1}) = V'_2$. For $0 \le i < j \le 3$, define

$$E_i = \sum_{\{w,y\}\subseteq V'_i} \left[d_\Gamma(w)^a d_\Gamma(y)^a d_\Gamma(w,y)^b - d_{\Gamma'}(w)^a d_{\Gamma'}(y)^a d_{\Gamma'}(w,y)^b\right];$$

$$E_{ij} = \sum_{w\in V'_i, y\in V'_j} \left[d_\Gamma(w)^a d_\Gamma(y)^a d_\Gamma(w,y)^b - d_{\Gamma'}(w)^a d_{\Gamma'}(y)^a d_{\Gamma'}(w,y)^b\right].$$

Thus, $Gut_{a,b}(\Gamma) - Gut_{a,b}(\Gamma') = \sum_{i=0}^{2} E_i + \sum_{i=0}^{3}\sum_{j=i+1}^{3} E_{ij}$. Note that, $d_\Gamma(v_i) = \kappa + n_1 - 1$, $d_{\Gamma'}(v_i) = k + n_1$ for $i = 1, 2, \dots, n_1$, $d_\Gamma(u_1) = \kappa + n_2 - 1$, $d_{\Gamma'}(u_1) = \kappa + n_1$, $d_\Gamma(u_i) = \kappa + n_2 - 1$, $d_{\Gamma'}(u_i) = \kappa + n_2 - 2$ for $i = 2, 3, \dots, n_2$, and $d_\Gamma(w_i) = d_{\Gamma'}(w_i) = n - 1$ for $i = 1, \dots, \kappa$. Therefore,

$E_0 = 0$;
$E_1 = \frac{n_1(n_1-1)}{2}\left[(\kappa + n_1 - 1)^{2a} - (\kappa + n_1)^{2a}\right]$;
$E_2 = \frac{(n_2-1)(n_2-2)}{2}\left[(\kappa + n_2 - 1)^{2a} - (\kappa + n_2 - 2)^{2a}\right]$;
$E_{01} = \kappa n_1(n-1)^a\left[(\kappa + n_1 - 1)^a - (\kappa + n_1)^a\right]$;
$E_{02} = \kappa(n_2 - 1)(n-1)^a\left[(\kappa + n_2 - 1)^a - (\kappa + n_2 - 2)^a\right]$;
$E_{03} = \kappa(n-1)^a\left[(\kappa + n_2 - 1)^a - (\kappa + n_1)^a\right]$;
$E_{12} = n_1(n_2 - 1)2^b\left[(\kappa + n_1 - 1)^a(\kappa + n_2 - 1)^a - (\kappa + n_1)^a(\kappa + n_2 - 2)^a\right]$;
$E_{13} = n_1\left[(\kappa + n_1 - 1)^a(\kappa + n_2 - 1)^a 2^b - (\kappa + n_1)^{2a}\right]$;
$E_{23} = (n_2 - 1)\left[(\kappa + n_2 - 1)^{2a} - (\kappa + n_1)^a(\kappa + n_2 - 2)^a 2^b\right]$.

Now,

$$\begin{aligned} E_1 + E_2 = {} & \frac{n_1(n_1-1)}{2}\left[(\kappa + n_1 - 1)^{2a} - (\kappa + n_1)^{2a}\right] \\ & + \frac{(n_2-1)(n_2-2)}{2}\left[(\kappa + n_2 - 1)^{2a} - (\kappa + n_2 - 2)^{2a}\right]. \end{aligned}$$

For $n_1 \ge n_2 \ge 2$ and $a > 1$, by Lemma 2.1, we have,
$(\kappa + n_1)^a - (\kappa + n_1 - 1)^a > (\kappa + n_2 - 1)^a - (\kappa + n_2 - 2)^a$. Thus, $E_1 + E_2 < 0$.

