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Research Article

Computation of Vertex-Based Topological Indices of Middle Graph of Alkane (C_tH_{2t+2})

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Alkanes are the primary constituents of methane or natural gas that can also be found in volcanic crust. As a result of methane as a heat source, humans may cook without using any fuel in a volcanic environment. Propane which is an alkane derivative is safer alternative to methane and is commonly present in gas cooking fuel, as well as a tiny amount of gasoline and matches. The primary ingredient in automobile especially gasoline is also alkane in the form of octane. Topological indices are largely applied in chemistry to improve the quantitative structure relationship in which the properties of the molecules can be linked with their chemical structures. In this research work, we will calculate the certain well-known topological indices of the middle graph of alkane based on vertex degree and also present a numerical and graphical comparison of computed topological indices.

1. Introduction and Preliminaries

Assume that $G = (V, E)$ is a simple and without loops molecular graph. The vertices represent the atoms of the molecule denoted by $V(G)$, while the edges $E(G)$ show chemical bonds. The edges in the graph (G) that connect to a vertex are referred as degree of vertex. A degree vertex is represented by d_u and d_v where $\{u, v \in V(G)\}$. For unspecified terminologies and notations, we recommended [1].

Chemical graph theory plays a vital role for the modeling of molecular structure, and it is also used to study chemical and physical properties of chemical compounds. Graph theory is used to assess the link between some graphs that are generated by using defined graph operations such as middle graph, double graph, and the strong double graph [2]. Topological indices offer significant information about the chemical structure, molecules, and quantitative structure-activity relationships. Topological index is numerical number or mathematical calculation that may be applied to several molecular graphs [3].

The symmetric division degree index (SD) of connected graph (G) [4] is defined as follows:

$$\mathrm{SD}(G) = \sum_{uv\in E(G)} \frac{d_u^2 + d_v^2}{d_u d_v}, \tag{1}$$

where d_u and d_v show the degree of vertex u and v in graph G.

A variant of the Randic connectivity index is sum-connectivity index [5], which is defined as follows:

$$\mathrm{SC}(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}. \tag{2}$$

Let G be molecular graph, then the Randic connectivity index [6] is defined as follows:

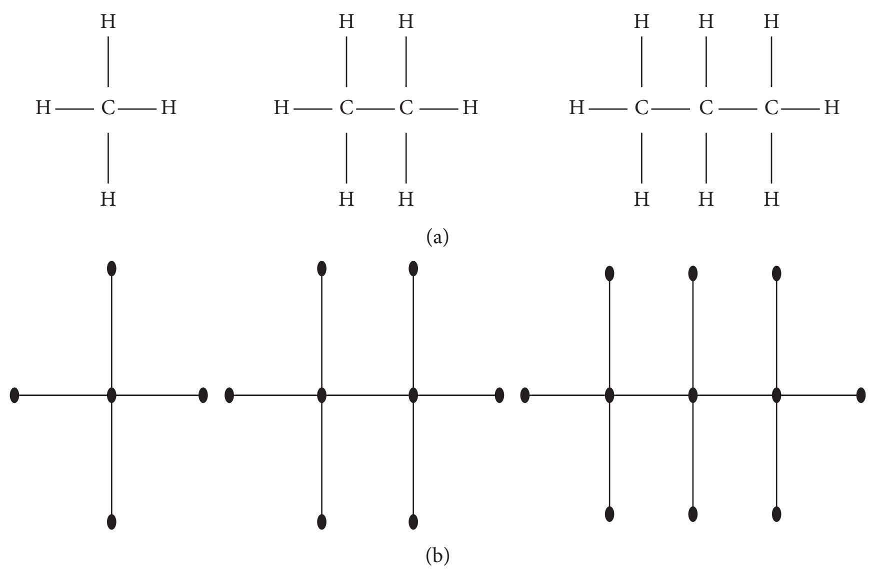

Figure 1: Alkanes (CH_4, C_2H_6, and C_3H_8).

