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Properties of Total Transformation Graphs for General Sum-Connectivity Index

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1. Introduction

Chemical graph theory [1] has given a massive area of research to chemists in which they apply graph theory to mathematical modeling of chemical phenomena. This area of research necessitates characteristics of structures, in which researchers deal with their grouping, properties, and ordering. The molecular graph furnishes a graph-theoretical depiction of the molecule and lays out gainful knowledge into the chemical phenomena. The atoms of a molecule are described as vertices, and links signify the covalent bonds between the atoms. A topological index is represented by a single number corresponding with a graph. There are a lot of categories of topological indices, some of them being distance-, counting-, eccentricity-, and degree-related indices and polynomials of graphs. Among the abovementioned categories of indices, the degree-dependent indices show a beneficial character in the chemical graph theory.

Here, we examine only simple and connected graphs. Let \( G \) be the graph with vertex and edge sets, \( V(G) \) and \( E(G) \), respectively. For a vertex \( q \) of \( G \), \( d^{(q)} \) denotes the degree of \( q \) which is described as the number of its incident edges. The Randić index was described in [2] as

\[
R(\mathcal{G}) = \sum_{q\in V(G)} \frac{1}{\sqrt{d^{(q)}d^{(q')}}}.
\]  

(1)

It is one of the most popular molecular invariants in the study of structure-property and activity relationships [3, 4]. The general Randić index is described as follows:

\[
R_\rho(\mathcal{G}) = \sum_{q\in V(G)} \left(d^{(q)}d^{(q')}\right)^\rho,
\]  

(2)

where \( \rho \) is a real number. The sum-connectivity index \( \chi_{\rho}(\mathcal{G}) = \sum_{q\in V(G)} (d^{(q)} + d^{(q')})^{-\rho/2} \) is introduced by Zhou and Trinajstić [5]. Zhou and Trinajstić [6] investigated the
idea of the general sum-connectivity index with the help of sum-connectivity index and defined it in following way:

\[ \chi_e(Q) = \sum_{q \in E(Q)} \left( d(q) + d(q') \right)^{\theta}, \]

(3)

where \( \rho \) is a real number. The Randić and sum-connectivity indices relate with the \( \pi \)-electron energy of benzenoid hydrocarbons [7]. A lot of extremal characteristics of the general sum-connectivity index for certain graph families were given [8–16]. For additional studies on extremal graphs with topological indices, we refer [17–23].

The total \( T(Q) \) graph is the graph with \( V(T(Q)) = V(Q) \cup E(Q) \) and \( Q \subseteq E(V(Q) \cup E(Q)) \) if and only if \( q \) and \( q' \) are either incident or linked in \( Q \). The total graphs of paths \( _n \mathcal{P} \) and cycle \( _n \mathcal{C} \) are shown in Figure 1. Some characteristics of total graphs are described in the literature [24–29].

A graph whose vertex set is converted into two linked vertex sets \( \mathcal{G}_1 \) and \( \mathcal{G}_2 \), such that every vertex in \( \mathcal{G}_1 \) is attached to every vertex in \( \mathcal{G}_2 \), is recognized as a complete bipartite \( K_{\mathcal{G}_1, \mathcal{G}_2} \) graph. A star graph \( \mathcal{S}_n \) is a complete bipartite \( K_{1,n} \) graph. The \( n \)-hypercube graph \( Q_n \) can be defined as a graph with vertices being a set of ordered \( l \)-tuples of \( 0/1 \)s and whose vertices are joined if and only if ordered \( l \)-tuples differ in exactly one partition.

## 2. Parametric Inequalities

This section provides certain important lemmas that will be beneficial in Section 3 to derive the smallest and largest general sum-connectivity index for different graphs corresponding to their total transformations.

**Lemma 1.** Let \( n \geq 3 \) be a positive integer; then, the function defined by

\[ f(v) = 2^{n-1}v(v-1)^{\rho+1}[1 - 2^{\rho}(v+1)], \]

(4)

is a strictly decreasing and a strictly increasing function for \( \rho > -3 \) and \( \rho < -3 \), respectively.

