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Research article

Extremal unicyclic and bicyclic graphs of the Euler Sombor index

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Abstract: Topological indices are widely used to analyze and predict the physicochemical properties of compounds, and have good application prospects. Recently, the Euler Sombor index was introduced, which is defined as

$$EP(G) = \sum_{v_i v_j \in E(G)} \sqrt{d(v_i)^2 + d(v_j)^2 + d(v_i)d(v_j)}.$$

As the latest index with geometry motivation, it has excellent discrimination and predictive ability for compounds, in addition to mathematical practicality. The unicyclic graphs and bicyclic graphs are composed of various chemical structures, and are of particular importance in the study of topological indices. In this paper, the maximal and minimal values of Euler Sombor index for all unicyclic and bicyclic graphs are determined, and the corresponding extremal graphs are characterized.

Keywords: extremal value; unicyclic graph; bicyclic graph; Euler Sombor index
Mathematics Subject Classification: 05C05, 05C09, 05C92

1. Introduction

As an important class of molecular descriptors, topological indices play a crucial role in mathematical chemistry as well as in graph theory. They have been applied to the physico-chemical properties, biological activity, and many other aspects of compounds [1, 2]. Among these topological indices, the vertex-degree-based (VDB) indices are undoubtedly the most widely investigated, and have new chemical and pharmacological applications, see [3–5]. In recent years, some new VDB indices with geometric interpretations have been discovered.

In 2021, the Sombor index was introduced by Gutman [5], defined as

$$SO(G) = \sum_{v_iv_j \in E(G)} \sqrt{d(v_i)^2 + d(v_j)^2}.$$

This is the first topological index with geometric significance, which has attracted a lot of attention. Many results have been gained in recent papers, such as the extremal values of the Sombor index for trees and any connected graph G [5], the extremal value of this index among all molecular trees [6], the correlation between this index and Zagreb index [7], and the upper and lower bounds of this index for unicyclic graphs as well as the extremal value of chemical unicyclic graphs with given girth [8]. Furthermore, a few new indices with geometric significance, such as the elliptic Sombor index [9], KG-Sombor index [10], etc. have been introduced. For more results on these indices, readers are referred to the review papers [11–13].

Recently, Gutman [14] and Tang et al. [15] proposed another index with geometric significance, defined as

$$EP(G) = \sum_{v_iv_j \in E(G)} \sqrt{d(v_i)^2 + d(v_j)^2 + d(v_i)d(v_j)}.$$

Due to its origin from an approximate expression of the perimeter of the ellipse, which was given by Euler in 1773, it is named the Euler Sombor index.

As the latest VDB index with geometric significance, the Euler Sombor index has irreplaceable importance. Formally an approximate expression of the perimeter for the ellipse, Gutman [14] determined some actual relations between the Euler Sombor index and Sombor index, and it can be used to estimate the Sombor index.

In [15], Tang, Li, and Deng fitted the boiling point (bp) and concentricity factor (AcenFac) with the Euler Sombor index of octane isomers, and showed that it has strong discriminability for compounds and is very effective in predicting physical and chemical properties. They also determined the extremal values for the Euler Sombor index among all (molecular) trees and characterized the corresponding extremal graphs.

Unicyclic graphs and bicyclic graphs are two important classic graphs in the study of topological indices, which are composed of various chemical structures. Cruz and Rada [16] attained the minimal values of (chemical) unicyclic and bicyclic graphs for the Sombor index and obtained an upper bound on the Sombor index of unicyclic and bicyclic graphs, but did not characterize the extremal graphs. In the same paper, they mentioned that the maximal graphs over the set of unicyclic and bicyclic graphs with respect to Sombor index is an interesting open problem. Very recently, Das completely solved these open problems in [17].

Inspired by these, we mainly study maximal and minimal values for the Euler Sombor index over all unicyclic and bicyclic graphs, and characterize corresponding extremum graphs. In Section 2, we present that C_n and $B_i(n, 1)(i = 2, 3)$, see Figure 1, are the only unicyclic and bicyclic graphs with the minimal value of $EP(G)$, respectively. Moreover, we obtain that S'_n is the unique unicyclic graph with the maximal value of $EP(G)$ in Section 3, and also determine that $C'_{n,4}$ is the only bicyclic graph with maximal value of $EP(G)$ in Section 4, where $n \geq 28$.

All graphs considered are simple and connected. Let $G = (V(G), E(G))$ be a graph with its vertex set $V(G)$ and edge set $E(G)$. The *degree* of a vertex v_i is denoted by $d_G(v_i)$ or $d(v_i)$. In particular, the maximal degree and the second maximal degree will be denoted by Δ and Δ_2, respectively. A vertex v_i is said to be *pendant* if $d(v_i) = 1$. Similarly, an edge $\{v_i v_j\}$ is called *pendant* if $d(v_i) = 1$ or $d(v_j) = 1$. The *neighbors* of vertex v_i, denoted by $N_G(v_i)$ or $N(v_i)$, are the set of vertices adjacent to v_i. For notations and terminology not mentioned, see [18].

Recall that a k-cyclic graph G with $|V(G)| = n$ vertices is a connected graph with $|E(G)| = n+k-1$ edges. We denote by $\mathcal{G}_{n,k}$ the set of k-cyclic graphs G with n vertices. In particular, $\mathcal{G}_{n,1}$ is the set of unicyclic graphs, while $\mathcal{G}_{n,2}$ is the set of bicyclic graphs. Let $C'_{n,4}$ be the graph obtained by attaching $(n-4)$ pendant edges to a vertex of degree three in $K_4 - e$, and S'_n the graph obtained from the star S_n by adding an edge. For convenience, an edge $\{v_i v_j\}$ in G with $(d(v_i), d(v_j)) = (x, y)$ (joining a vertex of degree x with a vertex of degree y) is called (x, y)-type, and $m_{x,y} = m_{x,y}(G)$ is the number of edges with (x, y)-type in G.

2. The minimal Euler Sombor index of unicyclic and bicyclic graphs

Let $\mathbb{P}_n = \{(x, y) \in \mathbb{N}\times\mathbb{N} : 1 \le x \le y \le n-1\} - \{(1, 1), (2, 2), (2, 3), (3, 2), (3, 3)\}$ and $\mathbb{P}_{n,k} = \{(x, y) \in \mathbb{P}_n : x + y \le n + k\}$.