Similarly,

$$\begin{aligned} E_{01} + E_{02} & = \kappa n_1(n-1)^a\left[(\kappa + n_1 - 1)^a - (\kappa + n_1)^a\right] \\ & \quad + \kappa(n_2 - 1)(n-1)^a\left[(\kappa + n_2 - 1)^a - (\kappa + n_2 - 2)^a\right] \\ & < 0. \end{aligned}$$

Consider

$$\begin{aligned} E_{13} + E_{23} = {} & 2^b\left[n_1(\kappa + n_1 - 1)^a(\kappa + n_2 - 1)^a - (n_2 - 1)(\kappa + n_2 - 2)^a(\kappa + n_1)^a\right] \\ & + \left[(n_2 - 1)(\kappa + n_2 - 1)^{2a} - n_1(\kappa + n_1)^{2a}\right] \\ & < 2^b\left[n_1(\kappa + n_1 - 1)^{2a} - (n_2 - 1)(\kappa + n_2 - 2)^{2a}\right] + \left[(n_2 - 1)(\kappa + n_2 - 1)^{2a} - n_1(\kappa + n_1)^{2a}\right]. \end{aligned}$$

Since $a > 1$ and $n_1 \geq n_2$, by Lemma 2.1, we get

$$n_1 \left[(\kappa + n_1)^{2a} - (\kappa + n_1 - 1)^{2a}\right] > (n_2 - 1) \left[(\kappa + n_2 - 1)^{2a} - (\kappa + n_2 - 2)^{2a}\right].$$

Therefore,

$$n_1(\kappa + n_1)^{2a} - (n_2 - 1)(\kappa + n_2 - 1)^{2a} > n_1(\kappa + n_1 - 1)^{2a} - (n_2 - 1)(\kappa + n_2 - 2)^{2a}.$$

Thus, $E_{13} + E_{23} < 0$ as $2^b \leq 1$.

Next, consider

$$\begin{aligned} E_{03} + E_{12} &= \kappa(n-1)^a \left[(\kappa + n_2 - 1)^a - (\kappa + n_1)^a\right] \\ &\quad + n_1(n_2 - 1)2^b \left[(\kappa + n_1 - 1)^a(\kappa + n_2 - 1)^a - (\kappa + n_1)^a(\kappa + n_2 - 2)^a\right] \\ &\leq \kappa(n-1)^a \left[(\kappa + n_1 - 1)^a - (\kappa + n_1)^a\right] \\ &\quad + n_1(n_2 - 1)2^b(\kappa + n_1 - 1)^a \left[(\kappa + n_2 - 1)^a - (\kappa + n_2 - 2)^a\right]. \end{aligned} \tag{4.1}$$

Since $b \leq 0$ and $|b| \leq \frac{\log \frac{4k}{(n-\kappa-1)^2}}{\log 2}$, $\kappa \geq n_1(n_2 - 1)2^b$. Hence, $E_{03} + E_{12} < 0$ by Lemma 2.1. Thus, $Gut_{a,b}(\Gamma) - Gut_{a,b}(\Gamma') < 0$, a contradiction.

Therefore, our claim is true, i.e., $n_2 = 1$, and consequently, $\Gamma \cong (K_{n-\kappa-1} \cup K_1) + K_\kappa$. Hence, the result follows from Lemma 4.1. □

5. Some bounds on general Gutman index

In this section, we obtain bounds on the general Gutman index in terms of the general Randić index, general Randić co-index, independence number, and diameter of graph G. The general Randić index [5] of a graph G is defined as

$$R_a(G) = \sum_{uv \in E(G)} [d_G(u)d_G(v)]^a,$$

where a is a real number. Its co-index is denoted by $\overline{R_a(G)}$, and is given by $\overline{R_a(G)} = \sum_{uv \notin E(G)} [d_G(u)d_G(v)]^a$.

Theorem 5.1. *Let G be a connected graph with n vertices and diameter D. For real numbers a and $b \geq 0$, where at least one of a and b is nonzero,*

$$R_a(G) + 2^b\, \overline{R_a(G)} \leq Gut_{a,b}(G) \leq R_a(G) + D^b\, \overline{R_a(G)},$$

Equality on both sides holds if, and only if, $D \leq 2$.

Proof. We have

$$\begin{aligned} Gut_{a,b}(G) &= \sum_{\{u,v\} \subseteq V(G)} [d_G(u)d_G(v)]^a \left[d_G(u,v)\right]^b \\ &= \sum_{uv \in E(G)} [d_G(u)d_G(v)]^a \left[d_G(u,v)\right]^b + \sum_{uv \notin E(G)} [d_G(u)d_G(v)]^a \left[d_G(u,v)\right]^b \end{aligned} \tag{5.1}$$

$$\leq \sum_{uv\in E(G)} [d_G(u)d_G(v)]^a + D^b \sum_{uv\notin E(G)} [d_G(u)d_G(v)]^a . \tag{5.2}$$
$$= R_a(G) + D^b\, \overline{R_a(G)}.$$

