


Research Article

Ve-Degree, Ev-Degree, and Degree-Based Topological Indices of Fenofibrate

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The molecular topology of a graph is described by topological indices, which are numerical measures. In theoretical chemistry, topological indices are numerical quantities that are used to represent the molecular topology of networks. These topological indices can be used to calculate several physical and chemical properties of chemical compounds, such as boiling point, entropy, heat generation, and vaporization enthalpy. Graph theory comes in handy when looking at the link between certain topological indices of some derived graphs. In the ongoing research, we determine ve-degree, ev-degree, and degree-based (D-based) topological indices of fenofibrate's chemical structure. These topological indices are the Zagreb index, general Randić index, modified Zagreb index, and forgotten topological index. These indices are very helpful to study the characterization of the given structure.

1. Introduction

Graph theory is a mathematical subfield. It begins in 1736 with the Königsberg bridge problem when Leonhard Euler publishes his work on the seven bridges of the city Königsberg. Graph theory is widely used in the study of networks, models, circuits, routes, etc.. This theory has found significant applications in computing, chemistry, physics, electricity and civil engineering, communication science, operations research, architecture, genetics, sociology, psychology, anthropology, linguistics, and economics. It is mostly used in organic chemistry and is called chemistry graph theory. Graph theory is based on vertices and edges; in chemical graph theory, vertices represent items and edges represent bonding. In graph theory, we understand the terms of quantitative structure-property relation (QSAR) and quantitative structure-activity relation (QSPR) for structure or formula of compound.

Topological indices are numerical values associated with a chemical structure and are used to correlate a chemical structure with many properties such as chemical stability, pharmacological activity, and physical properties. They are developed from molecular topology modeling and are divided into explicit structural descriptions such as chemical quantum and hidden structural descriptors such as hydrophobicity and electrical constants. The class of fenofibrate is referred to as antilipemic agents. It increases the natural processes to remove bad cholesterol from body. It decreases the fatty substances which are bad and also helps the fatty substances which are good for human body and reduces the risk of heart disease. Cholesterol has benefits when it remains in limit level, but when it increases from its level, it becomes a danger for the heart. In cholesterol, there are three main fats, low-density lipoprotein (LDL) and triglyceride are bad when increased but high-density lipoprotein (HDL) is known as good cholesterol.

Fenofibrate is used to reduce LDL and triglyceride levels along with a low-fat diet and exercise. The main purpose of our research is to control the heart disease with the help of fenofibrate using topological index. We calculate the formula via ve-degree, ev-degree, and degree-based topological indices. In chemical graph theory, vertices represent atoms and edges represent bonding. The graph of a chemical structure is a simple undirected graph. A graph is a combination of nonempty sets \mathfrak{V} and \mathfrak{E} . The members are vertices and edges, respectively. $\delta(\mathfrak{V})$ is the degree of vertex \mathfrak{V} and is the number of edges incident to \mathfrak{V} . The set of vertices which are connected to \mathfrak{V} is open neighborhood of \mathfrak{V} , denoted by $N(\mathfrak{V})$. $N(\mathfrak{V}) + \mathfrak{V}$ are the closed neighborhoods of \mathfrak{V} . A topological index is a unique number that defines the underlying structure of the molecular graph. These topological indices are used to study the quantitative structure-property and relationships. Scientists use the numerical parameters which are obtained from chemical graph network in QSPR and QSAR. In drug designs, its applications are in. The concept of topological index was firstly introduced by Wiener, and it was distance-based topological index. Later in 1972–75, D-based Zagreb index and Randić index were introduced. Recently, Chellali et al. [4] proposed two new degree concepts in topological indices, called ve-degree and ev-degree. Math concepts are discussed in [5]. The classical degree concepts (see [6–8]) have been converted to ve-degree and ev-degree such as Zagreb index, Randić index, modified Zagreb index, inverse degree index, and forgotten index (see [9–11]). It was found that they give better prediction results than classical indices [12, 13].

1.1. Motivation. In the last two years, COVID-19 has surged dramatically in numerous nations. Many pharmacists produced a variety of medications to aid in the management of COVID-19. Fenofibrate is a substance that is found in various anti-COVID-19 medications. In laboratories, studying its physicochemical properties is highly expensive and time consuming. We work on it and derive the mathematical equation utilising topological indices that are useful to chemists in order to improve it.