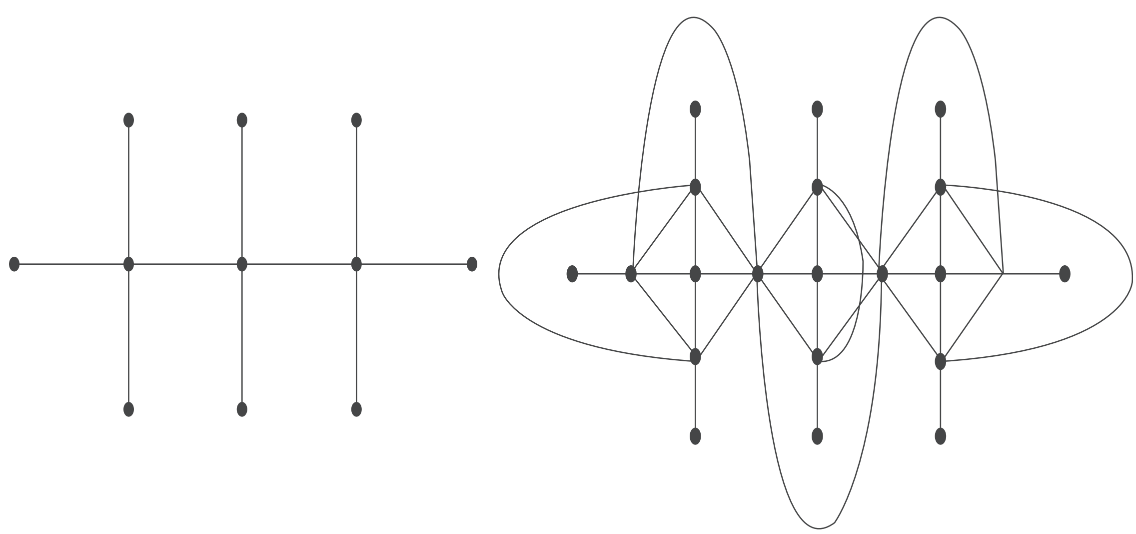

Figure 2: Alkane (C_3H_8) and its middle graph M (C_3H_8).

$$\mathrm{RC}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}. \tag{3}$$

The Harmonic index [7] is defined as follows:

$$H(G) = \sum_{uv \in E(G)} \frac{2}{(d_u + d_v)}. \tag{4}$$

The First-Zagreb index [8] is defined as follows:

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v). \tag{5}$$

The Second-Zagreb index [9] is defined as follows:

$$M_2(G) = \sum_{uv \in E(G)} (d_u d_v). \tag{6}$$

For more comprehensive discussion, we mention for the readers to read the following research articles [10–16].

Definition 1. The alkane contains carbon (C) and hydrogen (H) atoms in which all the carbon-carbon bonds are single where carbon and hydrogen are arranged in tree structure as shown in Figure 1(a) while the molecular structures are as shown in Figure 1(b). $C_tH_{(2t+2)}$ ($t \geq 1$) is chemical formula of the alkane [17]. Alkanes with 1–3 carbons do not exist in isomeric form because every formula has the same arrangement of atoms.

Definition 2. The middle graph $M[G]$ of a graph G is the graph, whose vertex set is $V[G]$ U $E[G]$, where two vertices are adjacent if and only if they are either adjacent edges of G or one is a vertex and the other is an edge incident with it

Table 1: Edge division based on the degree of end vertices of each edge.

$E[d_u, d_v]$	$E_{(1,5)}$	$E_{(5,5)}$	$E_{(4,5)}$	$E_{(4,8)}$	$E_{(5,8)}$	$E_{(8,8)}$
Number of edges	$2t+2$	$t+4$	$2t+2$	$2t-2$	$4t-2$	$t-2$

[18]. The middle graph of graph G is denoted by $M[G]$. For example, the middle graph of alkane C_3H_8 is depicted in Figure 2.

2. Degree-Based Topological Indices of Middle Graph of Alkane (C_tH_{2t+2})

Here, we determine degree-based indices for the middle graph of alkane (C_tH_{2t+2}), where $t \geq 2$. "

Theorem 1. *The symmetric division degree index of the middle graph of alkane is*

$$\mathrm{SD}[M(C_tH_{2t+2})] = \frac{182n}{5} - \frac{3}{20}. \tag{7}$$

Proof. The middle graph of alkane $M(C_tH_{2t+2})$ has $2t+2$ vertices of degree 1, 4 vertices of degree t, $2t+2$ vertices of degree 5, and $t-1$ vertices of degree 8. The edge set can be divided into different partitions of the form $E[d_u, d_v]$, where du and dv represent the degree of vertices u and v, respectively.

