

## Research Article

# On Minimum Generalized Degree Distance Index of Cyclic Graphs

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Topological index (TI) is a mapping that associates a real number to the under study (molecular) graph which predicts its various physical and chemical properties. The generalized degree distance index is the latest developed TI having compatible significance among the list of distance-based TIs. In this paper, the minimum generalized degree distance of unicyclic, bicyclic, and four cyclic graphs is determined. Mainly, the associated extremal (minimal) graphs are also identified among all the aforesaid classes of graphs.

## 1. Introduction

Let class of  $n$ -vertices connected graphs is denoted by  $G_n$ . Then,  $G_n^\alpha$  represents the subclass of  $G_n$  with  $\alpha$  linearly independent cycles and  $n + (\alpha - 1)$  edges. In this paper,  $\alpha = 1, 2, 4$  is considered. For any graph  $G \in G_n$ ,  $d(a, b)$  represents the shortest distance between the vertices  $a, b \in V(G)$ , and the maximum of  $d(a, b)$  for any  $a, b \in V(G)$  is defined to be the diameter of  $G$ , denoted by  $\text{diam}(G)$ . A well-known topological index is the Wiener index, which gives the sum of distances between all pairs of vertices of a graph. A new graph invariant named degree distance was introduced by Dobrynin and Kotchetova [1] and Gutman [2] and defined as

$$D'(G) = \sum_{\{a,b\} \subseteq V(G)} d(a,b)(d(a) + d(b)). \quad (1)$$

For a graph  $G$ , an additively weighted Harary index is given by [3]

$$H_A(G) = \sum_{\{a,b\} \subseteq V(G)} d^{-1}(a,b)(d(a) + d(b)). \quad (2)$$

For every vertex  $a$ , the generalized degree index denoted by  $H_\lambda(a)$  is defined as follows:

$$H_\lambda(a) = D^\lambda(a)d_G(a), \quad (3)$$

where  $D^\lambda(a) = \sum_{b \in V(G)} d^\lambda(a,b)$ . For a graph  $G$ ,

$$\begin{aligned} H_\lambda(G) &= \sum_{a \in V(G)} H_\lambda(a) = \sum_{\{a,b\} \subseteq V(G)} d^\lambda(a,b)(d(a) + d(b)) \\ &= \begin{cases} H_A(G), & \text{if } \lambda = -1, \\ 4m, & \text{if } \lambda = 0, \\ D'(G), & \text{if } \lambda = 1, \end{cases} \end{aligned} \quad (4)$$

where  $\lambda$  is a real number. Let  $\tau$  be a family of graphs a graph  $G' \in \tau$  is called extremal graph if  $\tau(G') \leq \tau(G') \forall G \in \tau$  or  $\tau(G') \geq \tau(G') \forall G \in \tau$ .

**1.1. Research Gaps and Motivation.** Asma et al. found the minimum generalized degree distance of tricyclic graphs in [5]. Moreover, Jianzhong et al. [6] have found degree distance topological indices for derived graphs. One can also find the results on the degree distance of strong products of graphs in [7]. This suggests that there is still room for the research on the topic of the minimum generalized degree distance of  $n$ -cyclic graphs for  $n = 1, 2$ , and 4.

1.2. *Novelty and Contributions.* In this paper, all the extremal unicyclic, bicyclic, and four cyclic graphs having minimum generalized degree distance are determined. Throughout this paper,  $G_n^1, G_n^2$  and  $G_n^4$  denote the class of unicyclic, bicyclic, and four cyclic graphs on  $n$  vertices, respectively.

### 2. Applications

The topological indices find their application in the areas of chemistry such as drug discovery, finding the physio-chemical properties of compounds such as melting point, boiling point, and  $\pi$ -electron energy. Also, they are helpful in providing the correlation between the aforesaid properties of chemical compound and thermodynamical properties. Moreover, it explains the molecular branching and cyclicity of chemical compound. Moreover, it also establishes correlations with various parameters of chemical compounds. To find more on their applications in chemical strata, see [4, 8, 9].

### 3. Classification of Cyclic Graphs

The characterizations of connected unicyclic, bicyclic, and 4-cyclic graphs by their degree sequence are given as follows.