Lemma 2.1. *Let*

$$g(x, y) = \sqrt{x^2 + y^2 + xy} + (18\sqrt{3} - 6\sqrt{19})\frac{x + y}{xy} + (4\sqrt{19} - 15\sqrt{3}).$$

Then $g(2, 2) < 0$, $g(2, 3) = g(3, 2) = g(3, 3) = 0$, *and* $g(x, y) > 0$ *for* $(x, y) \in \mathbb{P}_n$.

Proof. We can easily to check $g(2, 2) < 0$, and $g(2, 3) = g(3, 2) = g(3, 3) = 0$. Note that

$$\begin{aligned} g(x, y) &= \sqrt{x^2 + y^2 + xy} + (18\sqrt{3} - 6\sqrt{19})\frac{x + y}{xy} + (4\sqrt{19} - 15\sqrt{3}) \\ &> \sqrt{x^2 + y^2 + xy} + (4\sqrt{19} - 15\sqrt{3}) = g_1(x, y). \end{aligned}$$

For $5 \le x \le y$, immediately, $g(x, y) > g_1(5, 5) = \sqrt{75} + 4\sqrt{19} - 15\sqrt{3} > 0.11 > 0$. For $1 \le x \le 4$ and $y \ge 8$, we have $g(x, y) > g(1, 8) > g_1(5, 5) > 0$. Eventually, for $1 \le x \le 4$ and $2 \le y \le 7$, one can easily check that $g(x, y) > 0$ by tedious algebraic calculations. □

Lemma 2.2. *Let* $G \in \mathcal{G}_{n,k}$ *and* $k \in \{1, 2\}$. *Then*

$$EP(G) = (2\sqrt{19} - 3\sqrt{3})n - (4\sqrt{19} - 15\sqrt{3})(k-1) + g(2, 2)m_{2,2} + \sum_{(x,y)\in\mathbb{P}_{n,k}} g(x, y)m_{x,y},$$

where $g(x, y)$ *is defined as in Lemma 2.1.*

Proof. For $G \in \mathcal{G}_{n,k}$, it was proved in [16] that

$$\begin{aligned} m_{2,3} &= 2(n + 2 - 2k) - 2m_{2,2} + \sum_{(x,y)\in\mathbb{P}_{n,k}} (4 - 6\frac{x + y}{xy})m_{x,y}, \\ m_{3,3} &= 5k - n - 5 + m_{2,2} + \sum_{(x,y)\in\mathbb{P}_{n,k}} (5 - 6\frac{x + y}{xy})m_{x,y}. \end{aligned}$$

Substituting the above equations into $EP(G)$, it yields

$$\begin{aligned} EP(G) &= \sqrt{19}m_{2,3} + 3\sqrt{3}m_{3,3} + 2\sqrt{3}m_{2,2} + \sum_{(x,y)\in\mathbb{P}_{n,k}} \sqrt{x^2+y^2+xy}m_{x,y} \\ &= (2\sqrt{19} - 3\sqrt{3})n - (4\sqrt{19} - 15\sqrt{3})(k-1) + g(2,2)m_{2,2} \\ &+ \sum_{(x,y)\in\mathbb{P}_{n,k}} \left[\sqrt{x^2+y^2+xy} + (18\sqrt{3} - 6\sqrt{19})\frac{x+y}{xy} - (15\sqrt{3} - 4\sqrt{19})\right]m_{x,y} \\ &= (2\sqrt{19} - 3\sqrt{3})n - (4\sqrt{19} - 15\sqrt{3})(k-1) + g(2,2)m_{2,2} + \sum_{(x,y)\in\mathbb{P}_{n,k}} g(x,y)m_{x,y}. \end{aligned}$$

This completes the proof. □

Theorem 2.3. *Let $G \in \mathcal{G}_{n,1}$. Then,*

$$EP(G) \geq 2\sqrt{3}n,$$

with equality if and only if $G \cong C_n$.

Proof. First, by Lemma 2.2 and $k = 1$, we have

$$EP(G) = (2\sqrt{19} - 3\sqrt{3})n + (5\sqrt{3} - 2\sqrt{19})m_{2,2} + \sum_{(x,y)\in\mathbb{P}_{n,1}} g(x,y)m_{x,y}.$$

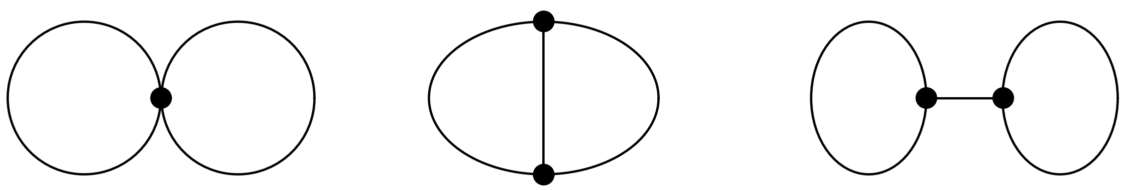
Using Lemma 2.1, one can easily obtain that $g(x,y) > 0$ for all $(x,y) \in \mathbb{P}_{n,1}$, and $5\sqrt{3} - 2\sqrt{19} = g(2,2) < -0.05 < 0$. Moreover, $m_{2,2} \leq n$ by $G \in \mathcal{G}_{n,1}$, and

$$EP(G) \geq (2\sqrt{19} - 3\sqrt{3})n + (5\sqrt{3} - 2\sqrt{19})n = 2\sqrt{3}n,$$

with equality if and only if $\mathbb{P}_{n,1} = \emptyset$ and $m_{2,2} = n$, i.e., $G \cong C_n$. □

The three bicyclic graphs B_1, B_2, and B_3 with n vertices are depicted in Figure 1, where two vertices of degree 3 in B_2 and B_3 are adjacent. One can easily obtain that

$$\begin{aligned} EP(B_1) &= 2\sqrt{3}n + 8\sqrt{7} - 6\sqrt{3}, \\ EP(B_2) &= EP(B_3) = 2\sqrt{3}n + 4\sqrt{19} - 5\sqrt{3}. \end{aligned}$$



B_1 B_2 B_3

Figure 1. Graphs B_1, B_2, and B_3.

Theorem 2.4. *Let $G \in \mathcal{G}_{n,2}$. Then,*

$$EP(G) \geq 2\sqrt{3}n + 4\sqrt{19} - 5\sqrt{3},$$

with equality if and only if $G \cong B_2$ or $G \cong B_3$.