2. Preliminaries

Here we give basic concepts. Consider a graph Δ with \mathfrak{V} vertex set and \mathfrak{E} edge set. The degree is the number of edges incident to vertex \mathfrak{V} , denoted as $\delta(\mathfrak{V})$. The ve-degree of vertex \mathfrak{V} is the number of edges which are incident to any vertex of close neighborhood of \mathfrak{V} , denoted by $\delta^{ve}(\mathfrak{V})$. The number of vertices in the union of closed neighborhoods of \mathfrak{V} and \mathfrak{V} is the ev-degree of edge $e = \mathfrak{V}\mathfrak{V}$, denoted by $\delta^{ev}(e)$.

The first Zagreb index [14] introduced in 1972 is defined as

$$M_1(\Delta) = \sum_{\mathfrak{V} \in \mathfrak{V}} \delta(\mathfrak{V})^2 = \sum_{\mathfrak{V}\mathfrak{V} \in \mathfrak{E}} (\delta(\mathfrak{V}) + \delta(\mathfrak{V})). \quad (1)$$

The ve-degree Zagreb beta index of graph Δ is defined as

$$M^{\beta ve}(\Delta) = \sum_{\mathfrak{V}\mathfrak{V} \in \mathfrak{E}} (\delta^{ve}(\mathfrak{V}) + \delta^{ve}(\mathfrak{V})). \quad (2)$$

The ve-degree Zagreb alpha index of Δ is defined as

$$M^{\alpha ve}(\Delta) = \sum_{\mathfrak{V} \in \mathfrak{V}} \delta^{ve}(\mathfrak{V})^2. \quad (3)$$

The ev-degree Zagreb index is defined as

$$M^{ev}(\Delta) = \sum_{e \in \mathfrak{E}} \delta^{ev}(e)^2. \quad (4)$$

The Randić index [15] is defined as

$$R(\Delta) = \sum_{\mathfrak{V}\mathfrak{V} \in \mathfrak{E}} (\delta(\mathfrak{V}) \times \delta(\mathfrak{V}))^{-(1/2)}. \quad (5)$$

The ve-degree Randić index of graph Δ is defined as

$$R^{ve}(\Delta) = \sum_{\mathfrak{V} \in \mathfrak{V}} \delta^{ve}(\mathfrak{V})^{-(1/2)}. \quad (6)$$

The ev-degree Randić index is defined as

$$R^{ev}(\Delta) = \sum_{e \in \mathfrak{E}} \delta^{ev}(e)^{-(1/2)}. \quad (7)$$

The ve-degree modified Zagreb index is defined as

$${}^m M^{ve}(\Delta) = \sum_{\mathfrak{V} \in \mathfrak{V}} \frac{1}{\delta^{ve}(\mathfrak{V})^2}. \quad (8)$$

The ev-degree modified Zagreb index of graph Δ is defined as

$${}^m M^{ev}(\Delta) = \sum_{e \in \mathfrak{E}} \frac{1}{\delta^{ev}(e)^2}. \quad (9)$$

The F index [16] is defined as

$$F(\Delta) = \sum_{\mathfrak{V} \in \mathfrak{V}} \delta(\mathfrak{V})^3 = \sum_{\mathfrak{V}\mathfrak{V} \in \mathfrak{E}} (\delta(\mathfrak{V})^2 + \delta(\mathfrak{V})^2). \quad (10)$$

The ve-degree F index is defined as

$$F_1^{ve}(\Delta) = \sum_{\mathfrak{V} \in \mathfrak{V}} \delta^{ve}(\mathfrak{V})^3. \quad (11)$$

The ev-degree F index of graph Δ is defined as

$$F_1^{ev}(\Delta) = \sum_{e \in \mathfrak{E}} \delta^{ev}(e)^3. \quad (12)$$

2.1. Applications of Topological Indices. Wiener created the idea of topology index while investigating alkane boiling points. Topological indices are used to studies the quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) to compare the topological similarities of different chemical compounds. Randić index has been closely correlated with many chemical properties, but the GA index is better than Randić connectivity index. Topological indices encode information regarding molecular size, shape, branching, and so on in numerical form, which is used for measuring topological similarity between chemical compounds and in (QSPR)/