**Proof.** However, we have

\[ f(v) = 2^{n-1}(v-1)^{\rho}[2v + \rho v - 1 - 2^{\rho}(3v^2 + \rho v^2 + \rho - 1)], \]

(5)

where the function \( g(v) \) is

\[ g(v) = 2v + \rho v - 1 - 2^{\rho}(3v^2 + \rho v^2 + \rho - 1). \]

(6)

Thus, we obtain

\[ g''(v) = -2^{\rho+1}(3 + \rho) < 0, \]

(7)

for \( \rho > -3 \), and

\[ g''(v) = -2^{\rho+1}(3 + \rho) > 0, \]

(8)

for \( \rho < -3 \). Consequently, we have \( f'(v) < 0 \) and \( f'(v) > 0 \) when \( \rho > -3 \) and \( \rho < -3 \), respectively. Therefore \( f(v) \) is a strictly decreasing function when \( \rho > -3 \) and is a strictly increasing function when \( \rho < -3 \), which finishes the proof.

**Lemma 2.** Let \( o, t \geq 2 \) be positive integers; then, the function defined by

\[ g(o, t) = t(o + t)^{\rho-1}(o + t + \rho o), \]

(9)

is a strictly increasing function for \( \rho > 0 \).

**Proof.** We obtain

\[ \frac{\partial g(o, t)}{\partial o} = pt(o + t)^{\rho-2}(o + 2t + \rho o) > 0, \]

(10)

for every \( \rho > 0 \), and

\[ \frac{\partial g(o, t)}{\partial t} = (o + t)^{\rho-2}[(1 + \rho)o^2 + \rho t^2 + (1 + \rho)ot + \rho^2 o] > 0, \]

(11)

if and only if we have \( (1 + \rho)o^2 + \rho t^2 + (1 + \rho)ot + \rho^2 o > 0 \) for \( o, t \geq 2 \) and \( \rho > 0 \). Hence, \( g(o, t) \) is a strictly increasing function when \( \rho > 0 \).

**Lemma 3.** Let \( o, t \geq 2 \) be positive integers; then, the function defined as

\[ \theta(o, t) = ot2^{\rho}(o + t)^{\rho}, \]

(12)

is a strictly increasing function for \( \rho > 0 \).

**Proof.** By taking derivative of \( \theta(o, t) \), we acquire

\[ \frac{\partial \theta(o, t)}{\partial o} = 2^{\rho}t(o + t)^{\rho-1}(o + t + \rho o) = 2^{\rho}t(o + t)^{\rho-1}\psi(o, t), \]

(13)

where \( \psi(o, t) = o + t + \rho o \). The function \( \psi(o, t) \) is increasing if and only if \( \rho > 0 \). Thus, we obtain \( (\partial \theta(o, t)/\partial o) < 0 \) and, similarly, we obtain \( (\partial \theta(o, t)/\partial t) > 0 \) when \( \rho > 0 \). Therefore, the function \( \theta(o, t) \) is strictly increasing function when \( \rho > 0 \).

**Lemma 4.** Let the function be defined by

\[ \phi(o, t) = ot(o + t)^{\rho}[1 - 2^{\rho}(o + 2)], \]

(14)

for \( o, t \geq 2 \), where \( o \) and \( t \) are the integers. Then, \( \phi(o, t) \) is a decreasing function when \( \rho > 0 \).

**Proof.** It is necessary to show that \( (\partial \phi(o, t)/\partial o) < 0 \) and \( (\partial \phi(o, t)/\partial t) < 0 \) for each \( o, t \geq 2 \). We acquire
\[
\frac{\partial \phi(o,t)}{\partial \rho} = t(o + t)^{\rho-1} (o + t + \rho o) \left[ 1 - 2^\rho (o + 2) \right] - \omega(t) o^\rho 2^\rho \\
= \omega(o,t) h(o) - \theta(o,t),
\]

where \( h(o) = 1 - 2^\rho (o + 2) \), and \( \omega(t) = o t(1 + t)^\rho 2^\rho \).

By Lemma 2, \( g(o,t) \) is a strictly increasing function when \( \rho > 0 \). Also, \( h'(o) = 1 - 2^\rho < 0 \) for each \( \rho > 0 \); therefore, \( h(o) \) is also a strictly decreasing function when \( \rho > 0 \).