**Lemma 1** (see [10]). *The degrees of vertices of a unicyclic graph are the integers  $n - 1 \geq a_1 \geq a_2 \geq \dots \geq a_n \geq 1$ , if and only if:*

- (i)  $n \geq 3$
- (ii)  $\sum_{j=1}^n a_j = 2n$
- (iii)  $a_j \geq 2$ , for at least three indices

**Lemma 2** (see [10]). *The degrees of the vertices of a bicyclic graph are the integers  $n - 1 \geq a_1 \geq a_2 \geq \dots \geq a_n \geq 1$  if and only if:*

- (i)  $n \geq 4$
- (ii)  $\sum_{j=1}^n a_i = 2n + 2$
- (iii)  $a_i \geq 2$ , for at least four indices
- (iv)  $a_1 \leq n - 1$ .

**Lemma 3** (see [11]). *The degrees of the vertices of a four cyclic graph are the integers  $n - 1 \geq a_1 \geq a_2 \geq \dots \geq a_n \geq 1$  if and only if:*

- (i)  $n \geq 5$
- (ii)  $\sum_{j=1}^n a_i = 2n + 6$
- (iii)  $a_i \geq 2$ , for at least five indices.

Let the number of vertices of graph  $G$  of degree  $i$  is denoted by  $b_i$ , for  $1 \leq i \leq n - 1$ . If  $d_G(v) = t$ , then

$$\begin{aligned}
 D^\lambda(a) &= \sum_{b \in V(G)} d^\lambda(a, b) = \sum_{\{a, b\} \subseteq V(G), d(a, b) = 1} d^\lambda(a, b) + \sum_{\{a, b\} \subseteq V(G), d(a, b) \geq 2} d^\lambda(a, b) \\
 &\geq 2^\lambda n - 2^\lambda(t + 1) + t, \\
 H_\lambda(G) &= \sum_{a \in V(G)} d_G(a) D_\lambda(a) \geq \sum_{t=1}^{n-1} t b_t (2^\lambda n - 2^\lambda(t + 1) + t).
 \end{aligned}
 \tag{5}$$

Let us denote

$$F_\lambda(b_1, b_2, \dots, b_{n-1}) = \sum_{t=1}^{n-1} t b_t (2^\lambda n - 2^\lambda(t + 1) + t). \tag{6}$$

To determine the minimum of  $F_\lambda(b_1, b_2, \dots, b_{n-1})$  over all integers  $b_1, b_2, \dots, b_{n-1}$ , which satisfy the conditions of above three lemmas.

Thus, Lemma 1-Lemma 3 with the help of aforesaid notions can be rewritten as follows:

**Lemma 4** (see [10]). *The integers  $b_1, \dots, b_{n-1} \geq 0$  are the multiplicities of the degrees of a unicyclic graph if and only if:*

- (i)  $n \geq 3$
- (ii)  $\sum_{i=1}^{n-1} b_i = n$
- (iii)  $\sum_{i=1}^{n-1} i b_i = 2n$
- (iv)  $b_1 \leq n - 3$

**Lemma 5** (see [10]). *For bicyclic graph, the integers  $b_1, \dots, b_{n-1} \geq 0$  represent the multiplicities of the degrees of vertices if and only if:*

- (i)  $n \geq 4$
- (ii)  $\sum_{i=1}^{n-1} b_i = n$
- (iii)  $\sum_{i=1}^{n-1} i b_i = 2n + 2$
- (iv)  $b_1 \leq n - 4$

**Lemma 6** (see [11]). *The integers  $b_1, \dots, b_{n-1} \geq 0$  are the multiplicities of the degrees of a four cyclic graph if and only if:*

- (i)  $n \geq 5$
- (ii)  $\sum_{i=1}^{n-1} b_i = n$
- (iii)  $\sum_{i=1}^{n-1} i b_i = 2n + 6$
- (iv)  $b_1 \leq n - 5$

The set of vectors  $(b_1, b_2, \dots, b_{n-1})$ , which satisfy the conditions of Lemma 4, 5, and 6, is denoted by  $\Delta_1, \Delta_2$ , and  $\Delta_3$ , respectively.

Now, we consider the transformation  $T_1$ , which is defined for  $i \geq 2, j > 0, i + j \leq n - 2, b_i \geq 1, b_j \geq 1$ , as follows [10]:  $T_1(b_1, \dots, b_{n-1}) = (b'_1, \dots, b'_{n-1}) = (b_1, \dots, b_{i-1} + 1, b_i - 1, \dots, b_{i+j} - 1, b_{i+j+1} + 1, \dots, b_{n-1})$ .