Proof. Since $G \in \mathcal{G}_{n,2}$, we have $m_{2,2} \leq n-3$, and the only graph with $m_{2,2} = n-3$ is the graph $B_1(n)$. Furthermore, one can check that $EP(B_1) > EP(B_2) = EP(B_3)$, and hence, we consider only the graphs with $m_{2,2} \leq n-4$.

By Lemma 2.2 and $k = 2$, we have

$$EP(G) = (2\sqrt{19} - 3\sqrt{3})n - (4\sqrt{19} - 15\sqrt{3}) + (5\sqrt{3} - 2\sqrt{19})m_{2,2} + \sum_{(x,y)\in\mathbb{P}_{n,2}} g(x,y)m_{x,y}.$$

On the other hand, Lemma 2.1 implies that $g(2,2) = 5\sqrt{3} - 2\sqrt{19} < -0.05 < 0$, and $g(x,y) > 0$ for $(x,y) \in \mathbb{P}_{n,2}$. With $m_{2,2} \leq n-4$, we obtain

$$\begin{aligned} EP(G) &\geq (2\sqrt{19} - 3\sqrt{3})n - (4\sqrt{19} - 15\sqrt{3}) + (5\sqrt{3} - 2\sqrt{19})(n-4) \\ &= 2\sqrt{3}n + 4\sqrt{19} - 5\sqrt{3}, \end{aligned}$$

with equality if and only if $\mathbb{P}_{n,2} = \emptyset$ and $m_{2,2} = n-4$, i.e., $G \cong B_2$ or $G \cong B_3$. □

3. The maximal Euler Sombor index of unicyclic graphs

In the remainder of this paper, we assume $f(x,y) = \sqrt{x^2 + y^2 + xy}$ with $x, y \geq 1$. Let $v_i, v_j \in V(G)$. Then

$$EP(G) = \sum_{v_iv_j\in E(G)} \sqrt{d(v_i)^2 + d(v_j)^2 + d(v_i)d(v_j)} = \sum_{v_iv_j\in E(G)} f(d(v_i), d(v_j)).$$

In this section, we use $\mathbb{U}_{n,k}$ to represent the set of unicyclic graphs with order n and girth k.

Lemma 3.1. *Let $f(x,y) = \sqrt{x^2 + y^2 + xy}$ with $x, y \geq 1$, and $x \geq y$. Then, $f(x,y) \leq (2-\sqrt{3})x + (\sqrt{3}-1)(x+y)$.*

Proof. It can be concluded that

$$\begin{aligned} (x + (\sqrt{3}-1)y)^2 &= x^2 + 2(\sqrt{3}-1)xy + (\sqrt{3}-1)^2y^2 \\ &= x^2 + (2\sqrt{3}-3)xy + xy + (4-2\sqrt{3})y^2 \\ &\geq x^2 + (2\sqrt{3}-3)y^2 + xy + (4-2\sqrt{3})y^2 \\ &= x^2 + y^2 + xy. \end{aligned}$$

So, $f(x,y) \leq x + (\sqrt{3}-1)y = (2-\sqrt{3})x + (\sqrt{3}-1)(x+y)$. □

Lemma 3.2. *Let $G \in \mathbb{U}_{n,k}$, $k \geq 3$, $G \ncong C_n$, and $v_i \neq v_j \in V(G)$.*
(1) If $G \in \mathbb{U}_{n,3}$, then $\Delta(G) \leq n-1$ and $d(v_i) + d(v_j) \leq n+1$.
(2) If $G \in \mathbb{U}_{n,4}$, then $\Delta(G) \leq n-2$ and $d(v_i) + d(v_j) \leq n$.
(3) If $G \in \mathbb{U}_{n,k}$ ($k \geq 5$), then $\Delta(G) \leq n-3$ and $d(v_i) + d(v_j) \leq n-1$.

Proof. $G \in \mathbb{U}_{n,k}$ implies that $|V(G)| = |E(G)| = n$. There are at least $(k-2)$ edges not incident with the vertex of degree Δ. Hence, $\Delta(G) \leq n-k+2$. By the condition $C_n \ncong G \in \mathbb{U}_{n,k}$, $E(G) = E(C_k) \cup \{e_1, e_2, \cdots, e_{n-k}\}$, where $e_1, e_2, \cdots, e_{n-k}$ are edges not on the cycle C_k. If all $e_1, e_2, \cdots, e_{n-k}$ are incident with at most two vertices on C_k, then we obtain that $d(v_i) + d(v_j) = n-k+4$. Otherwise, $d(v_i) + d(v_j) \leq n-k+3$. Therefore, (1)–(3) of this lemma hold. □

Lemma 3.3. *Let $G \in \mathbb{U}_{n,3}$ and $G \ncong C_n$. Then $EP(G) \leq EP(S'_n)$ with equality if and only if $G \cong S'_n$.*

Proof. From Lemma 3.2(1), we have $\Delta(G) \leq n-1$ and $d(v_i) + d(v_j) \leq n+1$ for any $v_i \neq v_j \in V(G)$.

If $\Delta = n-1$, then $G \cong S'_n$ and

$$\begin{aligned} EP(S'_n) &= \sum_{v_i v_j \in E(G)} f(d(v_i), d(v_j)) \\ &= (n-3)f(n-1,1) + 2f(n-1,2) + f(2,2) \\ &= (n-3)\sqrt{n^2-n+1} + 2\sqrt{n^2+3} + \sqrt{12}. \end{aligned}$$

If $\Delta = n-2$, then $G \cong F_{1,1}$ or $G \cong F_2$ (see Figure 2) since G contains a cycle C_3, and we can easily obtain

$$\begin{aligned} EP(F_{1,1}) &= \sum_{v_i v_j \in E(G)} f(d(v_i), d(v_j)) \\ &= (n-4)f(n-2,1) + f(n-2,3) + f(n-2,2) + f(3,2) + f(3,1) \\ &< (n-3)f(n-1,1) + 2f(n-1,2) + f(2,2) = EP(S'_n). \\ EP(F_2) &= (n-5)f(n-2,1) + 3f(n-2,2) + f(2,2) + f(2,1) \\ &< (n-3)f(n-1,1) + 2f(n-1,2) + f(2,2) = EP(S'_n). \end{aligned}$$

If $\Delta \leq n-3$, we assume that there is a graph $G \in \mathbb{U}_{n,3}$ with $EP(G) \geq EP(S'_n)$. Then the following claims will hold.