From Lemma 3, \( \theta(o,t) \) is an increasing function for \( \rho > 0 \), which implies that \( (\partial \phi(o,t)/\partial \rho) < 0 \) and, similarly, we have \( (\partial \phi(o,t)/\partial t) < 0 \) where \( \rho > 0 \) and \( o,t \geq 2 \). Hence, the function \( \phi(o,t) \) is a decreasing function for \( \rho > 0 \).

**Lemma 5.** Let \( u \geq 2 \) be a positive integer; then,

\[ f_1(u) = 2^{u+1} 1^u - (u + 2) 1^u, \]

is the strictly decreasing function for \( \rho > -3 \).

**Proof.** It is easily seen that

\[ f_1'(u) = 2^{u+1} 1^u [(u \ln 2 + \rho + 1) (1 - 2^\rho (u + 2)) - 2^\rho u] \\
= 2^{u+1} 1^u g(u),
\]

where \( g(u) = (u \ln 2 + \rho + 1) (1 - 2^\rho (u + 2)) - 2^\rho u \). Then, \( g''(u) = -2^{u+1} \ln 2 < 0 \) for \( \rho > -3 \). Consequently, we obtain that \( f_1'(u) < 0 \); thus, \( f_1(u) \) is the strictly decreasing function for \( \rho > -3 \).

**Lemma 6** (see [30]). Let \( w > 0 \) be a real number. If \( \rho < 0 \) or \( \rho > 1 \), then \( (1 + w)^\rho > 1 + pw \); but for \( 0 < \rho < 1 \), \( (1 + w)^\rho < 1 + pw \).

**Lemma 7.** Let \( u \geq 4 \) be a positive integer; then, the function defined as

\[ f(u) = (u - 1) \left[ 1 - 2^{u-1} u 2^\rho - (u + 2)^\rho - (3u - 2)^\rho \right], \]

is a strictly decreasing function for \( 2 \leq \rho < 3 \).

**Proof.** From \( f(u) \), we obtain

\begin{align*}
f'(u) &= (u - 1) \left[ u^{\rho-1} [(\rho + 1) u - \rho - 2^{\rho-1} u^2 (\rho + 1) + 2^{\rho-1} u (\rho - 1)] - (u + 2)^{\rho-1} (u + 2 + \rho) \right. \\
&\quad \left. + (3u - 2)^{\rho-1} (3u - 2 + \rho) \right],
\end{align*}

(19)

Since \( u^{\rho-1} \) is strictly convex, by using Jensen’s inequality, we acquire that

\[ (3u - 2)^{\rho-1} > 4u^{\rho-1} - (u + 2)^{\rho-1}, \]

(20)

which yields that
\[ f_r(u) < (u-1)\left[ u^{r-1}\left(\rho - 1\right) - 2(\rho + 1)u^2 \right] + 2^{r-1}u(\rho - 1) - 2(2u + 2)^{r-1}(2 - u) \]
\[ = (u-1)u^{r-1}\left[ (\rho - 11)u - 5\rho + 8 - 2^{r-1}u^2 (\rho + 1) \right] + 2^{r-1}u(\rho - 1) - 2(2 - u) \left( 1 + \frac{2^{r-1}}{u} \right). \]

(21)

Since \( 1 \leq \rho - 1 < 2 \), by Lemma 6, we obtain that
\[ (1 + (2u)\rho^{r-1}) > 1 + (2(\rho - 1)u) \text{.} \]
This implies that \( f_r(u) < (u-1)u^{r-1}g(u,\rho) \), where we obtain the function
\[ g(u,\rho) = \frac{1}{u} \left[ a(\rho)u^3 + b(\rho)u^2 + c(\rho)u + d(\rho) \right]. \]

(22)

In this result, an easy routine computation yields that
\[ a(\rho) = \rho + 2\rho^{r-1}(\rho + 1) - 9 < 0, \quad \text{and} \quad d(\rho) = -8(\rho - 1) < 0 \text{.} \]
Consequently, the function \( f_r(u) \) is a strictly decreasing function for
\[ 2 \leq \rho < 3. \]

\[ \square \]

3. Main results

The present section focuses on finding the general sum-connectivity \( \chi_p \) of total graphs of path \( P_n \) and cycle \( C_n \), complete \( K_n \) graph, complete bipartite \( K_{a,b} \) graph, hypercube graph \( Q_n \), star graph \( S_n \), and unicyclic graph with a fixed pendant vertex for different values of \( \rho \).

