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Research Article

Novel Degree-Based Topological Descriptors of Fenofibrate Using M-Polynomial

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Chemical graph theory is currently expanding the use of topological indices to numerically encode chemical structure. The prediction of the characteristics provided by the chemical structure of the molecule is a key feature of these topological indices. The concepts from graph theory are presented in a brief discussion of one of its many applications to chemistry, namely, the use of topological indices in quantitative structure-activity relationship (QSAR) studies and quantitative structure-property relationship (QSPR) studies. This study uses the M-polynomial approach, a newly discovered technique, to determine the topological indices of the medication fenofibrate. With the use of degree-based topological indices, we additionally construct a few novel degree based topological descriptors of fenofibrate structure using M-polynomial. When using M-polynomials in place of degree-based indices, the computation of the topological indices can be completed relatively quickly. The topological indices are also plotted. Using M-polynomial, we compute novel formulas for the modified first Zagreb index, modified second Zagreb index, first and second hyper Zagreb indices, SK index, SK_1 index, SK_2 index, modified Albertson index, redefined first Zagreb index, and degree-based topological indices.

1. Introduction

The study of graphs, which are mathematical constructions used to represent pairwise relationships between things, is known as graph theory in mathematics. Vertices (also known as nodes or points) make up a graph in this sense, which are connected by edges (also called links or lines). The shortest route in a network or on a road can be found using graph theory. The shortest path between two nodes is determined using graph theory in Google Maps, where various locations are represented as vertices or nodes and the highways are represented as edges. Molecules are theoretically modelled using graph theory to reveal the physical characteristics of these chemical substances. Some physical characteristics, such as boiling point, are connected to the compound's geometric structure. A chemical or molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory. A chemical graph is a graph with vertices and edges that represent the atoms of the compound and its chemical bonds, respectively. A topological index is an indicator of the topology of a graph is a topological index. This is an important attribute for analyzing the physicochemical properties of compound structures. We use fenofibrate to study the topological index via M-polynomial. Fenofibrate is used along with a proper diet to help lower "bad" cholesterol and fats and raise "good"

cholesterol in the blood. In the last two years, COVID-19 has surged dramatically in numerous nations. Many pharmacists have 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 utilizing topological indices that are useful to chemists in order to improve it. We derive the M-polynomials, which are a highly rapid way to determine topological indices, for the investigation of its many physicochemical characteristics [1, 2]. Fenofibrate is a fabric acid derivative indicated for use in treatment of primary hypercholesterolemia and mixed dyslipidemia.

A sizable number of people have died as a result of the severe acute respiratory syndrome corona virus-2 (SARS-CoV-2) pandemic, which has also disrupted society globally. We created a screen to monitor the dimidiation of the angiotensin-converting enzyme 2 (ACE2), the main receptor for the virus, in order to find medications that could be repurposed to treat SARS-CoV-2 infections. The active metabolite of fenofibrate, fenofibric acid, was discovered by this screening. In addition, fenofibric acid reduced the ability of the viral spike protein's receptor-binding domain (RBD) to bind to ACE2 in ELISA and whole cell-binding experiments. Two distinct SARS-CoV-2 isolates were used to examine the effects of fenofibrate and fenofibric acid on the infection of cultivated Vero cells. Chemicals like fenofibrate are used by chemists to develop different medicines [3]. It takes too long and is too pricey. Now, in order to save time and money, we study it with the aid of graph theory. The fenofibrate polymer's mathematical form is driven by M-polynomial form. Drugs containing fenofibrate may be more effective in treating existing problems like COVID-19 and preventing high cholesterol levels [4, 5].

1.1. Motivation. The COVID-19 pandemic, which was brought on by the SARS-CoV-2 virus, began in December 2019 when a severe pneumonia-like illness first appeared in Wuhan, China. Numerous therapy regimens are being recommended to help address this issue because of the increase in infectivity and mortality brought on by the virus. The SARS-CoV2 virus's capacity to connect to the ACE II receptors on host cells via its viral spike protein (S protein) and cause entry into the target cell is what gives it its infectious properties. Fenofibrate's actions on ACE II receptors as well as how its medicinal characteristics can aid COVID-19 patients by preventing viral entry and ultimately reducing severity. The risk-to-benefit analysis shows that this medication is advantageous for patients with severe SARS-CoV2 infection since it has a favourable profile and is generally safe to use. We use this chemical structure to aid chemists in their research into the chemical properties of fenofibrate.