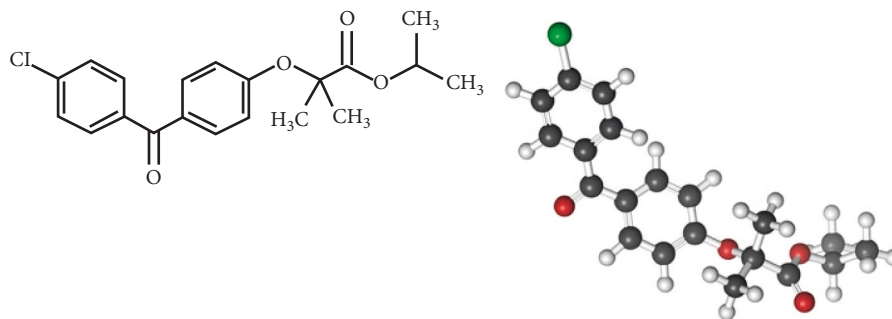


FIGURE 1: 2D and 3D structures of fenofibrate.

TABLE 1: Edge division of fenofibrate.

$(\delta(\nabla), \delta(\beth))$	(1, 3)	(1, 4)	(2, 2)	(2, 3)	(2, 4)	(3, 3)	(3, 4)
Edge partition	$\Xi_1(\Delta)$	$\Xi_2(\Delta)$	$\Xi_3(\Delta)$	$\Xi_4(\Delta)$	$\Xi_5(\Delta)$	$\Xi_6(\Delta)$	$\Xi_7(\Delta)$
Frequency	5	2	4	11	1	2	1

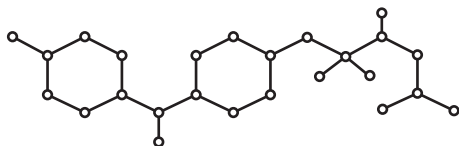


FIGURE 2: 2D and 3D structures of fenofibrate.

(QSAR) studies. Randić index has been closely correlated with many chemical properties and found to parallel the boiling point and Kovats constants. For certain physico-chemical properties, the predictive power of GA index is somewhat better than predictive power of the Randić connectivity index.

3. Methods

To calculate results, we use the vertex segment technique, edge partition technique, degree checking technique, and degree of neighbors strategy. We use Maple 16 for verification of calculations.

3.1. Fenofibrate ($C_{20}H_{21}ClO_4$) · 2D Structure. The 2D molecular graph of fenofibrate is given in Figure 1. For the computation of above given formulas for fenofibrate ($C_{20}H_{21}ClO_4$), we use a unit cell. To find topological indices, we partitioned edges. There are 5 $\nabla\eth$ edges in the first edge division, where $\delta(\nabla) = 1$ and $\delta(\beth) = 3$. There are 2 $\nabla\eth$ edges in second edge division, where $\delta(\nabla) = 1$ and $\delta(\beth) = 4$. There are 4 $\nabla\eth$ edges in the third edge division, where $\delta(\nabla) = 2$ and $\delta(\beth) = 2$. There are 11 $\nabla\eth$ edges in the fourth edge division, where $\delta(\nabla) = 2$ and $\delta(\beth) = 3$. There is 1 $\nabla\eth$ edge in the fifth edge division, where $\delta(\nabla) = 2$ and $\delta(\beth) = 4$. There are 2 $\nabla\eth$ edges in the sixth edge division, where $\delta(\nabla) = 3$ and $\delta(\beth) = 3$. There is 1 $\nabla\eth$ edge in the seventh edge division,

where $\delta(\nabla) = 3$ and $\delta(\beth) = 4$. Table 1 shows the edge partition of fenofibrate.

The molecular graph of fenofibrate is shown in Figure 2.