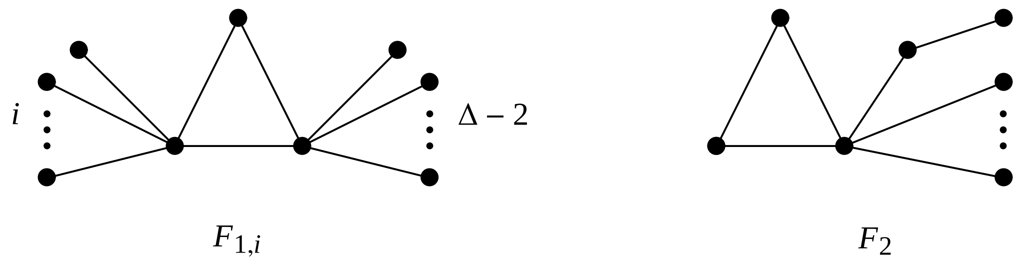


Figure 2. Graphs $F_{1,i}$ and F_2.

Claim 1. $\Delta \geq n-8$ and there exists $v_i \neq v_j \in V(G)$ with $d(v_i) + d(v_j) = n+1$ for $n-8 \leq \Delta \leq n-6$.

Proof. Otherwise, $\Delta \leq n-9$. From Lemma 3.1, we have

$$\begin{aligned} f(d(v_i), d(v_j)) &\leq (2-\sqrt{3})\Delta + (\sqrt{3}-1)(d(v_i) + d(v_j)) \\ &\leq (2-\sqrt{3})(n-9) + (\sqrt{3}-1)(n+1) \\ &< (n - \frac{3}{2}). \end{aligned}$$

Using this result, we can deduce that

$$\begin{aligned} EP(G) &= \sum_{v_iv_j\in E(G)} f(d(v_i), d(v_j)) \\ &< n(n-\frac{3}{2}) < (n-3)(n-\frac{1}{2}) + 2n \\ &< (n-3)\sqrt{n^2-n+1} + 2\sqrt{n^2+3} + \sqrt{12} = EP(S'_n), \end{aligned}$$

a contradiction to $EP(G) \geq EP(S'_n)$. So, $\Delta \geq n-8$.

Next, we will prove the rest of the claim. Otherwise, let $n-8 \leq \Delta \leq n-6$ and $d(v_i) + d(v_j) \leq n$ for all $v_i \neq v_j \in V(G)$. Then,

$$\begin{aligned} f(d(v_i), d(v_j)) &\leq (2-\sqrt{3})\Delta + (\sqrt{3}-1)(d(v_i)+d(v_j)) \\ &\leq (2-\sqrt{3})(n-6) + (\sqrt{3}-1)n \\ &< (n-\frac{3}{2}), \end{aligned}$$

and

$$EP(G) = \sum_{v_iv_j\in E(G)} f(d(v_i), d(v_j)) < n(n-\frac{3}{2}) < (n-3)(n-\frac{1}{2}) + 2n < EP(S'_n),$$

a contradiction to $EP(G) \geq EP(S'_n)$. Claim 1 is proved. □

Claim 2. If $n-5 \leq \Delta \leq n-3$, then there exist two vertices $v_i \neq v_j \in V(G)$ such that $d(v_i)+d(v_j) = n+1$ or n. In particular, if there are two vertices $v_i \neq v_j \in V(G)$ such that $d(v_i) + d(v_j) = n$, then G has no $(1,2)$-type or $(2,2)$-type edge.

Proof. Otherwise, $d(v_i) + d(v_j) \leq n-1$ for any $v_i \neq v_j \in V(G)$. We have

$$\begin{aligned} f(d(v_i), d(v_j)) &\leq (2-\sqrt{3})\Delta + (\sqrt{3}-1)(d(v_i)+d(v_j)) \\ &\leq (2-\sqrt{3})(n-3) + (\sqrt{3}-1)(n-1) \\ &< (n-\frac{3}{2}), \end{aligned}$$

and

$$EP(G) < n(n-\frac{3}{2}) < (n-3)(n-\frac{1}{2}) + 2n < EP(S'_n),$$

a contradiction to $EP(G) \geq EP(S'_n)$.

In the following, we will show that G has no $(1,2)$-type or $(2,2)$-type edge if there are two vertices $v_i \neq v_j \in V(G)$ such that $d(v_i) + d(v_j) = n$. Otherwise, there is an edge $v_kv_l \in E(G)$ such that $f(d(v_k), d(v_l)) \leq \sqrt{12}$. By Lemma 3.1,

$$\begin{aligned} f(d(v_i), d(v_j)) &\leq (2-\sqrt{3})\Delta + (\sqrt{3}-1)(d(v_i)+d(v_j)) \\ &\leq (2-\sqrt{3})(n-3) + (\sqrt{3}-1)n < (n-\frac{1}{2}). \end{aligned}$$

Consequently, we obtain

$$EP(G) < (n-1)(n-\frac{1}{2}) + \sqrt{12} < EP(S'_n),$$

a contradiction to $EP(G) \geq EP(S'_n)$. □

Based on Claims 1 and 2, we have the following in two cases.

Case 1. $n-8 \leq \Delta \leq n-3$. Then, there exists two vertices $v_i \neq v_j \in V(G)$ such that $d(v_i)+d(v_j) = n+1$.