1.2. The Goal of the Study and the Task Involved. The purpose of this research is to help out the chemist with the study of the physicochemical properties of fenofibrate that are used in medication. Experimental expenses are too high to have an effect on the cost of the medicine. So, the cost of medicine can be controlled with the help of mathematical chemistry. It is much more expensive and time-consuming for a chemist to conduct experiments in the lab to study the properties of the chemical, while a mathematician can do this study by the structure of the chemical, which has no cost and makes it much easier to find the properties with less time. The medication is taken orally, costs less, and is readily available throughout the world. It can be especially helpful for low- and middle-income countries (LMIC). Vaccination campaigns have helped to stop the spread of COVID-19, but not everyone has access to the vaccine, and adoption rates are not uniform.

Some consequential endowments of the current study are as follows:

(1) First, introduce a concept of fenofibrate

(2) Also explore the fundamental uses of fenofibrate

(3) To develop the study fenofibrate, we find Novel degree based topological indices y the help of M-polynomial that are very easy to find the mathematical equations that are used to study the physicochemical properties

(4) At the end, we compared all topological indices with the help of graph

The remainder of this article is structured as follows. Section 2 briefly reviewed the literature of the graph theory and topological indices. Applications of the topological indices are described in Section 3. Our purposed research and some proofs are presented in Section 4. Section 5 presents a graphical comparison analysis. Section 6 concludes this study.

2. Literature Review

The M-polynomial [6, 7] of G is illustrate as follows:

$$M(G; x, y) = \sum_{\delta \le i \le j \le \Delta} m_{ij}(G) x^i y^j, \tag{1}$$

where $\delta = \mathrm{Min}\{\eth_\Phi : \Phi \in V(G)\}$, $\Delta = \mathrm{Max}\{\eth_\Psi : \Psi \in V(G)\}$, and $m_{ij}(G)$ is the edge $\Phi\Psi \in E(G)$ for which $\{\eth_\Psi, \eth_\Phi\} = \{i, j\}$.

The Zagreb indices [8] are one of the oldest degree-based topological descriptors. They were conceived in 1972. First Zagreb index [8] is illustrated as follows:

$$M_1 = \sum_{\Phi\Psi \in E(G)} [\eth_\Phi + \eth_\Psi]. \tag{2}$$

Modified First Zagreb index [9] is illustrated as follows:

$$M_1^* = \sum_{\Psi \in E(G)} (\eth_\Psi)^2. \tag{3}$$

Second Zagreb index [8] is illustrated as follows:

$$M_2 = \sum_{\Phi\Psi \in E(G)} (\eth_\Phi \cdot \eth_\Psi). \tag{4}$$

Modified second Zagreb index [8, 10] is illustrated as follows:

$$M_1^* = \sum_{\Psi \in E(G)} (\eth_\Psi)^2. \tag{5}$$

Fath Taber [11], in 2011, introduced new graph invariant, third Zagreb index, which is illustrated as follows:

$$M_2 = \sum_{\Phi\Psi \in E(G)} |\eth_\Phi - \eth_\Psi|. \tag{6}$$

The first and second hyper Zagreb indices were introduced several years ago [12]. Also, studied by many researchers as [13, 14]. They are illustrated as follows:

$$\begin{aligned} HM_1 &= \sum_{\Phi\Psi \in E(G)} (\eth_\Phi + \eth_\Psi)^2, \\ HM_2 &= \sum_{\Phi\Psi \in E(G)} (\eth_\Phi . \eth_\Psi)^2. \end{aligned} \tag{7}$$

SK index [15] is illustrated as follows:

$$SK(G) = \sum_{\Phi\Psi \in E(G)} \frac{\eth_\Phi + \eth_\Psi}{2}. \tag{8}$$

SK_1 index [15, 16] is defined as follows:

$$SK_1(G) = \sum_{\Phi,\Psi \in E(G)} \frac{\eth_\Phi . \eth_\Psi}{2}. \tag{9}$$

SK_2 index [15] is illustrated as follows:

$$SK_2(G) = \sum_{\Phi\Psi \in E(G)} \left(\frac{\eth_\Phi + \eth_\Psi}{2}\right)^2. \tag{10}$$