We have  $b_m = b'_m$  for  $m \neq \{i - 1, i, i + j, i + j + 1\}$ .

Let  $2 \leq i \leq i - 2$  and  $b_i \geq 2$  the transformation  $T_2$  defined as  $T_2(b_1, \dots, b_{n-1}) = (b'_1, \dots, b'_{n-1}) = (b_1, \dots, b_{i-1} + 1, b_i - 2, b_{i+1} + 1, \dots, b_{n-1})$  for  $b_m = b'_m$  for  $m \neq \{i - 1, i, i + 1\}$ .

**Lemma 7.** Suppose  $\lambda$  is a positive integer and  $(b_1, b_2, \dots, b_{n-1}) \in \Delta_i$ , for  $i = 1, 2, 3$ .

- (a)  $T_1(b_1, b_2, \dots, b_{n-1}) \in \begin{cases} \Delta_1 \text{ or } \Delta_2, & \text{if } m \neq 2, \text{ and } b_1 \neq n - 3 \\ \Delta_3, & \text{if } m \neq 2, \text{ and } b_1 \neq n - 5 \end{cases}$
- (b)  $F_\lambda(T_1(b_1, b_2, \dots, b_{n-1})) < F_\lambda(b_1, b_2, \dots, b_{n-1})$

*Proof*

- (a) As  $\sum_{i=1}^{n-1} b_i = \sum_{i=1}^{n-1} b'_i$  and  $\sum_{i=1}^{n-1} i b_i = \sum_{i=1}^{n-1} i b'_i$ . If  $(b_1, \dots, b_{n-1}) \in \Delta_i$ , for  $i = 1, 2$  and  $m = 2$  and  $b_1 = n - 3$ , then  $b'_1 > n - 3$  a contradiction. Also, if  $(b_1, \dots, b_{n-1}) \in \Delta_3$ , and  $m = 2$  and  $b_1 = n - 5$ , then  $b'_1 > n - 5$  a contradiction.

- (b) By simple calculations,  $F_\lambda(b_1, \dots, b_{n-1}) - F_\lambda(T_1(b_1, \dots, b_{n-1})) = (2^\lambda - 1)(2j + 2) > 0$ .  $\square$

**Lemma 8.** Suppose  $\lambda \geq 0$  and  $(b_1, \dots, b_{n-1}) \in \Delta_i, i = 1, 2, 3$ .

- (a)  $T_2(b_1, b_2, \dots, b_{n-1}) \in \begin{cases} \Delta_1 \text{ or } \Delta_2, & \text{if } m \neq 2, \text{ and } b_1 \neq n - 3 \\ \Delta_3, & \text{if } m \neq 2, \text{ and } b_1 \neq n - 5 \end{cases}$

$$\min H_\lambda(G) = F_\lambda(n - 3, 2, 0, \dots, 1) = 2^\lambda(n^2 - n - 6) + (n^2 - n + 6), \tag{8}$$

and the unique extremal graphs is  $K_{1,n-1} + e$ .  $\square$

**Theorem 10** (see [10]). For every  $n \geq 3$  and  $\in G_n^1$  it holds that

$$\min D'(G) = \begin{cases} 12, & \text{if } n = 3, \\ 3n^2 - 3n - 6, & \text{if } n \geq 4. \end{cases} \tag{9}$$

*Proof.* By putting  $\lambda = 1$  in Theorem 9, the above result is proved, and the result is the same as Theorem 3.1 in [10].  $\square$

**Theorem 11.** For every  $n \geq 4$  and  $G \in G_n^2$  it holds that

$$\min H_\lambda(G) = 2^\lambda(n^2 + n - 16) + (n^2 - n + 14), \tag{10}$$

$$\min H_\lambda(G) = F_\lambda(n - 6, 2, 1, 0, \dots, 1) = 2^\lambda(n^2 + n - 16) + (n^2 - n + 14), \tag{11}$$

$$(b) F_\lambda(T_2(b_1, \dots, b_{n-1})) < F_\lambda(b_1, \dots, b_{n-1})$$

*Proof.* (a) Proof of (a) is the same as above

- (b) By putting  $p = 0$  in the above, it holds that  $F_\lambda(T_2(b_1, \dots, b_{n-1})) < F_\lambda(b_1, \dots, b_{n-1})$   $\square$

#### 4. Main Result

This section deals with the main results related to our finding of the minimum generalized degree distance index for the different families of the cyclic graphs.