If $\Delta = n-3$, then $G \cong F_{1,2}$, where $n \geq 7$. Similarly, it can be concluded that $G \cong F_{1,1+k}$ if $\Delta = n-(3+k)$, where $1 \leq k \leq 5$ and $n \geq 7+2k$. Consequently, $G \cong F_{1,i}$ (shown in Figure 2), where $2 \leq i \leq 7$. We deduce that

$$\begin{aligned}
EP(F_{1,2}) &= \sum_{v_iv_j\in E(G)} f(d(v_i), d(v_j)) \\
&= (n-5)f(n-3,1) + f(n-3,4) + f(n-3,2) + 2f(4,1) + f(4,2) \\
&< (n-3)f(n-1,1) + 2f(n-1,2) + f(2,2) = EP(S'_n). \\
EP(F_{1,3}) &= (n-6)f(n-4,1) + f(n-4,5) + f(n-4,2) + 3f(5,1) + f(5,2) \\
&< (n-3)f(n-1,1) + 2f(n-1,2) + f(2,2) = EP(S'_n). \\
EP(F_{1,4}) &= (n-7)f(n-5,1) + f(n-5,6) + f(n-5,2) + 4f(6,1) + f(6,2) \\
&< (n-3)f(n-1,1) + 2f(n-1,2) + f(2,2) = EP(S'_n). \\
EP(F_{1,5}) &= (n-8)f(n-6,1) + f(n-6,7) + f(n-6,2) + 5f(7,1) + f(7,2) \\
&< (n-3)f(n-1,1) + 2f(n-1,2) + f(2,2) = EP(S'_n). \\
EP(F_{1,6}) &= (n-9)f(n-7,1) + f(n-7,8) + f(n-7,2) + 6f(8,1) + f(8,2) \\
&< (n-3)f(n-1,1) + 2f(n-1,2) + f(2,2) = EP(S'_n). \\
EP(F_{1,7}) &= (n-10)f(n-8,1) + f(n-8,9) + f(n-8,2) + 7f(9,1) + f(9,2) \\
&< (n-3)f(n-1,1) + 2f(n-1,2) + f(2,2) = EP(S'_n).
\end{aligned}$$

Case 2. $n-5 \leq \Delta \leq n-3$. Then, there exist two vertices $v_i \neq v_j \in V(G)$ such that $d(v_i)+d(v_j) = n$, and there is no edge with $(1,2)$-type or $(2,2)$-type.

If $\Delta = n-3$, then $G \cong F_3$, where $n \geq 6$. Similarly, if $\Delta = n-4$ or $\Delta = n-5$, then $G \cong F_4$ or $G \cong F_5$, where $n \geq 8$ and $n \geq 10$, see Figure 3. We obtain

$$\begin{aligned}
EP(F_3) &= \sum_{v_iv_j\in E(G)} f(d(v_i), d(v_j)) \\
&= (n-5)f(n-3,1) + 2f(n-3,3) + f(3,3) + 2f(3,1) \\
&< (n-3)f(n-1,1) + 2f(n-1,2) + f(2,2) = EP(S'_n). \\
EP(F_4) &= (n-6)f(n-4,1) + f(n-4,3) + f(n-4,3) + f(4,3) + 2f(4,1) + f(3,1) \\
&< (n-3)f(n-1,1) + 2f(n-1,2) + f(2,2) = EP(S'_n).
\end{aligned}$$

$$\begin{aligned}
EP(F_5) &= (n-7)f(n-5,1) + f(n-5,5) + f(n-5,3) + f(5,3) + 3f(5,1) + f(3,1) \\
&< (n-3)f(n-1,1) + 2f(n-1,2) + f(2,2) = EP(S'_n).
\end{aligned}$$

Therefore, together with Cases 1 and 2, Lemma 3.3 is done. □

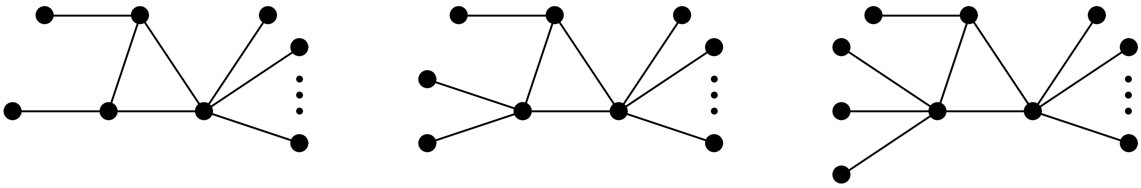


Figure 3. Graphs F_3, F_4 and F_5.

Lemma 3.4. *Let $G \in \mathbb{U}_{n,4}$ and $G \ncong C_n$. Then $EP(G) < EP(S'_n)$.*

Proof. By Lemma 3.2(2), $\Delta \le n-2$, and $d(v_i)+d(v_j) \le n$ for $v_i \ne v_j \in V(G)$. We will prove the lemma by contradiction, and assume there exists a graph $G \in \mathbb{U}_{n,4}$ such that $EP(G) \ge EP(S'_n)$. We give the following claims at first.

Claim 1. There is no edge with $(1,2)$-type and $(2,2)$-type.

Proof. Otherwise, there exists an edge $e = v_kv_l$ such that $f(d(v_k), d(v_l)) \le f(2,2) = \sqrt{12}$. By Lemma 3.1, we have

$$\begin{aligned} f(d(v_i), d(v_j)) &\le (2-\sqrt{3})\Delta + (\sqrt{3}-1)(x+y) \\ &\le (2-\sqrt{3})(n-2) + (\sqrt{3}-1)n < (n-\frac{1}{2}). \end{aligned}$$

And

$$\begin{aligned} EP(G) &= \sum_{v_iv_j \in E(G)} f(d(v_i), d(v_j)) \\ &< (n-1)(n-\frac{1}{2}) + \sqrt{12} \\ &< (n-3)\sqrt{n^2-n+1} + 2\sqrt{n^2+3} + \sqrt{12} = EP(S'_n). \end{aligned}$$

So, Claim 1 is done. □

Claim 2. $n-5 \le \Delta \le n-2$ and there exists two vertices v_i and v_j in G with $d(v_i)+d(v_j) = n$.

Proof. Otherwise, $\Delta \le n-6$. From Lemma 3.1, we have

$$\begin{aligned} f(d(v_i), d(v_j)) &\le (2-\sqrt{3})\Delta + (\sqrt{3}-1)(d(v_i)+d(v_j)) \\ &\le (2-\sqrt{3})(n-6) + (\sqrt{3}-1)n \\ &< (n-\frac{3}{2}), \end{aligned}$$

and

$$EP(G) < n(n-\frac{3}{2}) < (n-3)(n-\frac{1}{2}) + 2n < EP(S'_n),$$

a contradiction. Consequently, $n-5 \le \Delta \le n-2$.

Next, we will prove there exists two vertices $v_i \ne v_j \in V(G)$ such that $d(v_i)+d(v_j) = n$.

If $\Delta = n-2$, then $G \cong H_{1,0}$, as shown in Figure 4, and there exists two vertices v_i and v_j such that $d(v_i) + d(v_j) = n$.