Since $d_G(u,v) \geq 2$ for $uv \notin E(G)$, from Eq (5.1), we get

$$Gut_{a,b} \geq \sum_{uv\in E(G)} [d_G(u)d_G(v)]^a + 2^b \sum_{uv\notin E(G)} [d_G(u)d_G(v)]^a . \tag{5.3}$$
$$= R_a(G) + 2^b\, \overline{R}_a(G).$$

Further, the equality in Eqs (5.2) and (5.3) holds if, and only if, $D \leq 2$. This completes the proof. □

Theorem 5.2. *Let G be a connected graph with n vertices and diameter D. For real numbers a and $b \leq 0$, where at least one of a and b is nonzero,*

$$R_a(G) + D^b\, \overline{R_a(G)} \leq Gut_{a,b}(G) \leq R_a(G) + 2^b\, \overline{R_a(G)}.$$

Equality on both sides holds if, and only if, $D \leq 2$.

Proof. We omit the details of the proof as it is similar to that of Theorem 5.1. □

A vertex independent set of a graph G is a set of pair-wise nonadjacent vertices in G. The independence number of G, denoted by $\beta_0(G)$, is the maximum order of a vertex independent set of G.

The following lemma can be obtained by direct calculation.

Lemma 5.3. *Let $G \cong \overline{K_{\beta_0}} + K_{n-\beta_0}$. Then,*
$Gut_{a,b}(G) = \frac{(n-\beta_0)(n-\beta_0-1)}{2}(n-1)^{2a} + \beta_0(n-\beta_0)^a\left[(n-1)^a(n-\beta_0) + (n-\beta_0)^a(\beta_0-1)2^{b-1}\right].$

Theorem 5.4. *Let G be a connected graph with n vertices and independence number β_0. For $a \geq 0$ and $b \leq 0$, where at least one of a and b is nonzero, $Gut_{a,b} \leq Gut_{a,b}(\overline{K}_{\beta_0} + K_{n-\beta_0}) = \frac{(n-\beta_0)(n-\beta_0-1)}{2}(n-1)^{2a} + \beta_0(n-\beta_0)^a\left[(n-1)^a(n-\beta_0) + (n-\beta_0)^a(\beta_0-1)2^{b-1}\right]$.*

Proof. Let H be a connected graph with n vertices, vertex independence number β_0, and having maximum general Gutman index for $a \geq 0$ and $b \leq 0$. Let S be a maximum vertex independent set of H. Then, $|S| = \beta_0$. Let $S' = V(H)\backslash S$. Assume that the vertices x and y belonging to S' are nonadjacent. Then, the graph $H + xy$ has vertex independence number β_0, and also by Lemma 2.2, $Gut_{a,b}(H + xy) > Gut_{a,b}(H)$, a contradiction. Thus, every pair of vertices, in S' are adjacent. By a similar argument, each vertex in S is adjacent to every vertex in S'. Thus, $H \cong \overline{K}_{\beta_0} + K_{n-\beta_0}$, and by Lemma 5.3, the result follows. □

Let S be a subset of $V(G)$. The induced sub-graph $G[S]$ is the graph whose vertex set is S and edge set consists of all those edges of G whose both end points are in S. We denote by kG, the k disjoint copies of G.

Theorem 5.5. *Let G be a connected graph with n vertices. For $a \geq 0$ and $b \leq 0$, where at least one of a and b is nonzero,*

$Gut_{a,b}(G) \leq (n-2\eta)(n-1)^a\left[\frac{(n-2\eta-1)}{2}(n-1)^a + 2\eta(n-2\eta+1)^a\right] + \eta(n-2\eta+1)^{2a}\left[1 + (2\eta-2)2^b\right],$
where η is the maximum positive integer such that ηK_2 is an induced sub-graph of G.

Proof. Let S be a subset of $V(G)$ such that $G[S] = \eta K_2$. Let $S' = V(G)\backslash S$. Denote by H the graph obtained from G by adding edges between the nonadjacent vertices in S' and then joining each vertex of S with every nonadjacent vertex in S'. Therefore, $H \cong \eta K_2 + K_{n-2\eta}$, and also by Lemma 2.2, $Gut_{a,b}(G) \leq Gut_{a,b}(H)$. Now,