**Theorem 9.** For every  $n \geq 3$  and  $G \in G_n^1$  it holds that

$$\min H_\lambda(G) = 2^\lambda(n^2 - n - 6) + (n^2 - n + 6), \tag{7}$$

and the unique extremal graphs is  $K_{1,n-1} + e$ .

*Proof.* For  $n = 3$ , the only unicyclic graph is  $C_3$  and  $H_\lambda(C_3) = 12$ .

For  $n \geq 4$ , if  $b_{n-1} > 1$ , we will get at least two cycles that do not satisfy the hypothesis. Thus,  $b_{n-1} \leq 1$ . Next, we investigate the values of  $b_i$  for  $3 \leq i \leq n - 2$ . If  $b_i \geq 1$  and  $b_j \geq 1$ , then by applying the transformation  $T_1$  at position  $i$  and  $j$ , we get a smaller value of  $F_\lambda(T_1(b_2, b_2, \dots, b_{n-1}))$ . Now, for  $b_3 = b_4 = \dots = b_{n-2} = 0$ , the value of  $b_2 \neq 0$ . If  $b_2 = 0$ , then  $b_1 = n - 2$  which is not possible. Since  $b_{n-1} \leq 1$ , first we consider  $b_{n-1} = 0$ , then  $b_1 + b_2 = n$  and  $b_1 + 2b_2 = 2n$  imply that  $b_1 = 0$  and  $b_2 = n$  which corresponds to the graph  $C_n$ . If  $b_{n-1} = 1$ , then the conditions of Lemma 4 imply that  $b_1 = n - 3$  and  $b_2 = 2$ , and hence,

and the unique extremal graphs are obtained from  $K_{1,n-1}$  by adding two edges of common extremity.

*Proof.* For  $n = 4$ , the unique bicyclic graph is  $C_4$  with an edge and  $H_\lambda(C_4 \text{ with an edge}) = 34$ .

For  $n \geq 5$ , it holds that we have  $b_{n-1} \leq 1$  and  $b_4 = b_5 = \dots = b_{n-2} = 0$ . Since  $b_{n-1} = \{0, 1\}$ , first we consider  $b_{n-1} = 0$ , then  $b_1 + b_2 + b_3 = n$  and  $b_1 + 2b_2 + 3b_3 = 2n + 2$  imply that  $b_1 = b_3 - 2$ . If  $b_3 \geq 2$ , then by action of transformation  $T_2$  at position 3, a smaller value for  $F$  is determined. Consider if  $b_{n-1} = 1$ , then  $b_1 + b_2 + b_3 = n - 1$  and  $b_1 + 2b_2 + 3b_3 = n + 3$ . If  $b_3 = 0$ , we have  $(n - 5, 4, 0, \dots, 1)$  and  $T_2(n - 5, 4, 0, \dots, 1) = (n - 6, 2, 1, 0, \dots, 1)$ . If  $b_3 = 1$ , then we get  $(n - 6, 2, 1, 0, \dots, 1)$ , and hence,

and the unique extremal graphs is  $K_{1,n-1}$  with two edges of the common vertex.  $\square$

**Theorem 12** (see [10]). For every  $n \geq 3$  and  $\in G_n^2$ , it holds that

$$\min D'(G) = \begin{cases} 34, & \text{if } n = 4, \\ 3n^2 + n - 18, & \text{if } n \geq 5. \end{cases} \quad (12)$$

*Proof.* By putting  $\lambda = 1$  in Theorem 11, the above result is proved, and the result is the same as Theorem 3.2 in [10].  $\square$

**Theorem 13.** For  $n \geq 5, \lambda \geq 0$  and  $G \in G_n^4$ , it holds that

$$\min H_\lambda(G) = 2^\lambda(n^2 + 5n - 42) + (n^2 - n + 36). \quad (13)$$

Then, all the extremal graphs are isomorphic to  $A_1$ . The graph  $A_1$  is obtained by identifying the center of star  $S_n$  with an arbitrary vertex of degree 5.