In the next theorem, we determine the graphs having the smallest and largest general sum-connectivity (GSC) index in the case of total transformation of path \( P_n \).

**Theorem 1.** Let \( T(P_n) \) be the total graph of path \( P_n \) where \( n \geq 4 \). Then, \( P_n \) has the smallest and largest general sum-connectivity (GSC) index when \( \rho > -2 \) and \( \rho < -2 \), respectively.

**Proof.** It can be easily seen that
\[ \chi_p(P_n) - \chi_p(T(P_n)) = (n-3)4^\rho - 4n - 13)^8^\rho + 2 \cdot 3^\rho - 2 \cdot 5^\rho - 2 \cdot 6^\rho - 4 \cdot 7^\rho. \]

(23)

For \( u \geq 4 \), the function defined as \( \theta(u) = (u-3)4^\rho - (u - 13)8^\rho \) is strictly decreasing when \( \rho > -2 \). Therefore,
\[ \chi_p(P_n) - \chi_p(T(P_n)) \leq \theta(u) \leq \theta(4) \]
and
\[ \theta(4) = 4^\rho - 3 \cdot 8^\rho + 2 \cdot 3^\rho - 2 \cdot 5^\rho - 2 \cdot 6^\rho - 4 \cdot 7^\rho \]
\[ = 2(3^\rho - 5^\rho - 6^\rho) - (3 \cdot 8^\rho + 4 \cdot 7^\rho - 4^\rho) < 0. \]

(25)

This implies that \( \chi_p(P_n) < \chi_p(T(P_n)) \). Similarly, we obtain \( \chi_p(P_n) > \chi_p(T(P_n)) \) for \( \rho < -2 \), which finishes the proof.

In Theorem 2, we investigate the graphs with the smallest and largest general sum-connectivity (GSC) index in the case of total transformation of \( C_n \).

**Theorem 2.** For every \( n \geq 3 \), let \( T(C_n) \) be the total graph of cycle \( C_n \). Then, the cycle \( C_n \) has a smallest and largest general sum-connectivity (GSC) index when \( \rho > -2 \) and \( \rho < -2 \), respectively. Moreover,
\[ \chi_p(C_n) = \chi_p(T(C_n)). \]

(26)

if and only if \( \rho = -2 \).

**Proof.** We have
\[ \chi_p(C_n) - \chi_p(T(C_n)) = n \cdot 4^\rho - 4n \cdot 8^\rho. \]

(27)

For every \( u \geq 3 \), the function \( \psi(u) = (4^\rho - 4 \cdot 8^\rho)u \). Then, we acquire that \( \psi(u) = 4^\rho - 4 \cdot 8^\rho < 0 \), which shows that \( \psi(u) \) is a decreasing function. Thus,
\[ \chi_p(C_n) - \chi_p(T(C_n)) \leq \psi(u) \leq \psi(3). \]

(28)

Also, \( \psi(3) = 3 \cdot 4^\rho - 12 \cdot 8^\rho < 0 \) if and only if \( (1/2)^\rho < 4 \) which is proved for \( \rho > -2 \). Then, we obtain \( \chi_p(C_n) < \chi_p(T(C_n)) \) finally.

Moreover, it can be easily seen that \( \psi(3) = 3 \cdot 4^\rho - 12 \cdot 8^\rho > 0 \) if and only if \( (1/2)^\rho > 4 \), which is obeyed for \( \rho < -2 \). Then, we obtain in this case that \( \chi_p(C_n) > \chi_p(T(C_n)) \). For \( \rho = -2 \), we have \( \chi_p(C_n) = \chi_p(T(C_n)) \), which finishes the proof.

In the upcoming theorem, we determine graphs with the smallest and largest GSC index for the total transformation of the complete graph \( K_n \).

**Theorem 3.** For \( n \geq 3 \), let \( T(K_n) \) be the total transformation of \( K_n \). Then, \( K_n \) has the smallest and largest GSC index for \( \rho > -3 \) and \( \rho < -3 \), respectively. Moreover,
\[ \chi_p(K_n) = \chi_p(T(K_n)). \]

(29)

if and only if we have \( \rho = -3 \) and \( n = 3 \).