$$\begin{aligned}
Gut_{a,b}(H) &= \sum_{\{w,y\}\subseteq S'} d(w)^a d(y)^a d(w,y)^b + \sum_{\{w,y\}\subseteq S} d(w)^a d(y)^a d(w,y)^b + \sum_{\substack{w\in S\\ y\in S'}} d(w)^a d(y)^a d(w,y)^b \\
&= \frac{(n-2\eta)(n-2\eta-1)}{2}(n-1)^{2a} + \eta(n-2\eta+1)^{2a} \\
&+ \eta(\eta-1)(n-2\eta+1)^{2a}\, 2^{b+1} + 2\eta(n-2\eta)(n-1)^a(n-2\eta+1)^a \\
&= (n-2\eta)(n-1)^a\left[\frac{(n-2\eta-1)}{2}(n-1)^a + 2\eta(n-2\eta+1)^a\right] \\
&+ \eta(n-2\eta+1)^{2a}\left[1 + (\eta-1)2^{b+1}\right].
\end{aligned}$$

This completes the proof. □

6. QSPR analysis of some anticancer drugs

We consider the general Gutman index $Gut_{1,1}(G), Gut_{1,-1}(G), Gut_{-1,1}(G)$ and $Gut_{-1,-1}(G)$ for modeling four representative physical properties (boiling point (BP), melting point (MP), enthalpy (E) and molar refraction (MR)) of 10 anticancer drugs. The exact values of these properties are taken from Chem Spider and are also listed in [3, 17]. The molecular graphs of the anticancer drug, namely, Carmustine, Caulibugulone E, Convolutamine F, Perfragilin A, Melatonin, Convolutamydine A, Tambjamine K, Pterocellin B, Amathaspiramide E, Aspidostomide E, Aminopterin, Podophyllotoxin, Convolutamide A, Deguelin, Minocycline, Daunorubicin, and Raloxifene, are as depicted in Figure 3. Table 1 gives the experimental values of these compounds. The general Gutman index of these anticancer drugs is given in Table 2.

A linear regression through Microsoft Excel is performed on the dataset. We consider the linear regression model

$$P = A(TI) + B, \tag{6.1}$$

where P is the physical property of the anticancer drug, A is the regression coefficient, TI represents the topological index, and B is a constant.