The redefined first Zagreb index [17] of graph G is illustrated as follows:

$$RZG_1(G) = \sum_{\Phi\Psi \in E(G)} \frac{\eth_\Phi + \eth_\Psi}{\eth_\Phi . \eth_\Psi}. \tag{11}$$

The modified Albertson index [18] of graph G is illustrated as follows:

$$mA(G) = \sum_{\Phi\Psi \in E(G)} (\eth_\Phi)^2 + (\eth_\Psi)^2. \tag{12}$$

3. Applications of Topological Indices

Using the first Zagreb index, Gutman and Trinajstic looked at the association between the total *pi*-electron energy and the structure of a molecule. The second Zagreb index was created by Gutman et al. when they expanded on their research and created another TI for molecular structures. Following that, numerous lengthy publications on these invariants have been published. This TI was reevaluated by Ali and Trinajstic, who gave it the new name modified first Zagreb connection index (ZCI). They added that it had more accurate correlation coefficient values for the different octane isomers. The first, second, and modified first (ZCI) of the S-sum graphs were calculated by Tang et al. When researching the boiling point of paraffin, Harry Wiener created the Wiener index, which was the first TI. Trinajstic and Gutman discovered a formula for the total energy of electrons in molecules in 1972, and it appeared as the sum of the squares of the valences at the molecular structure's vertices. Today, this amount is referred to as the first Zagreb index. The general first Zagreb index, along with the second, third, modified first, hyper Zagreb, SK_1, SK_2, and modified Albertson index are all aspects of the first Zagreb index that are discussed in this study.

4. Research Methods and Proof

In this section, first, we construct Table 1 for M-polynomials of the topological indices using the graph of fenofibrate as shown in Figure 1. After that, we define the formulas for calculation of the indices. Then, we apply the all described formulas for check the physicochemical properties of the fenofibrate that give us the numeric equations. Derivations of some topological indices from M-polynomial are stated as follows:

$$\begin{aligned} D_x M(x,y) &= x\frac{\partial}{\partial x} M(x,y), \\ D_y M(x,y) &= y\frac{\partial}{\partial y} M(x,y), \\ S_x M(x,y) &= \int \frac{M(x,y)}{x} dx, \\ S_y M(x,y) &= \int \frac{M(x,y)}{y} dy, \\ JM(x,y) &= f(x,x), \\ Q_\alpha M(x,y) &= x^\alpha M(x,y), \\ L_x M(x,y) &= f\left(x^2, y\right), \\ L_y M(x,y) &= f\left(x, y^2\right), \end{aligned} \tag{13}$$

$$D_x^{(1/2)} M(x,y) = \sqrt{x\frac{\partial M(x,y)}{\partial x}}.\sqrt{M(x,y)},$$

$$D_y^{(1/2)} M(x,y) = \sqrt{y\frac{\partial M(x,y)}{\partial y}}.\sqrt{M(x,y)},$$

$$S_x^{(1/2)} M(x,y) = \sqrt{\int \frac{M(x,y)}{x} dx}.\sqrt{M(x,y)},$$

$$S_y^{(1/2)} M(x,y) = \sqrt{\int \frac{M(x,y)}{y} dy}.\sqrt{M(x,y)}.$$

Theorem 1. *Let "G" be the graph, then "first Zagreb index" is*

$$mM_1(G) = 142n - 16. \tag{14}$$

Table 1: Derivation of some topological indices from M-polynomial.