*Proof.* In order to find  $\min H_\lambda(G)$ , it is enough to find  $\min F(b_1, \dots, b_{n-1})$ , where  $(b_1, \dots, b_{n-1}) \in \Delta_3$ . Let  $n = 5$ , only graphs  $B_1, B_2 \in G_n^4$  (see Figure 1). Also,  $H_\lambda(B_1) = 74$  and  $H_\lambda(B_2) = 76$ . Let us consider  $n \geq 6$ . For  $n = 6$ , all graphs  $G \in G_6^4$  are  $A_i$  where  $1 \leq i \leq 10$  shown in Figure 2. For these graphs  $\min H_\lambda(A_i) = 3 \cdot 2^{\lambda+3} + 66$  which hold for the graph  $A_1$ .

Finally, for  $n \geq 7$ . If  $b_{n-1} \geq 2$ , Then, we have at least five cycles; hence,  $b_{n-1}$  must be less than or equal to one.

Now, we investigate the possible values of  $b_6, b_7, \dots, b_{n-2}$ . If there exists  $6 \leq l < m \leq n - 2$ , such that  $b_l \geq 1$  and  $b_m \geq 1$ , then by the action of  $T_1$  at position  $l$  and  $m$ , a new vector  $(b'_1, \dots, b'_{n-1}) \in \Delta_3$  for which  $F(b'_1, \dots, b'_{n-1}) < F(b_1, \dots, b_{n-1})$  is obtained.

Similarly, if there exists  $6 \leq l \leq n - 2$  such that  $b_l \geq 2$ , a new degree sequence in  $\Delta_3$  is determined by which  $F_\lambda(b'_1, \dots, b'_{n-1}) < F_\lambda(b_1, \dots, b_{n-1})$ . Now, we consider two cases:  $\square$

*Case 14.* Consider distinct indices  $6 \leq l \leq n - 2$  and  $m$  such that  $b_l = 1$  and  $b_m = 0$ . If  $b_5 = 0$ , since  $b_{n-1} \in \{0, 1\}$ , we will analyze the two cases separately.

$$F_\lambda(n - 6, 4, 0, 0, 1, 0, \dots, 0, 1) = 2^\lambda(n^2 + 5n - 42) + (n^2 - n + 36). \quad (14)$$

Next, consider if  $b_5 = 0$ , then  $b_2 + 2b_3 + 3b_4 = 8$ . There are only two possible solutions that satisfy the conditions of four cyclic graph. These graphical sequences are

$$F_\lambda(n - 5, 1, 2, 1, 0, \dots, 0, 1) = 2^\lambda(n^2 + 5n - 40) + (n^2 - n + 34). \quad (15)$$

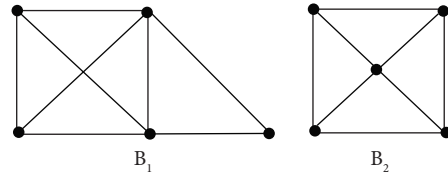


FIGURE 1: The graphs having 5 vertices in  $G_n^4$ .

- (a) In this case,  $b_{n-1} = b_l = 1$ , where  $l \geq 6$  and  $b_4 = 0$ . By considering different vertices  $p, q, r, s, t, w, z \in V(G)$  in such a way that  $d(p) = n - 1, d(q) = j \geq 6$ . The vertices  $r, s, t, w, z$  are adjacent to  $p$  and  $q$ . Also,  $p$  and  $q$  are adjacent. Then, there exist five cycles which contradicts the hypothesis.
- (b) Suppose  $b_{n-1} = 0$ , then  $b_4 = 0$  and  $b_i = 1, (6 \leq i \leq n - 2)$  and  $\Delta_3$  is characterized by the equations  $b_1 + b_2 + b_3 = n - 1$  and  $b_1 + 2b_2 + 3b_3 = 2n + 6 - i$ , which implies that  $b_2 + 2b_3 = n + 7 - i$ , by solving for  $b_2$  and  $b_3$ , and then by applying the transformation for position 2 or 3, we obtain a smaller value of  $F$ .