3.2. Proof of the Topological Indices

3.2.1. D-Based Zagreb Index. We calculate degree-based Zagreb index using Table 1.

$$\begin{aligned}
 M_1(\Delta) &= \sum_{\nabla\eth \in \Xi(\Delta)} (\delta(\nabla) + \delta(\beth)) \\
 &= 5(1 + 3) + 2(1 + 4) + 4(2 + 2) + 11(2 + 3) \\
 &\quad + (2 + 4) + 2(3 + 3) + (3 + 4) \\
 &= 126.
 \end{aligned} \tag{13}$$

3.2.2. Ev-D-Based Zagreb Index. We calculate ev-degree Zagreb index using Table 2.

$$\begin{aligned}
 M^{ev}(\Delta) &= \sum_{e \in \Xi(\Delta)} \delta_{ev}(e)^2 \\
 &= 8 \times 4^2 + 13 \times 5^2 + 3 \times 6^2 + 7^2 \\
 &= 610.
 \end{aligned} \tag{14}$$

3.2.3. Ve-Degree-Based Zagreb Index. Using Table 3, we calculate ve-degree Zagreb alpha indices.

Zagreb alpha index:

$$\begin{aligned}
 M_1^{ave}(\Delta) &= \sum_{\beth \in V(\Delta)} \delta_{ve}(\beth)^2 \\
 &= 5(3^2) + 2(4^2) + 8(5^2) + (6^2) + (7^2) \\
 &\quad + (4^2) + (5^2) + (6^2) + 4(7^2) + (7^2) \\
 &= 684.
 \end{aligned} \tag{15}$$

Zagreb beta index can be calculated by using Table 4.

TABLE 2: Ev-degree of fenofibrate.

$\{\delta(\neg), \delta(\natural)\}$	Ev-degree	Frequency
(1, 3)	4	5
(1, 4)	5	2
(2, 2)	4	4
(2, 3)	5	11
(2, 4)	6	1
(3, 3)	6	2
(3, 4)	7	1

TABLE 3: Numerical calculations of *TIs* for fenofibrate.

Topological indices	<i>D</i> -based	Ve-degree	Ev-degree
$M_1(\Delta)$	126	$M^\alpha = 684/M^\beta = 286$	610
$R_1(\Delta)$	143	791	1.22
$R_{1/2}(\Delta)$	59.897	141.029	55.064
$R_{-(1/2)}(\Delta)$	11.686	4.975	11.417
$R_{-1}(\Delta)$	5.431	0.992	5.243
${}^mM(\Delta)$	10.34	1.28	1.124
$F(\Delta)$	340	$F_1 = 3942/F = 1662$	3128

$$\begin{aligned}
 M_1^{\beta ve}(\Delta) &= \sum_{\neg \natural \in E(\Delta)} (\delta(\neg) + \delta(\natural)) \\
 &= 2(3 + 4) + (3 + 5) + 2(3 + 7) + (4 + 6) \\
 &\quad + 2(4 + 7) + 6(5 + 5) + 2(5 + 6) \\
 &\quad + 4(5 + 7) + 2(6 + 7) + 4(7 + 7) \\
 &= 286.
 \end{aligned}
 \tag{16}$$

3.2.4. *D*-Based General Randić Index. Using Table 1, we calculate *D*-based general Randić index

$$\begin{aligned}
 R_\alpha(\Delta) &= \sum_{\neg \natural \in E(\Delta)} (\delta(\neg) \times \delta(\natural))^\alpha \\
 &= 5(1 + 3)^\alpha + 2(1 + 4)^\alpha + 4(2 + 2)^\alpha + 11(2 + 3)^\alpha \\
 &\quad + (2 + 4)^\alpha + 2(3 + 3)^\alpha + (3 + 4)^\alpha.
 \end{aligned}
 \tag{17}$$

For $\alpha = 1$,

$$R_1(\Delta) = 143. \tag{18}$$

For $\alpha = (1/2)$,

$$R_{1/2}(\Delta) = 59.8972. \tag{19}$$

For $\alpha = -(1/2)$,

$$R_{-(1/2)}(\Delta) = 11.6864. \tag{20}$$

For $\alpha = -1$,

$$R_{-1}(\Delta) = 5.4306. \tag{21}$$

TABLE 4: Ve-degree of end vertex of each edge of fenofibrate.

$(\delta(\neg), \delta(\natural))$	Ve-degree	Frequency
(1, 3)	(3, 4)	2
(1, 3)	(3, 5)	1
(1, 3)	(3, 7)	2
(1, 4)	(4, 7)	2
(2, 2)	(5, 5)	4
(2, 3)	(4, 6)	1
(2, 3)	(5, 5)	2
(2, 3)	(5, 6)	2
(2, 3)	(5, 7)	4
(2, 3)	(6, 7)	2
(2, 4)	(7, 7)	1
(3, 3)	(7, 7)	2
(3, 4)	(7, 7)	1

TABLE 5: Vertex degree and corresponding frequency.