If $n-5 \le \Delta \le n-3$, and $d(v_i) + d(v_j) \le n-1$ for any vertices $v_i \ne v_j \in V(G)$, then we have

$$\begin{aligned} f(d(v_i), d(v_j)) &\le (2-\sqrt{3})\Delta + (\sqrt{3}-1)(d(v_i)+d(v_j)) \\ &\le (2-\sqrt{3})(n-3) + (\sqrt{3}-1)(n-1) < (n-\frac{3}{2}), \end{aligned}$$

and

$$EP(G) < n(n-\frac{3}{2}) < (n-3)(n-\frac{1}{2}) + 2n < EP(S_n'),$$

a contradiction. Claim 2 is proved. □

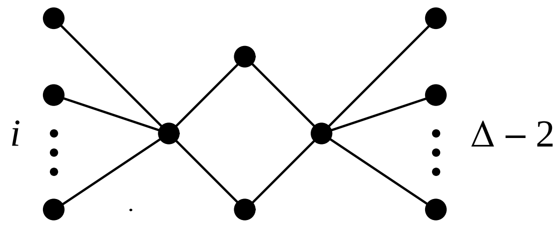


Figure 4. Graph $H_{1,i}$ $(0 \le i \le 3)$.

Now, we consider the following cases according to Claims 1 and 2.

If $\Delta = n-2$, then $G \cong H_{1,0}$, and this graph contains edges of $(2,2)$-type, which contradicts with Claim 1.

If $\Delta = n-3$, there exists $v_i \ne v_j \in V(G)$ with $d(v_i)+d(v_j) = n$, and there is no edge with $(2,2)$-type. Then $G \cong H_{1,1}$, see Figure 4.

If $\Delta = n-4$ or $\Delta = n-5$, then we have only $G \cong H_{1,2}$ or $G \cong H_{1,3}$, as shown in Figure 4.

Therefore, we deduce that

$$\begin{aligned} EP(H_{1,1}) &= (n-5)f(n-2,1) + 2f(n-2,2) + 2f(3,2) + f(3,1) \\ &< (n-3)\sqrt{n^2-n+1} + 2\sqrt{n^2+3} + \sqrt{12} = EP(S_n'). \\ EP(H_{1,2}) &= (n-6)f(n-3,1) + 2f(n-3,2) + 2f(4,2) + f(4,1) \\ &< (n-3)\sqrt{n^2-n+1} + 2\sqrt{n^2+3} + \sqrt{12} = EP(S_n'). \\ EP(H_{1,3}) &= (n-7)f(n-5,1) + 2f(n-5,2) + 2f(5,2) + f(5,1) \\ &< (n-3)\sqrt{n^2-n+1} + 2\sqrt{n^2+3} + \sqrt{12} = EP(S_n'). \end{aligned}$$

So, the assumption is not true, and this completes the proof. □

Theorem 3.5. *Let $G \in \mathcal{G}_{n,1}$, $n \ge 4$. Then,*

$$EP(G) \le (n-3)\sqrt{n^2-n+1} + 2\sqrt{n^2+3} + \sqrt{12},$$

with equality if and only if $G \cong S_n'$.

Proof. If $G \cong C_n$, then

$$EP(G) = \sqrt{12}n < (n-3)\sqrt{n^2-n+1} + 2\sqrt{n^2+3} + \sqrt{12} = EP(S'_n),$$

and the theorem holds.

Next, let $G \in \mathbb{U}_{n,k}$ and $G \ncong C_n$.

Using Lemmas 3.3 and 3.4, the theorem holds for $G \in \mathbb{U}_{n,3}$ and $G \in \mathbb{U}_{n,4}$, especially, with equality if $G \cong S'_n$. Otherwise, $G \in \mathbb{U}_{n,k}$ and $k \geq 5$. Lemma 3.2 implies that $\Delta \leq n-3$, and $d(v_i) + d(v_j) \leq n-1$ for $v_i, v_j \in G$. With Lemma 3.1, we deduce that

$$\begin{aligned} f(d(v_i), d(v_j)) &\leq (2-\sqrt{3})\Delta + (\sqrt{3}-1)(d(v_i)+d(v_j)) \\ &\leq (2-\sqrt{3})(n-3) + (\sqrt{3}-1)(n-1) < (n-\frac{3}{2}), \end{aligned}$$

and

$$EP(G) < n(n-\frac{3}{2}) < (n-3)(n-\frac{1}{2}) + 2n < EP(S'_n).$$

□

4. The maximal Euler Sombor index of bicyclic graphs

In this section, we establish the upper bound of $EP(G)$ for bicyclic graphs, as well as characterize the extremal graph, where $n \geq 28$.

Theorem 4.1. *Let $G \in \mathcal{G}_{n,2}$, $n \geq 28$. Then,*

$$EP(G) \leq (n-4)\sqrt{n^2-n+1} + 2\sqrt{n^2+3} + \sqrt{n^2+n+7} + 2\sqrt{19},$$

with equality if and only if $G \cong C'_{n,4}$.

Proof. Let $v_i \neq v_j \in V(G)$. We divide into the following three cases.

Case 1. $3 \leq \Delta \leq n-13$.

For $3 \leq \Delta \leq 14$, we have

$$f(d(v_i), d(v_j)) \leq \Delta\sqrt{3} \leq 14\sqrt{3} < 24.3.$$

With $n \geq 28$, we deduce that

$$\begin{aligned} EP(G) &< 24.3(n+1) \\ &< (n-4)(n-\frac{1}{2}) + 2n + (n+\frac{1}{2}) + 2\sqrt{19} \\ &< (n-4)\sqrt{n^2-n+1} + 2\sqrt{n^2+3} + \sqrt{n^2+n+7} + 2\sqrt{19} \\ &= EP(C'_{n,4}). \end{aligned}$$

For $15 \leq \Delta \leq n-13$, we assume that $d(v_i) \geq d(v_j)$. Because G is a bicyclic graph, $d(v_i) + d(v_j) \leq n+2$. Let $g(x) = x^2 - (n+2)x + (n+2)^2$. Then, $g(x)$ is monotonically decreasing for $x \in [15, \frac{n+2}{2}]$, and monotonically increasing for $x \in [\frac{n+2}{2}, n-13]$. Therefore,

$$\begin{aligned} f(d(v_i), d(v_j)) &\leq \sqrt{d(v_i)^2 + (n+2-d(v_i))^2 + d(v_i)(n+2-d(v_i))} \\ &= \sqrt{max\{g(15), g(n-13)\}} \\ &\leq \sqrt{g(n-13)} \\ &= \sqrt{n^2 - 11n + 199}. \end{aligned} \tag{4.1}$$