In $M(C_tH_{2t+2})$, we get edge of type $E_{(1,5)}$, $E_{(5,5)}$, $E_{(4,5)}$, $E_{(4,8)}$, $E_{(5,8)}$, and $E_{(8,8)}$; the edges of these types are given in Table.

Now, by using Table 1 and equation (1),

$$\mathrm{SD}(G) = \sum_{uv\in E(G)} \frac{d_u^2 + d_v^2}{d_u d_v},$$

$$\begin{aligned}
\mathrm{SD}[M(C_tH_{2t+2})] = {} & |E_{(1,5)}| \sum_{uv\in E(M(C_tH_{2t+2}))} \frac{d_u^2 + d_v^2}{d_u d_v} + |E_{(5,5)}| \sum_{uv\in E(M(C_tH_{2t+2}))} \frac{d_u^2 + d_v^2}{d_u d_v} \\
& + |E_{(4,5)}| \sum_{uv\in E(M(C_tH_{2t+2}))} \frac{d_u^2 + d_v^2}{d_u d_v} + |E_{(4,8)}| \sum_{uv\in E(M(C_tH_{2t+2}))} \frac{d_u^2 + d_v^2}{d_u d_v} \\
& + |E_{(5,8)}| \sum_{uv\in E(M(C_tH_{2t+2}))} \frac{d_u^2 + d_v^2}{d_u d_v} + |E_{(8,8)}| \sum_{uv\in E(M(C_tH_{2t+2}))} \frac{d_u^2 + d_v^2}{d_u d_v},
\end{aligned} \tag{8}$$

$$\begin{aligned}
\mathrm{SD}[M(C_tH_{2t+2})] = {} & (2t+2)\frac{25}{5} + (t+4)\frac{(5)^2 + (5)^2}{25} + (2t+2)\frac{(4)^2 + (5)^2}{20} \\
& + (2t-2)\frac{(4)^2 + (8)^2}{32} + (4t-2)\frac{(5)^2 + (8)^2}{40} + (t-2)\frac{(8)^2 + (8)^2}{20},
\end{aligned}$$

$$\mathrm{SD}[M(C_tH_{2t+2})] = 17t + 13 + \frac{41t}{10} + \frac{41}{10} + \frac{89t}{10} - \frac{89}{20} + \frac{32t}{5} - \frac{64}{5},$$

$$\mathrm{SD}[M(C_tH_{2t+2})] = \frac{182t}{5} - \frac{3}{20}.$$

□

Theorem 2. *The sum-connectivity index of middle graph of Alkane is*

$$\mathrm{SC}[M(C_tH_{2t+2})] = (2t+2)\frac{1}{\sqrt{6}} + (t+4)\frac{1}{\sqrt{10}} + (t-1)\frac{1}{\sqrt{3}} + \frac{11t}{12} + \frac{1}{6} + (2t-1)\frac{2}{\sqrt{13}}. \tag{9}$$