*Case 15.* Suppose that  $b_6 = b_7 = \dots = b_{n-1} = 0$  holds, the degree sequence is  $(b_1, b_2, b_3, b_4, 0, 0, \dots, 0, b_{n-1})$ . As  $b_{n-1} \in \{0, 1\}$ , so we have to analyze two cases:

- (a) If  $b_{n-1} = 0$ , then  $b_2 + 2b_3 + 3b_4 + 4b_5 = n + 6$ . This equation does not hold. If all  $b_2, b_3, b_4$ , and  $b_5$  are not greater than 2, then  $b_2 + 2b_3 + 3b_4 + 4b_5 \leq 20$ , which contradicts the hypothesis  $n \geq 7$ . If  $b_j > 2$  for any  $j = 2, 3, 4, 5$  by applying  $T_2$  at position  $j$ , the minimum value of  $F$  is obtained.
- (b) If  $b_{n-1} = 1$ , then  $b_2 + 2b_3 + 3b_4 + 4b_5 = 8$ . If  $b_5 \geq 3$ , then  $b_2 + 2b_3 + 3b_4 + 4b_5 \geq 12$ . So  $b_5 \leq 2$ , if  $b_5 = 2$ , then  $b_2 + 2b_3 + 3b_4 = 0$ , which implies that  $b_2 = b_3 = b_4 = 0$ , and  $b_1 = n - 3$  which is a contradiction as  $b_1 \leq n - 5$ . So,  $b_5 < 2$ . Thus, either  $b_5 = 0$  or  $b_5 = 1$ .

If  $b_5 = 1$ , then  $b_2 + 2b_3 + 3b_4 = 4$ , the only possible solution that follows Lemma 6 and gives a graphical degree sequence is  $b_2 = 4, b_3 = 0, b_4 = 0$ . Thus,  $(b_1, b_2, \dots, b_{n-1}) = (n - 6, 4, 0, 0, 1, 0, \dots, 0, 1)$  and

$(n - 5, 0, 4, 0, \dots, 0, 1)$  and  $(n - 5, 2, 0, 2, 0, \dots, 0, 1)$ . By applying  $T_2$  at position 3 of  $(n - 5, 0, 4, 0, \dots, 0, 1)$ , we obtain a degree sequence  $(n - 5, 2, 0, 2, 0, \dots, 0, 1)$  and

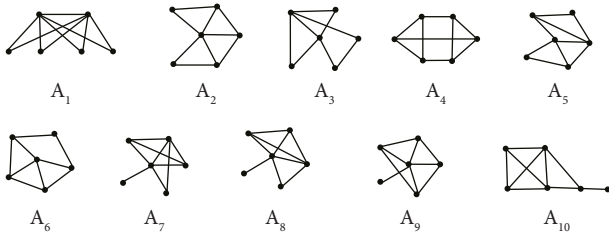


FIGURE 2: The graphs  $A_i$  for  $1 \leq i \leq 6$  existing in the family of graphs  $G_n^4$ .

Since  $2^\lambda(n^2 + 5n - 42) + (n^2 - n + 36) = 2^\lambda(n^2 + 5n - 40) + (n^2 - n + 34) - 2(2^\lambda - 1) < 2^\lambda(n^2 + 5n - 40) + (n^2 - n + 34)$ . Hence,

$$\min H_\lambda(G) = 2^\lambda(n^2 + 5n - 42) + (n^2 - n + 36). \quad (16)$$

and the unique extremal graph is obtained by identifying the center of graph  $K_{1,n-4}$  with an arbitrary degree 4 vertex of graph  $A_1$  (Figure 2).

**Theorem 16.** Let  $G \in G_n^4$ , then

$$\min D'(G) = \begin{cases} 74, & \text{if } n = 5, \\ 3n^2 + 9n - 48, & \text{if } n \geq 6. \end{cases} \quad (17)$$

*Proof.* By putting  $\lambda = 1$  in Theorem 13, the above result is proved, and the result is the same as Theorem 12 in [11].  $\square$

### 5. Conclusion

In this note, we have computed the minimum generalized degree distance indices in the different families of unicyclic, bicyclic, and four cyclic graphs. The extremal graphs having minimum generalized degree distance indices are also characterized among these families of graphs. However, the problem is still open to compute this index for various families of  $\alpha$ -cyclic graphs for  $\alpha = 3$  and  $\alpha \geq 5$  [12–17].

### Data Availability

The data supporting the current study are available from the corresponding author upon request.

### Conflicts of Interest

The authors declare that they have no conflicts of interest.

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