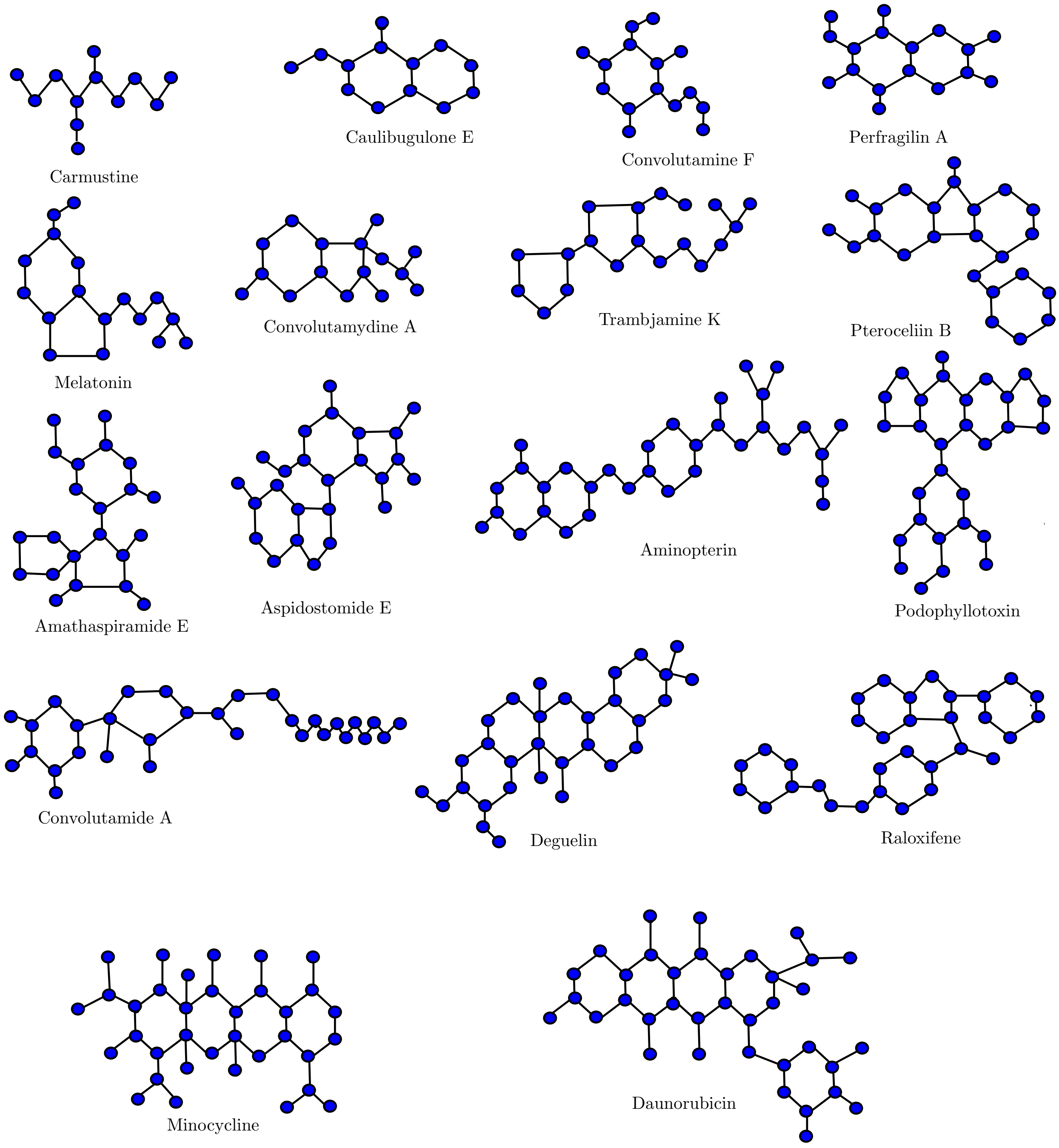

Figure 3. Molecular graph of some anticancer drugs.

Table 1. Some anticancer drugs with its physicochemical property value.

Drug	BP	MP	E	MR
Carmustine	309.6	120.99	63.8	46.6
Caulibugulone E	373	129.46	62	52.2
Convolutamine F	387.7	128.67	63.7	73.8
Perfragilin A	431.5	187.62	68.7	63.6
Melatonin	512.8	182.51	78.4	67.6
Convolutamydine A	504.9	199.2	81.6	68.2
Trambjamine K	391.7	-	64.1	76.6
Pterocellin B	521.6	199.88	79.5	87.4
Amathaspiramide E	572.7	209.72	90.3	89.4
Aspidostomide E	798.8	-	116.2	116
Aminopterin	782.27	344.45	-	114
Podophyllotoxin	597.9	235.86	93.6	104.3
Convolutamide A	629.9	-	97.9	130.1
Deguelin	560.1	213.39	84.3	105.1
Minocycline	803.3	326.3	122.5	116
Daunorubicin	770	208.5	117.6	130
Raloxifene	728.2	289.58	110.1	136.6

Table 2. Some anticancer drugs with general Gutman index values for some a and b.

Drug	a=1, b=1	a=1, b= -1	a= -1, b=1	a= -1, b= -1
Carmustine	691	107.7226	101.5278	9.244048
Caulibugulone E	1104	205.169	90.8333	10.44967
Convolutamine F	1248	161.7524	154.1667	13.0582
Perfragilin A	1768	289.1083	189.1111	14.46911
Melatonin	1900	245.727	185.2778	12.75701
Convolutamydine A	1759	278.4524	192.125	16.21925
Trambjamine K	3264	276.8154	255.7222	14.63814
Pterocellin B	5843	493.6581	342.0556	20.1794
Amathaspiramide E	3802	437.6786	324.8333	21.89983
Aspidostomide E	6291	585.3044	488.0556	26.92546
Aminopterin	14985	569.3475	1232.8056	32.7608
Podophyllotoxin	9455	673.7335	527.75	28.2706
Convolutamide A	14313	516.5041	1175.7778	34.4201
Deguelin	10998	713.369	826.4583	36.9371
Minocycline	14001	803.7356	1105	63.73204
Daunorubicin	17335	937.3948	1325.1111	49.9052
Raloxifene	18138	728.2362	774	28.2997

Using Eq (6.1), we can get the different linear fittings; see Figures 4–7 for the general Gutman index for some values of a and b, and the value of R^2 is also listed below.