Proof. Now, by using Table and equation (2), we get

$$\begin{aligned}
\mathrm{SC}(G) &= \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u+d_v}},\\
\mathrm{SC}[M(\mathrm{C}_t\mathrm{H}_{2t+2})] &= |E_{(1,5)}| \sum_{uv\in E(M(\mathrm{C}_t\mathrm{H}_{2t+2}))} \frac{1}{\sqrt{d_u+d_v}} + |E_{(5,5)}| \sum_{uv\in E(M(\mathrm{C}_t\mathrm{H}_{2t+2}))} \frac{1}{\sqrt{d_u+d_v}}\\
&\quad + |E_{(4,5)}| \sum_{uv\in E(M(\mathrm{C}_t\mathrm{H}_{2t+2}))} \frac{1}{\sqrt{d_u+d_v}} + |E_{(4,8)}| \sum_{uv\in E(M(\mathrm{C}_t\mathrm{H}_{2t+2}))} \frac{1}{\sqrt{d_u+d_v}}\\
&\quad + |E_{(5,8)}| \sum_{uv\in E(M(\mathrm{C}_t\mathrm{H}_{2t+2}))} \frac{1}{\sqrt{d_u+d_v}} + |E_{(8,8)}| \sum_{uv\in E(M(\mathrm{C}_t\mathrm{H}_{2t+2}))} \frac{1}{\sqrt{d_u+d_v}},\\
\mathrm{SC}[M(\mathrm{C}_t\mathrm{H}_{2t+2})] &= (2t+2)\frac{1}{\sqrt{6}} + (t+4)\frac{1}{\sqrt{10}} + (2t+2)\frac{1}{\sqrt{9}} + (2t-2)\frac{1}{\sqrt{12}}\\
&\quad + (4t-2)\frac{1}{\sqrt{13}} + (t-2)\frac{1}{\sqrt{16}},\\
\mathrm{SC}[M(\mathrm{C}_t\mathrm{H}_{2t+2})] &= (2t+2)\frac{1}{\sqrt{6}} + (t+4)\frac{1}{\sqrt{10}} + (t-1)\frac{1}{\sqrt{3}} + \frac{11t}{12} + \frac{1}{6} + (2t-1)\frac{2}{\sqrt{13}}.
\end{aligned} \tag{10}$$

□

Theorem 3. *The Randic connectivity index of the middle graph of alkane is*

$$\begin{aligned}
\mathrm{RC}[M(\mathrm{C}_t\mathrm{H}_{2t+2})] &= \frac{3}{\sqrt{5}}(t+1) + \frac{1}{4\sqrt{2}}(2t-2)\\
&\quad + \frac{1}{\sqrt{10}}(2t-1) + \frac{13t}{40} + \frac{11}{20}.
\end{aligned} \tag{11}$$

Proof. Now, by using Table and equation (3), we get

$$\begin{aligned}
\mathrm{RC}(G) &= \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}},\\
\mathrm{RC}[M(\mathrm{C}_t\mathrm{H}_{2t+2})] &= |E_{(1,5)}| \sum_{uv\in E(M(\mathrm{C}_t\mathrm{H}_{2t+2}))} \frac{1}{\sqrt{d_u d_v}} + |E_{(5,5)}| \sum_{uv\in E(M(\mathrm{C}_t\mathrm{H}_{2t+2}))} \frac{1}{\sqrt{d_u d_v}}\\
&\quad + |E_{(4,5)}| \sum_{uv\in E(M(\mathrm{C}_t\mathrm{H}_{2t+2}))} \frac{1}{\sqrt{d_u d_v}} + |E_{(4,8)}| \sum_{uv\in E(M(\mathrm{C}_t\mathrm{H}_{2t+2}))} \frac{1}{\sqrt{d_u d_v}}\\
&\quad + |E_{(5,8)}| \sum_{uv\in E(M(\mathrm{C}_t\mathrm{H}_{2t+2}))} \frac{1}{\sqrt{d_u d_v}} + |E_{(8,8)}| \sum_{uv\in E(M(\mathrm{C}_t\mathrm{H}_{2t+2}))} \frac{1}{\sqrt{d_u d_v}},\\
\mathrm{RC}[M(\mathrm{C}_t\mathrm{H}_{2t+2})] &= (2t+2)\frac{1}{\sqrt{5}} + (t+4)\frac{1}{\sqrt{25}} + (2t+2)\frac{1}{\sqrt{20}} + (2t-2)\frac{1}{\sqrt{32}},\\
&\quad + (4t-2)\frac{1}{\sqrt{40}} + (t-2)\frac{1}{\sqrt{64}},\\
\mathrm{RC}[M(\mathrm{C}_t\mathrm{H}_{2t+2})] &= \frac{3}{\sqrt{5}}(t+1) + \frac{1}{4\sqrt{2}}(2t-2) + \frac{1}{\sqrt{10}}(2t-1) + \frac{13t}{40} + \frac{11}{20}.
\end{aligned} \tag{12}$$