If $n \geq 32$, then $\sqrt{n^2 - 11n + 199} < \sqrt{n^2 - 5n + \frac{25}{4}} = (n - \frac{5}{2})$, and

$$\begin{aligned} EP(G) &< 24.3(n+1) < (n+1)(n - \frac{5}{2}) \\ &< (n-4)\sqrt{n^2 - n + 1} + 2\sqrt{n^2+3} + \sqrt{n^2+n+7} + 2\sqrt{19} \\ &= EP(C'_{n,4}). \end{aligned}$$

If $28 \leq n \leq 31$, then we can also conclude that $EP(G) < EP(C'_{n,4})$ by (4.1), and the detailed results see Table 1.

Table 1. Upper bounds of $(n+1)\sqrt{n^2 - 11n + 199}$ and $EP(C'_{n,4})$.

orders n	Upper bounds of $(n+1)\sqrt{n^2 - 11n + 199}$	$EP(C'_{n,4})$
28	753.443	753.772
29	805.543	809.264
30	859.656	866.758
31	921.911	926.253

Case 2. $n - 12 \leq \Delta \leq n - 3$.

Recall that Δ_2 is the second maximal degree in G. Since $G \in \mathcal{G}_{n,2}$, $\Delta + \Delta_2 \leq n + 2$. Next, we will consider two subcases.

Subcase 2.1. $\Delta_2 = n + 2 - \Delta$.

In this case, $G \cong G_{1,n-1-\Delta}$, as shown in Figure 5. Consequently,

$$\begin{aligned} EP(G) &= (\Delta - 3)f(\Delta, 1) + 2f(\Delta, 2) + f(\Delta, \Delta_2) + (\Delta_2 - 3)f(\Delta_2, 1) + 2f(\Delta_2, 2) \\ &= (\Delta - 3)f(\Delta, 1) + 2f(\Delta, 2) + f(\Delta, n+2-\Delta) \\ &+ (n-1-\Delta)f(n+2-\Delta, 1) + 2f(n+2-\Delta, 2). \end{aligned} \tag{4.2}$$

For $n - 12 \leq \Delta \leq n - 3$, we have the following relations:

$$\begin{aligned} &f(\Delta, 1) < f(\Delta, 2) \leq f(n-3, 2) < f(n-1, 1), \\ &f(n+2-\Delta, 1) < f(n+2-\Delta, 2) \leq f(14, 2) < f(n-1, 1), \\ &f(\Delta, n+2-\Delta) \leq f(n-3, 5) < f(n-1, 1). \end{aligned}$$

Together with (4.2), we have

$$\begin{aligned} EP(G) &< (n-3)f(n-1, 1) + 2f(14, 2) + 2f(14, 1) \\ &< (n-4)\sqrt{n^2 - n + 1} + 2\sqrt{n^2+3} + \sqrt{n^2+n+7} + 2\sqrt{19} \ (n \geq 28) \\ &= EP(C'_{n,4}). \end{aligned}$$

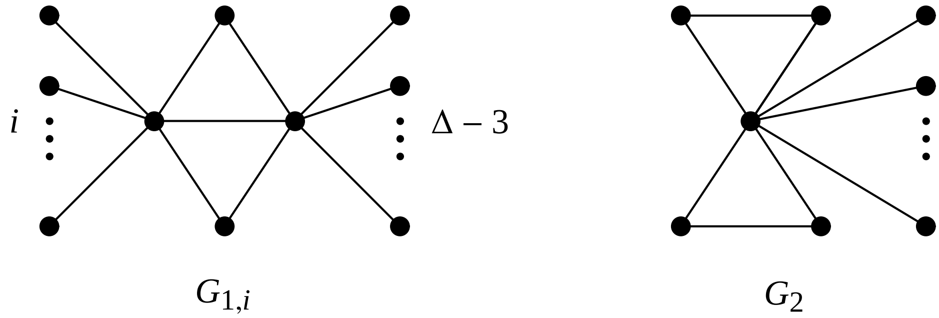


Figure 5. Graphs $G_{1,i}$ and G_2.

Subcase 2.2. $\Delta_2 \leq n + 1 - \Delta$.

For any $v_i \neq v_j \in V(G)$, $d(v_i) + d(v_j) \leq n + 1$. If $n - 12 \leq \Delta \leq n - 9$, then

$$\begin{aligned} f(d(v_i), d(v_j)) &\leq \sqrt{d(v_i)^2 - (n+1)d(v_i) + (n+1)^2} \\ &\leq \sqrt{(n-9)^2 - (n+1)(n-9) + (n+1)^2} \\ &< (n - \frac{5}{2}) \ (n \geq 28). \end{aligned}$$

In this case, we obtain

$$EP(G) \leq (n+1)(n - \frac{5}{2}) < (n-4)(n - \frac{1}{2}) + 2n + (n + \frac{1}{2}) + 2\sqrt{19} < EP(C'_{n,4}).$$

If $n - 8 \leq \Delta \leq n - 3$, then we deduce that

$$EP(G) = \sum_{\{v_i v_j\} \in E(G)} f(d(v_i), d(v_j)) \leq \Delta \sqrt{\Delta^2 + \Delta_2^2 + \Delta\Delta_2} + \Delta_2 \sqrt{3\Delta_2^2}. \tag{4.3}$$

Furthermore, we have the relations

$$\begin{aligned} \sqrt{\Delta^2 + \Delta_2^2 + \Delta\Delta_2} &\leq \sqrt{(n-3)^2 - (n+1)(n-3) + (n+1)^2} \\ &= \sqrt{n^2 - 2n + 13} < (n - \frac{1}{2}), \end{aligned}$$

and

$$\sqrt{3\Delta_2^2} \leq \sqrt{3}(n + 1 - \Delta) \leq \sqrt{3}(n + 1 - n + 8) = 9\sqrt{3},$$

Thus, the Eq (4.3) yields that

$$\begin{aligned} EP(G) &\leq (n - \frac{1}{2})\Delta + 9\sqrt{3}\Delta_2 = (n - \frac{1}{2})\Delta + 9\sqrt{3}(n + 1 - \Delta) \\ &= (n - 9\sqrt{3} - \frac{1}{2})\Delta + 9\sqrt{3}(n+1) \\ &< n^2 - 3.4n + 64 < n^2 - \frac{3}{2}n + 11.2 \ (n \geq 28) \\ &< (n-4)\sqrt{n^2 - n + 1} + 2\sqrt{n^2 + 3} + \sqrt{n^2 + n + 7} + 2\sqrt{19} \\ &= EP(C'_{n,4}). \end{aligned}$$

Case 3. $n - 2 \leq \Delta \leq n - 1$.