$\delta(\neg)$	Total vertex
1	7
2	10
3	7
4	1

TABLE 6: Ve-degree of fenofibrate.

$\delta(\neg)$	Ve-degree	Frequency
1	3	5
1	4	2
2	5	8
2	6	1
2	7	1
3	4	1
3	5	1
3	6	1
3	7	4
4	7	1

3.2.5. *Ev-D*-Based General Randić Index. Using Table 2, we calculate *D*-based general Randić index:

$$\begin{aligned}
 R_\alpha^{ev}(\Delta) &= \sum_{e \in E(\Delta)} \delta_{ev}(e)^\alpha \\
 &= 8 \times 4^\alpha + 13 \times 5^\alpha + 3 \times 6^\alpha + 7^\alpha.
 \end{aligned}
 \tag{22}$$

For $\alpha = 1$,

$$R_1(\Delta) = 122. \tag{23}$$

For $\alpha = (1/2)$,

$$R_{1/2}(\Delta) = 55.064. \tag{24}$$

For $\alpha = -(1/2)$,

$$R_{-(1/2)}(\Delta) = 11.417. \tag{25}$$

For $\alpha = -1$,

$$R_{-1}(\Delta) = 5.2429. \tag{26}$$

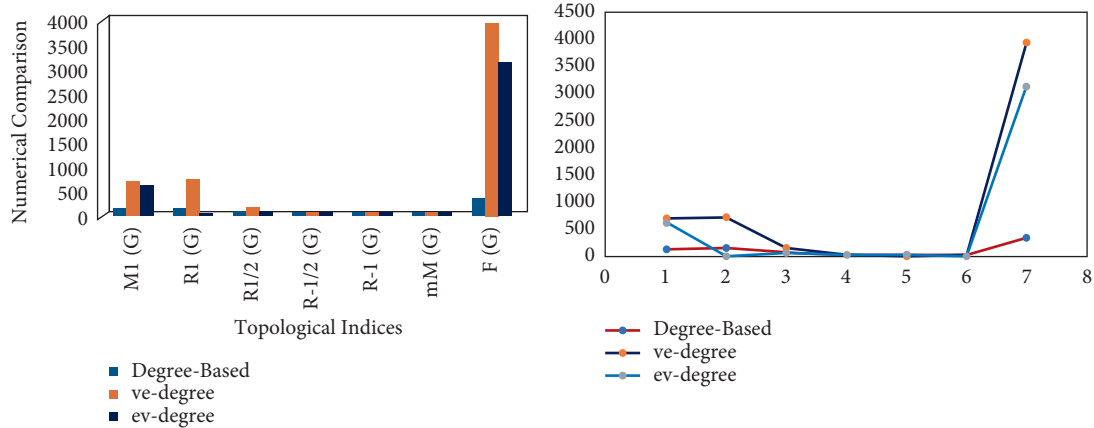


FIGURE 3: Graphical analysis of the topological indices.

3.2.6. *Ve-Degree-Based General Randić Index.* Using Table 4, we calculate ve-degree general Randić index:

$$\begin{aligned}
 R_{\alpha}^{ve}(\Delta) &= \sum_{\tau \in \Xi(\Delta)} (\delta(\tau) + \delta(\tau))^{\alpha} \\
 &= 2(3+4)^{\alpha} + (3+5)^{\alpha} + 2(3+7)^{\alpha} + (4+6)^{\alpha} \\
 &\quad + 2(4+7)^{\alpha} + 6(5+5)^{\alpha} + 2(5+6)^{\alpha} \\
 &\quad + 4(5+7)^{\alpha} + 2(6+7)^{\alpha} + 4(7+7)^{\alpha}.
 \end{aligned} \tag{27}$$

For $\alpha = 1$,

$$R_1(\Delta) = 791. \tag{28}$$

For $\alpha = (1/2)$,

$$R_{1/2}(\Delta) = 141.0286. \tag{29}$$

For $\alpha = -(1/2)$,

$$R_{-(1/2)}(\Delta) = 4.9754. \tag{30}$$

For $\alpha = -1$,

$$R_{-1}(\Delta) = 0.9919. \tag{31}$$

3.2.7. *D-Based Modified Zagreb Index.* Using Table 5, we calculate D-based modified Zagreb index

$$\begin{aligned}
 {}^mM(\Delta) &= \sum_{\tau \in V(\Delta)} \frac{1}{\delta(\tau)^2} \\
 &= 7 + \frac{10}{2^2} + \frac{7}{3^2} + \frac{1}{4^2} \\
 &= 10.34.
 \end{aligned} \tag{32}$$