□

Theorem 4. *The Harmonic index of the middle graph of alkane is*

$$H[M(C_tH_{2t+2})] = \frac{11161}{4680}t + \frac{2387}{2340}. \tag{13}$$

Proof. Now, by using Table and equation (4), we get

$$\begin{aligned}
H(G) &= \sum_{uv\in E(G)} \frac{2}{(d_u + d_v)},\\
H[M(C_tH_{2t+2})] &= |E_{(1,5)}| \sum_{uv\in E(M(C_tH_{2t+2}))} \frac{2}{(d_u + d_v)} + |E_{(5,5)}| \sum_{uv\in E(M(C_tH_{2t+2}))} \frac{2}{(d_u + d_v)}\\
&\quad + |E_{(4,5)}| \sum_{uv\in E(M(C_tH_{2t+2}))} \frac{2}{(d_u + d_v)} + |E_{(4,8)}| \sum_{uv\in E(M(C_tH_{2t+2}))} \frac{2}{(d_u + d_v)}\\
&\quad + |E_{(5,8)}| \sum_{uv\in E(M(C_tH_{2t+2}))} \frac{2}{(d_u + d_v)} + |E_{(8,8)}| \sum_{uv\in E(M(C_tH_{2t+2}))} \frac{2}{(d_u + d_v)},\\
H[M(C_tH_{2t+2})] &= (2t+2)\frac{2}{6} + (t+4)\frac{2}{10} + (2t+2)\frac{2}{9}\\
&\quad + (2t-2)\frac{2}{12} + (4t-2)\frac{2}{13} + (t-2)\frac{2}{16},\\
H[M(C_tH_{2t+2})] &= \left(\frac{2t}{3} + \frac{2}{3}\right) + \left(\frac{t}{5} + \frac{4}{5}\right) + \left(\frac{4t}{9} + \frac{4}{9}\right) + \left(\frac{t}{3} - \frac{1}{3}\right) + \left(\frac{8t}{13} - \frac{4}{13}\right) + \left(\frac{t}{8} - \frac{1}{4}\right),\\
H[M(C_tH_{2t+2})] &= \frac{11161}{4680}t + \frac{2387}{2340}.
\end{aligned} \tag{14}$$

□

Theorem 5. *The First-Zagreb index of middle graph of alkane is*

$$M_1[M(C_tH_{2t+2})] = 132t - 12. \tag{15}$$

Proof. Now, by using Table and equation (5), we get

$$\begin{aligned}
M_1(G) &= \sum_{uv\in E(G)} (d_u + d_v),\\
M_1[M(C_tH_{2t+2})] &= |E_{(1,5)}| \sum_{uv\in E(M(C_tH_{2t+2}))} (d_u + d_v) + |E_{(5,5)}| \sum_{uv\in E(M(C_tH_{2t+2}))} (d_u + d_v)\\
&\quad + |E_{(4,5)}| \sum_{uv\in E(M(C_tH_{2t+2}))} (d_u + d_v) + |E_{(4,8)}| \sum_{uv\in E(M(C_tH_{2t+2}))} (d_u + d_v)\\
&\quad + |E_{(5,8)}| \sum_{uv\in E(M(C_tH_{2t+2}))} (d_u + d_v) + |E_{(8,8)}| \sum_{uv\in E(M(C_tH_{2t+2}))} (d_u + d_v),\\
M_1[M(C_tH_{2t+2})] &= (2t+2)6 + (t+4)10 + (2t+2)9 + (2t-2)12 + (4t-2)13 + (t-2)16,\\
M_1[M(C_tH_{2t+2})] &= 12t + 12 + 10t + 40 + 18t + 18 + 24t - 24 + 52t - 26 + 16t - 32,\\
M_1[M(C_tH_{2t+2})] &= 132t - 12.
\end{aligned} \tag{16}$$

□

Theorem 6. *The Second-Zagreb index of middle graph of alkane is*

$$M_2[M(C_tH_{2t+2})] = 363t - 122. \tag{17}$$

Table 2: Numerical representation of topological indices of middle graph of alkane (C_tH_{2t+2}).