Gutman index

$$BP = 0.0213[Gut(G)] + 410.49, R^2 = 0.6747,$$
$$MP = 0.0083[Gut(G)] + 151.85, R^2 = 0.6293,$$
$$E = 0.0027[Gut(G)] + 67.926, R^2 = 0.6632,$$
$$MR = 0.0042[Gut(G)] + 61.209, R^2 = 0.8649.$$

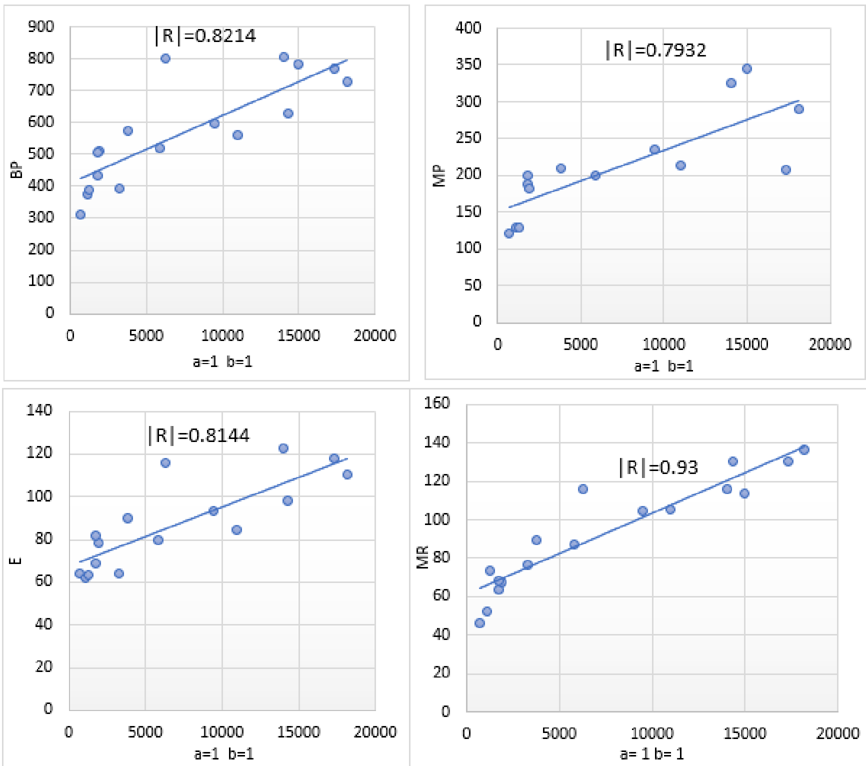

Figure 4. Linear fitting of the Gutman index with BP, MP, E, and MR.

General Gutman index for $a = 1$ and $b = -1$

$$
\begin{aligned}
BP =& 0.5647[Gut_{1,-1}(G)] + 302.65, R^2 = 0.7387,\\
MP =& 0.1824[Gut_{1,-1}(G)] + 126, R^2 = 0.5041,\\
E =& 0.0716[Gut_{1,-1}(G)] + 53.768, R^2 = 0.7653,\\
MR =& 0.1027[Gut_{1,-1}(G)] + 44.321, R^2 = 0.7905.
\end{aligned}
$$