Topological indexes	Derivative from $M(G;x,y)$
First Zagreb	$(D_x + D_y)M(G;x,y)\|_{x=y=1}$
Second Zagreb	$(D_xD_y)M(G;x,y)\|_{x=y=1}$
3rd Zagreb index	$(D_y - D_x)M(G;x,y)\|_{x=y=1}$
Modified first Zagreb index	$D_y^2M(G;x,y)\|_{x=y=1}$
Hyper 2nd Zagreb index	$D_x^2D_y^2M(G;x,y)\|_{x=y=1}$
SK index	$1/2D_xJM(G;x,y)\|_{x=y=1}$
SK_1 index	$(D_xD_y/2)M(G;x,y)\|_{x=y=1}$
SK_2 index	$((D_x^2/4) + (D_y^2/4) + (D_xD_y/2))M(G;x,y)\|_{x=y=1}$
Hyper 1st Zagreb index	$(D_y^2 + D_x^2 + 2D_xD_y)M(G;x,y)\|_{x=y=1}$
Redefined 1st Zagreb index	$(S_x + S_y)M(G;x,y)\|_{x=y=1}$
Modified Albertson index	$(D_y^2 - D_x^2)M(G;x,y)\|_{x=y=1}$

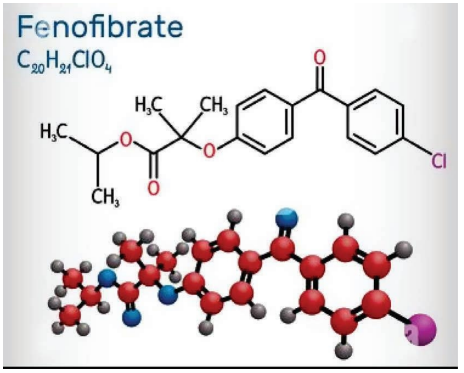

Figure 1: Fenofibrate chemical structure.

Proof

$$\begin{aligned} M(G;x,y) &= (3n+2)xy^3 + 2nxy^4 + (3n+1)x^2y^2 + (13n-2)x^2y^3 + nx^2y^4 \\ &\quad + (5n-3)x^3y^3 + nx^3y^4, \\ (D_x + D_y)M(G;x,y) &= (12n+8)xy^3 + 10nxy^4 + (12n+4)x^2y^2 + (65n-10)x^2y^3 \\ &\quad + 6nx^2y^4 + (30n-18)x^3y^3 + 7nx^3y^4, \\ (D_y + D_x)M(G;x,y)|_{x=y=1} &= 142n - 16. \end{aligned} \tag{15}$$

The first Zagreb index is plotted in 2D and 3D in Figure 2, which reveals how it depends on the relevant parameters. The graph's behavior in the xy-plane vertically upward changed when we increased the value of n. □

Theorem 2. *Let "G" be the graph, then the "second Zagreb index" is*

$$mM_2(G) = 172n - 29. \tag{16}$$

Proof

$$\begin{aligned} M(G;x,y) &= (3n+2)xy^3 + 2nxy^4 + (3n+1)x^2y^2 + (13n-2)x^2y^3 + nx^2y^4 + (5n-3)x^3y^3 + nx^3y^4, \\ (D_yD_x)M(G;x,y) &= (9n+6)xy^3 + 8nxy^4 + (12n+4)x^2y^2 + (78n-12)x^2y^3 + 8nx^2y^4 \\ &\quad + (45n-27)x^3y^3 + 12nx^3y^4, \\ (D_yD_xM(G;x,y))|_{x=y=1} &= 172n - 29. \end{aligned} \tag{17}$$

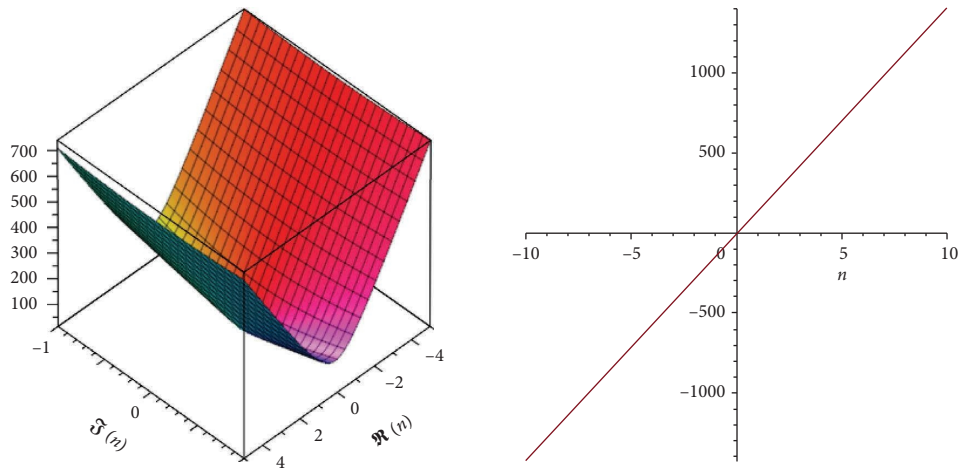

Figure 2: 2-D and 3-D structure of first Zagreb index.