t	2	3	4	5	6	7	8
$SD[M(C_tH_{2t+2})]$	72.650	109.05	145.45	181.85	218.25	254.65	291.05
$SC[M(C_tH_{2t+2})]$	8.5884	12.324	16.061	19.796	23.533	27.269	31.005
$RC[M(C_tH_{2t+2})]$	6.5273	9.1799	11.832	14.485	17.138	19.790	22.443
$H[M(C_tH_{2t+2})]$	5.7897	8.1746	10.559	12.944	15.329	17.714	20.099
$M_1[M(C_tH_{2t+2})]$	252.00	384.00	516.00	648.00	780.00	912.00	1044.0
$M_2[M(C_tH_{2t+2})]$	604.00	967.00	1330.0	1693.0	2056.0	2419.0	2782.0

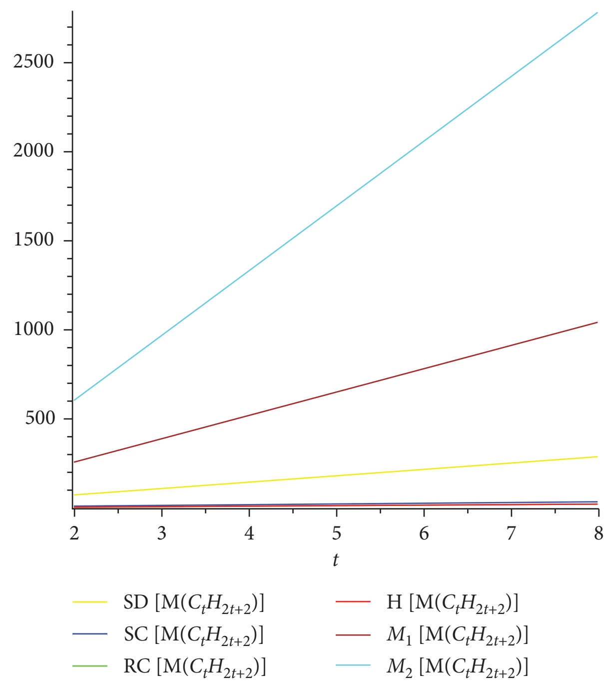

Figure 3: Graphically representation of middle graph of alkane (C_tH_{2t+2}).

Proof. Now, by using Table and equation (6), we get

$$\begin{aligned}
M_2(G) &= \sum_{uv\in E(G)} (d_u d_v),\\
M_2[M(C_tH_{2t+2})] &= |E_{(1,5)}| \sum_{uv\in E(M(C_tH_{2t+2}))} (d_u d_v) + |E_{(5,5)}| \sum_{uv\in E(M(C_tH_{2t+2}))} (d_u d_v)\\
&\quad + |E_{(4,5)}| \sum_{uv\in E(M(C_tH_{2t+2}))} (d_u d_v) + |E_{(4,8)}| \sum_{uv\in E(M(C_tH_{2t+2}))} (d_u d_v)\\
&\quad + |E_{(5,8)}| \sum_{uv\in E(M(C_tH_{2t+2}))} (d_u d_v) + |E_{(8,8)}| \sum_{uv\in E(M(C_tH_{2t+2}))} (d_u d_v),\\
M_2[M(C_tH_{2t+2})] &= (2t+2)5 + (t+4)25 + (2t+2)20\\
&\quad + (2t-2)32 + (4t-2)40 + (t-2)64\\
&= 10t + 10 + 25t + 100 + 40t + 40 + 64t - 64 + 160t - 80 + 64t - 128,\\
M_2[M(C_tH_{2t+2})] &= 363t - 122.
\end{aligned} \tag{18}$$

□

3. Comparison

Here, in Table 2 and Figure 3, we express the numerical and graphical comparison of topological indices involved symmetric division degree index (SD), sum-connectivity index (SC), Randic connectivity index (RC), First-Zagreb index (M_1), Second-Zagreb index (M_2), and Harmonic index (H) for $t = 2, 3, \ldots, 8$ of middle graph of alkane (C_tH_{2t+2}).

4. Conclusion

We have calculated the closed formulae of degree-based topological indices like as symmetric division degree index (SD), sum-connectivity index (SC), Randic connectivity index (RC), First-Zagreb index (M_1), Second-Zagreb index (M_2), and Harmonic index (H) of middle graph of alkane (C_tH_{2t+2}), where $t \geq 2$. Chemical compounds can be computed by these degree-based indices in order to identify their several properties. The comparison and geometric structure of attained results are presented numerically and graphically.

Data Availability

No data were used in this manuscript.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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