**Proof.** As we have
\[ \chi_p(K_n) - \chi_p(T(K_n)) = 2^{n-1}(n-1)^{\rho+1}[1 - 2^\rho(n+1)], \]

(30)

for every \( u \geq 3 \), the function \( \varphi(u) = 2^{n-1}u(n-1)^{\rho+1}[1 - 2^\rho(n+1)] \) is a decreasing function when \( \rho > -3 \) and increasing function for \( \rho < -3 \) by Lemma 1. Then, we acquire
\[ \chi_p(K_n) - \chi_p(T(K_n)) \leq \varphi(u) \leq \varphi(3). \]

(31)

For all \( \rho \), we have \( \varphi(3) = 3(4^\rho - 4 \cdot 8^\rho) < 0 \) if and only if \( (1/2)^\rho < 4 \), which is proved for \( \rho > -3 \). Then, \( \chi_p(K_n) > \chi_p(T(K_n)) \). Similarly, \( \varphi(3) = 3(4^\rho - 4 \cdot 8^\rho) > 0 \) if and only if \( (1/2)^\rho > 4 \), which is obeyed for \( \rho < -3 \). Thus, we finally obtain that \( \chi_p(K_n) > \chi_p(T(K_n)) \) with equality if and only if we have \( \rho = -3 \) and \( n = 3 \).

In the upcoming theorem, we derive graphs with the smallest GSC index for the total transformation of \( K_{a,b} \).

**Theorem 4.** For \( a, b \geq 2 \), let \( T(K_{a,b}) \) be the total transformation of \( K_{a,b} \). Then, the complete bipartite graph \( K_{a,b} \) has the
smallest GSC index for $\rho > 0$ with equality if and only if $\rho = -2$ and $a, b = 2$.

Proof. We have

$$\chi_\rho(K_{a,b}) - \chi_\rho(T(K_{a,b})) = ab(a + b)\rho(1 - 2^\rho(a + 2)).$$

(32)

Let the function $\phi(u, v) = uv(u + v)^\rho[1 - 2^\rho(u + 2)]$ for $u, v \geq 2$. By Lemma 4, we obtain that $\phi(u, v)$ is a decreasing function for $\rho > 0$. Thus, we have

$$\chi_\rho(K_{a,b}) - \chi_\rho(T(K_{a,b})) \leq \phi(x, y) \leq \phi(2, 2).$$

(33)

This is because for all $\rho$, we obtain $\phi(2, 2) = 4(4^\rho - 4 \cdot 8^\rho) < 0$ if and only if $(1/2)^\rho < 4$, which is satisfied for $\rho > 0$. Thus, we obtain that

$$\chi_\rho(K_{a,b}) < \chi_\rho(T(K_{a,b})),$$

(34)

for $x, y \geq 2$ and $\rho > 0$ with equality if and only if $\rho = -2$ and $a = b = 2$.

In the next theorem, we derive graphs with the smallest general sum-connectivity (GSC) index for the total transformation of the hypercubes $Q_n$.

Theorem 5. Let $Q_n$ be the hypercube and $T(Q_n)$ be the total transformation of the hypercube. For every $n \geq 2$ and $\rho > -3$, the hypercube $Q_n$ has the smallest general sum-connectivity (GSC) index and also

$$\chi_\rho(Q_n) = \chi_\rho(T(Q_n)), $$

(35)

if and only if $n = 2$ and $\rho = -2$.

Proof. As we know,

$$\chi_\rho(Q_n) - \chi_\rho(T(Q_n)) = 2^{n+1} - 2^{n+1}[1 - 2^{n+1}(n + 2)].$$

(36)

As the function defined by $f_1(u) = 2^{n+1} - 2^{n+1}[1 - 2^{n+1}(u + 2)]$ is the strictly decreasing function by Lemma 5, $f_1(2) = 4(4^\rho - 4 \cdot 8^\rho) < 0$ if and only if $(1/2)^\rho < 4$, where $u \geq 2$ and $\rho > -3$. Thus, we acquire

$$\chi_\rho(Q_n) - \chi_\rho(T(Q_n)) \leq f_1(u) \leq f_1(2).$$

(37)

For all $\rho$, we have $f_1(2) = 4(4^\rho - 4 \cdot 8^\rho) < 0$ if and only if $(1/2)^\rho < 4$, which is satisfied for $\rho > -3$. Therefore,

$$\chi_\rho(Q_n) < \chi_\rho(T(Q_n)),$$

(38)

with equality if and only if we have $n = 2$ and $\rho = -2$, which finishes the proof.