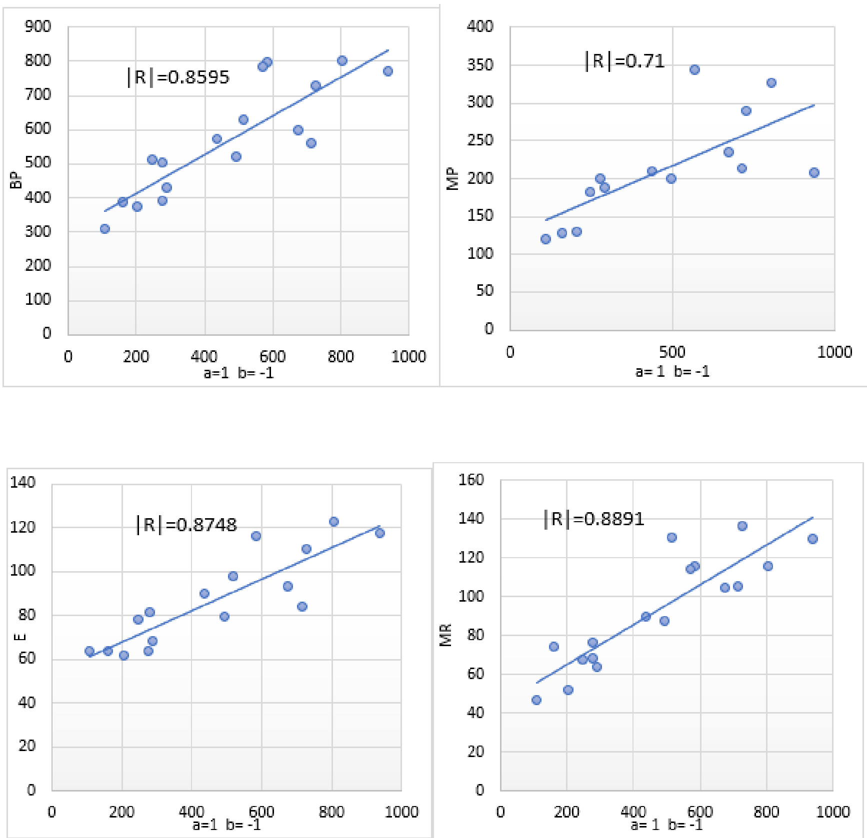

Figure 5. Linear fitting of the $Gut_{1,-1}$ with BP, MP, E, and MR.

General Gutman index for $a = -1$ and $b = 1$

$$BP = 0.3029[Gut_{-1,1}(G)] + 403.62, R^2 = 0.6606,$$
$$MP = 0.1206[Gut_{-1,1}(G)] + 149.06, R^2 = 0.6078,$$
$$E = 0.0407[Gut_{-1,1}(G)] + 66.67, R^2 = 0.6464,$$
$$MR = 0.057[Gut_{-1,1}(G)] + 61.651, R^2 = 0.7564.$$

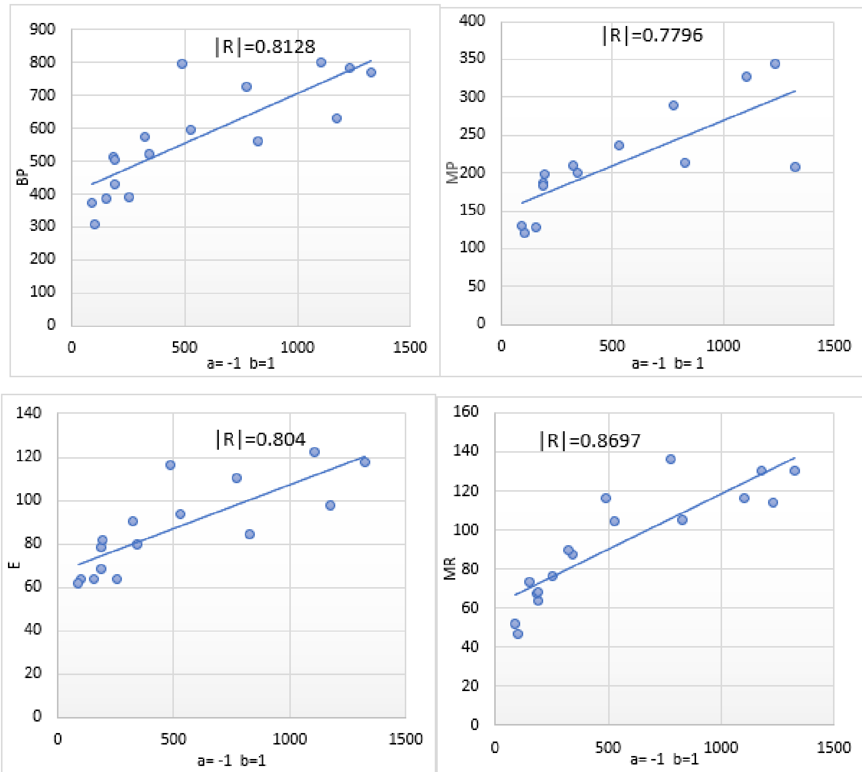

Figure 6. Linear fitting of the $Gut_{-1,1}(G)$ with BP, MP, E, and MR.

General Gutman index for $a = -1$ and $b = -1$

$$\begin{aligned} BP &= 8.8591[Gut_{-1,-1}(G)] + 342.92, R^2 = 0.6533, \\ MP &= 3.0602[Gut_{-1,-1}(G)] + 134.29, R^2 = 0.5085, \\ E &= 1.1504[Gut_{-1,-1}(G)] + 58.283, R^2 = 0.7053, \\ MR &= 1.5078[Gut_{-1,-1}(G)] + 54.287, R^2 = 0.6123. \end{aligned}$$