3.2.8. *Ev-D-Based Modified Zagreb Index.* Using Table 2, we calculate ev-degree modified Zagreb index:

$$\begin{aligned}
 {}^mM^{ev}(\Delta) &= \sum_{e \in \Xi(\Delta)} \frac{1}{\delta_{ev}(e)^2} \\
 &= 8 \times \frac{1}{4^2} + 13 \times \frac{1}{5^2} + 3 \times \frac{1}{6^2} + \frac{1}{7^2} \\
 &= 1.1237.
 \end{aligned} \tag{33}$$

3.2.9. *Ve-Degree-Based Modified Zagreb Index.* Using Table 4, we calculate ve-degree modified Zagreb index

$$\begin{aligned}
 {}^mM^{ve}(\Delta) &= \sum_{\tau \in V(\Delta)} \frac{1}{\delta_{ve}(\tau)^2} \\
 &= \frac{5}{3^2} + \frac{2}{4^2} + \frac{8}{5^2} + \frac{1}{6^2} + \frac{1}{7^2} + \frac{1}{4^2} + \frac{1}{5^2} + \frac{1}{6^2} + \frac{4}{7^2} + \frac{1}{7^2} \\
 &= 1.28.
 \end{aligned} \tag{34}$$

3.2.10. *D-Based F Index.* Using Table 5, we calculate D-based F index

$$\begin{aligned}
 F(\Delta) &= \sum_{\tau \in V(\Delta)} \delta(\tau)^3 \\
 &= 7 + 10(2^3) + 7(3^3) + 4^3 \\
 &= 340.
 \end{aligned} \tag{35}$$

3.2.11. *Ev-D-Based F Index.* Using Table 2, we calculate ev-degree F index

$$\begin{aligned}
 F_1^{ev}(\Delta) &= \sum_{e \in \Xi(\Delta)} \delta_{ev}(e)^3 \\
 &= 8 \times 4^3 + 13 \times 5^3 + 3 \times 6^3 + 7^3 \\
 &= 3128.
 \end{aligned} \tag{36}$$

3.2.12. *Ve-Degree-Based F Index.* Using Table 6, we calculate ve-degree F index

$$\begin{aligned} F_1^{ve}(\Delta) &= \sum_{\lambda \in V(\Delta)} \delta_{ve}(\lambda)^3 \\ &= 5(3^3) + 2(4^3) + 8(5^3) + 6^3 + 7^3 + 4^3 \\ &\quad + 5^3 + 6^3 + 4(7^3) + 7^3 \\ &= 3942. \end{aligned} \quad (37)$$

In Figure 3, all the derived indices are shown in the graphical ways. The different behaviors of the indices can be seen in the figure. In table 3 results of these TIs are given.

4. Conclusion

Topological descriptors have an important role in the study of QSPR/QSAR and predict the properties of chemical compounds. Fenofibrate is a drug that is used in conjunction with a healthy diet to lower cholesterol and triglyceride (fat-like substance) levels in the blood. This could help prevent pancreatitis (inflammation or swelling of the pancreas) caused by excessive triglyceride levels in the blood. In this study, we compute D -based first Zagreb index, ve-degree Zagreb α index, Zagreb β index, ev-degree Zagreb index, Randić index, ve-degree Randić index, ev-degree Randić index, modified Zagreb index, ve-degree modified Zagreb index, ev-degree modified Zagreb index, F index, ve-degree F index, and ev-degree F index for fenofibrate. With the help of these, we can study the physicochemical properties of the fenofibrate. Chemical compound testing in a lab is very expensive and time-consuming, whereas TIs are simple to obtain. The production of the drug fenofibrate can be obtained in very low cost, which can be frequently used everywhere. Future work may be done to investigate TI for other drugs.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors' Contributions

Each author made an equal contribution. The manuscript has been read by all authors, and they have all agreed that it should be published.

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