Subcase 3.1. $\Delta = n - 2$.

One can easily check that $\Delta_2 \leq 4$. If $\Delta_2 = 4$, then we deduce that $G \cong G_{1,1}$, shown in Figure 5. Recall that $n \geq 28$. We obtain

$$\begin{aligned} EP(G) &< (n-5)\sqrt{(n-2)^2 + 1 + (n-2)} + 2\sqrt{(n-2)^2 + 4 + 2(n-2)} \\ &+ \sqrt{(n-2)^2 + 16 + 4(n-2)} + 2\sqrt{28} + \sqrt{21} \\ &< (n-4)\sqrt{n^2 - n + 1} + 2\sqrt{n^2 + 3} + \sqrt{n^2 + n + 7} + 2\sqrt{19} \\ &= EP(C'_{n,4}). \end{aligned}$$

Next, we assume $\Delta_2 = 3$. In this case, $G \cong G_3$ or $G \cong G_4$ (see Figure 6). Since $n \geq 28$, we have an immediate consequence by calculation:

$$\begin{aligned} EP(G_3) &= (n-5)\sqrt{(n-2)^2 + 1 + (n-2)} + 2\sqrt{(n-2)^2 + 9 + 3(n-2)} \\ &+ \sqrt{(n-2)^2 + 4 + 2(n-2)} + \sqrt{27} + \sqrt{19} + \sqrt{13} \\ &< (n-4)\sqrt{n^2 - n + 1} + 2\sqrt{n^2 + 3} + \sqrt{n^2 + n + 7} + 2\sqrt{19} \\ &= EP(C'_{n,4}). \\ EP(G_4) &= (n-6)\sqrt{(n-2)^2 + 1 + (n-2)} + 3\sqrt{(n-2)^2 + 4 + 2(n-2)} \\ &+ 2\sqrt{19} + \sqrt{27} + \sqrt{7} \\ &< (n-4)\sqrt{n^2 - n + 1} + 2\sqrt{n^2 + 3} + \sqrt{n^2 + n + 7} + 2\sqrt{19} \\ &= EP(C'_{n,4}). \end{aligned}$$

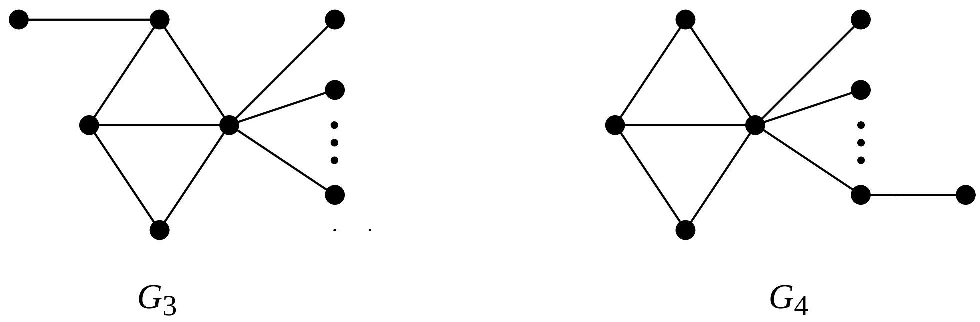


Figure 6. Graphs G_3 and G_4.

Otherwise, $\Delta_2 \leq 2$, we deduce that

$$\begin{aligned} EP(G) &\leq (n-2)\sqrt{(n-2)^2 + 4 + 2(n-2)} + 3\sqrt{12} \\ &< (n-4)\sqrt{n^2 - n + 1} + 2\sqrt{n^2 + 3} + \sqrt{n^2 + n + 7} + 2\sqrt{19} \\ &= EP(C'_{n,4}). \end{aligned}$$

Subcase 3.2. $\Delta = n - 1$.

If $G \cong C'_{n,4}$, then

$$EP(G) = EP(C'_{n,4}) = (n-4)\sqrt{n^2-n+1} + 2\sqrt{n^2+3} + \sqrt{n^2+n+7} + 2\sqrt{19}.$$

Otherwise, $G \cong G_2$, where G_2 is shown in Figure 5. Noting that $\sqrt{n^2-n+1} + \sqrt{n^2+n+7} \geq 2\sqrt{n^2+3}$, we have

$$\begin{aligned} EP(G_2) &= (n-5)\sqrt{n^2-n+1} + 4\sqrt{n^2+3} + 2\sqrt{12} \\ &< (n-4)\sqrt{n^2-n+1} + 2\sqrt{n^2+3} + \sqrt{n^2+n+7} + 2\sqrt{19} \\ &= EP(C'_{n,4}), \end{aligned}$$

and the theorem is proved. □

5. Conclusions

Topological indices are commonly molecular structure descriptors that can be used to simulate and predict the physical, chemical, and biological properties of compounds, and they promoted the development of applied disciplines such as chemistry and pharmacology. Recently, the Euler Sombor index derived from geometry, has been shown to have excellent discriminability for compounds and has therefore received much attention.

In this paper, we present C_n, and $B_i(n,1)(i = 2,3)$ are the only graphs with the minimum Euler Sombor index among all unicyclic and bicyclic graphs, respectively. Moreover, we completely obtain that S'_n is the unique unicyclic graph with the maximum value of $EP(G)$, and also determine that $C'_{n,4}$ is the only bicyclic graph with maximal value of $EP(G)$, where $n \geq 28$. The extremal values of the Euler Sombor index among multi-cyclic graphs, as well as its chemical applications in compounds, may be the research interests of mathematics and chemistry in the future.

Author contributions

Zhenhua Su: Writing-original draft preparation, Writing-review and editing; Zikai Tang: Formal analysis, Methodology. All authors have read and agreed to the published version of the manuscript.

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 conflict of interest.

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