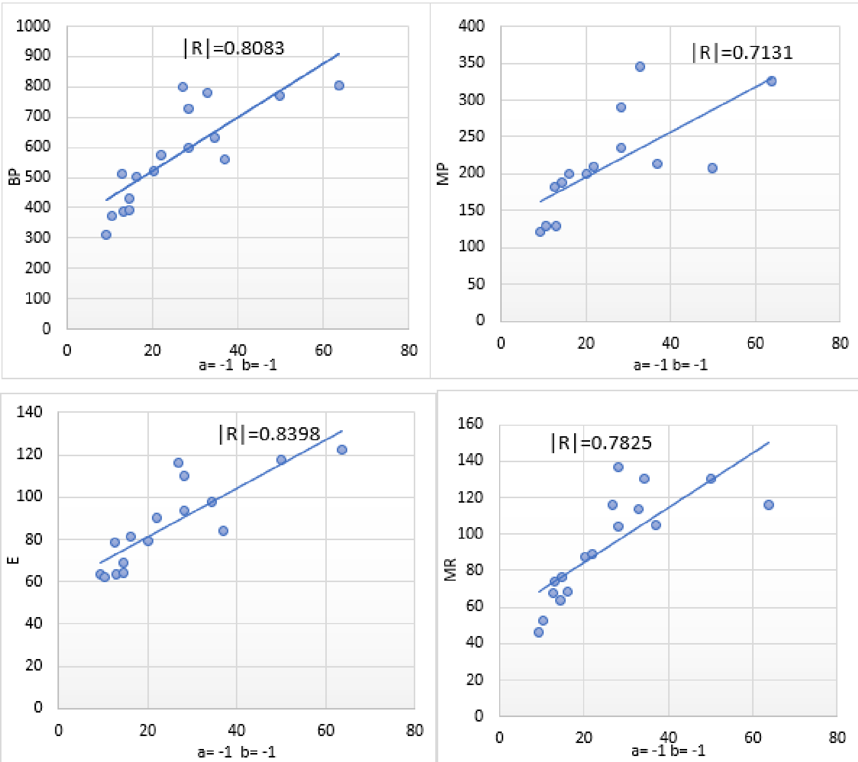

Figure 7. Linear fitting of the $Gut_{-1,-1}(G)$ with BP, MP, E, and MR.

The correlation coefficient of the general Gutman index for some values of a and b with BP, MP, E, and MR is given in Table 3. The numbers highlighted in bold font indicates a high correlation between the general Gutman index and the physicochemical properties of anticancer drugs considered in the study.

Table 3. Correlation coefficient value of general Gutman index with BP, MP, E, and MR of anticancer drugs.

General Gutman index	BP	MP	E	MR
$Gut_{1,1}(G)$	0.8214	**0.7932**	0.8144	**0.93**
$Gut_{1,-1}(G)$	**0.8595**	0.71	**0.8748**	0.8891
$Gut_{-1,1}(G)$	0.8128	0.7796	0.804	0.8697
$Gut_{-1,-1}(G)$	0.8083	0.7131	0.8398	0.7895

From the above linear regression model, it can be seen that the general Gutman index $Gut_{1,1}(G)$ has higher positive correlation with melting point and molar refraction value. Also, the index $Gut_{1,-1}(G)$ correlates well with boiling point and enthalpy. Further, it is observed that $Gut_{1,1}(G)$ and $Gut_{1,-1}$ have a high correlation with melting point and enthalpy respectively than that of other degree-based topological indices considered in [3, 17].

7. Conclusions

In this work, we have obtained extremal unicyclic graphs for the general Gutman index $Gut_{a,b}(G)$ (for some values of a and b). Also, we have obtained bounds for the general Gutman index in terms of vertex connectivity, independence number, and general Randić index. These results indeed answer some of the open problems posed by Das and Vetrík. A comparative study of the general Gutman index with other topological indices would be an interesting problem for future work. At last, QSPR analysis of some anticancer drugs is carried out. It is observed that for some specified values of a and b, $Gut_{a,b}(G)$ index is found to correlate well with some physicochemical properties (namely, boiling point, melting point, enthalpy, and molar refractivity) of anticancer drugs. Hence, it would be interesting to conduct QSPR analysis on various drugs with a general Gutman index.

Author contributions

Swathi Shetty, B. R. Rakshith and Sayinath Udupa N. V. : Conceptualization, Writing-original draft, Writing-review, editing. All authors have read and approved the final version of the manuscript for publication.

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Conflict of interest

All authors declare no conflicts of interest in this paper.

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