Next, we present graphs with the smallest GSC index for the total transformation of the star graph $S_n$.

Theorem 6. For every $n \geq 4$, let $T(S_n)$ be the total transformation of star graph $S_n$. Then, the star graph $S_n$ has the smallest GSC index where $2 \leq \rho < 3$.

Proof. We easily acquire that

$$\chi_\rho(S_n) - \chi_\rho(T(S_n)) = (n - 1)(1 - 2^{\rho - 1}n)^\rho - (n + 2)^\rho - (3n - 2)^\rho.$$ 

(39)

For every $u \geq 4$, let $f(u) = (u - 1)(1 - 2^{\rho - 1}u)^\rho - (u + 2)^\rho - (3u - 2)^\rho$. Then, by using Lemma 7, the function $f(u)$ is a strictly decreasing function. Hence,

$$\chi_\rho(S_n) - \chi_\rho(T(S_n)) \leq f(u) \leq f(4) < 0.$$ 

(40)

This is because we have $f(4) = 3 \cdot (4^\rho - 3 \cdot 6^\rho - 6 \cdot 8^\rho - 3 \cdot 10^\rho < 0$ and only if $(4^\rho + 6^\rho)/(2 \cdot 8^\rho + 10^\rho) = 1$, which is satisfied by $2 \leq \rho < 3$. This implies that the star $S_n$ has the smallest general sum-connectivity (GSC) index when $2 \leq \rho < 3$.

In the next theorem, we obtain graphs with the smallest and largest general sum-connectivity (GSC) index for the total transformation of the $U_n^1$, where $U_n^1$ is the unicyclic graph acquired by connecting a pendant vertex to a unique vertex of $C_n$.

Theorem 7. Let $T(U_n^1)$ be the total transformation of $U_n^1$. Then, for every $n \geq 3$, $U_n^1$ has the smallest and largest general sum-connectivity (GSC) index when $\rho > -2$ and $\rho < -2$, respectively.

Proof. We acquire

$$\chi_\rho(U_n^1) - \chi_\rho(T(U_n^1)) = (n - 1)4^\rho - (4n - 8)8^\rho + 2 \cdot 5^\rho - 6^\rho + 6 \cdot 9^\rho - 4 \cdot 10^\rho - 2 \cdot 11^\rho.$$ 

(41)

For every $u \geq 3$, let $f(u) = (u - 1)4^\rho - (4u - 8)8^\rho$ be a strictly decreasing function for $\rho > -2$. Then,

$$\chi_\rho(U_n^1) - \chi_\rho(T(U_n^1)) \leq f(u) \leq f(3).$$

(42)

For $\rho > -2$, we acquire

$$f(3) = 2 \cdot 4^\rho - 8 \cdot 8^\rho + 2 \cdot 5^\rho - 6^\rho - 6 \cdot 9^\rho - 4 \cdot 10^\rho - 2 \cdot 11^\rho = 2(4^\rho + 5^\rho - 11^\rho) - 2(4 \cdot 8^\rho + 3 \cdot 9^\rho + 2 \cdot 10^\rho) - 6^\rho < 0.$$ 

(43)

It follows that $\chi_\rho(U_n^1) < \chi_\rho(T(U_n^1))$. Similarly, one can also prove that

$$\chi_\rho(U_n^1) > \chi_\rho(T(U_n^1)),$$

(44)

for $\rho < -2$, which completes the proof.

4. Conclusion

In this manuscript, we focus on finding the general sum-connectivity index in case of total graphs for a path $P_n$ and cycle $C_n$, complete graph, complete bipartite graph $K_{a,b}$, hypercube graph $Q_n$, star graphs $S_n$, and unicyclic graph with a fixed pendant vertex for different values of $\rho$. It would be most appealing to compute beneficial results for the extremal general sum-connectivity index of different graphs with fixed parameters and also to work on the Mostar, edge
Mostar and weighted Mostar indices for total graphs and certain transformations of graphs.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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