The second Zagreb index is plotted in 2D and 3D in the accompanying Figure 3, which reveals how it depends on the relevant parameters. The graph's behavior in the xy-plane vertically upward changed when we increased the value of n. □

Theorem 3. *Let "G" be the graph, then the "3rd Zagreb index" is*

$$mM_3(G) = 28n + 2. \tag{18}$$

Proof

$$\begin{aligned} M(G;x,y) &= (3n+2)xy^3 + 2nxy^4 + (3n+1)x^2y^2 + (13n-2)x^2y^3 + nx^2y^4 \\ &\quad + (5n-3)x^3y^3 + nx^3y^4, \\ \left(D_y - D_x\right)M(G;x,y) &= 2(3n+2)xy^3 + 3.2nxy^4 + 0.(3n+1)x^2y^2 + (13n-2)x^2y^3 + 2nx^2y^4 \\ &\quad + 0.(5n-3)x^3y^3 + nx^3y^4, \\ \left(D_y - D_x\right)M(G;x,y)|_{x=y=1} &= 28n + 2. \end{aligned} \tag{19}$$

The third Zagreb index is plotted in 2D and 3D in Figure 4, which reveals how it depends on the relevant parameters. The graph's behavior in the xy-plane vertically upward changed when we increased the value of n. □

$$mMM_1(G) = 265n - 23. \tag{20}$$

Proof

Theorem 4. *Let "G" be the graph, then the "modified first Zagreb index" is*

$$\begin{aligned} M(G;x,y) &= (3n+2)xy^3 + 2nxy^4 + (3n+1)x^2y^2 + (13n-2)x^2y^3 + nx^2y^4 \\ &\quad + (5n-3)x^3y^3 + nx^3y^4, \\ D_y^2M(G;x,y) &= 9(3n+2)xy^3 + 16.2nxy^4 + 4(3n+1)x^2y^2 + 9(13n-2)x^2y^3 + 16nx^2y^4 \\ &\quad + 9(5n-3)x^3y^3 + 16nx^3y^4, \\ D_y^2M(G;x,y)|_{x=y=1} &= 265n - 23. \end{aligned} \tag{21}$$

The modified first Zagreb index is plotted in 2D and 3D in Figure 5, which reveals how it depends on the relevant parameters. The graph's behavior in the xy-plane vertically upward changed when we increased the value of n. □

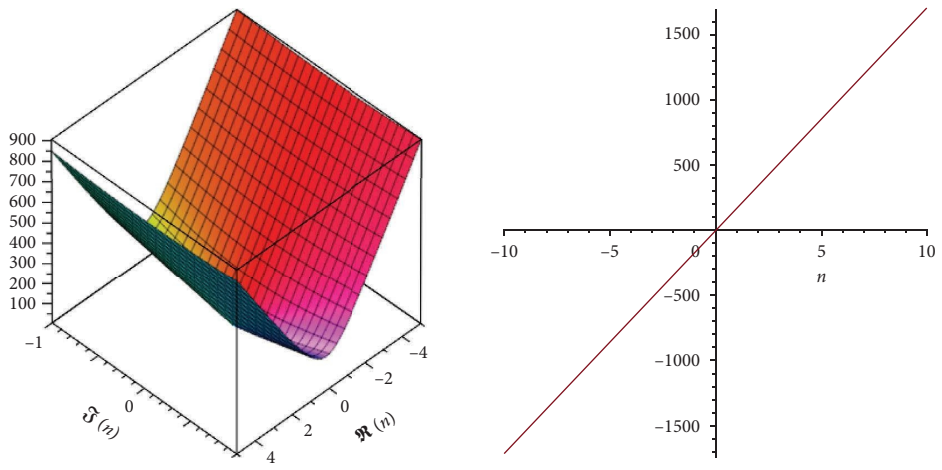

Figure 3: 2-D and 3-D structure of second Zagreb index.

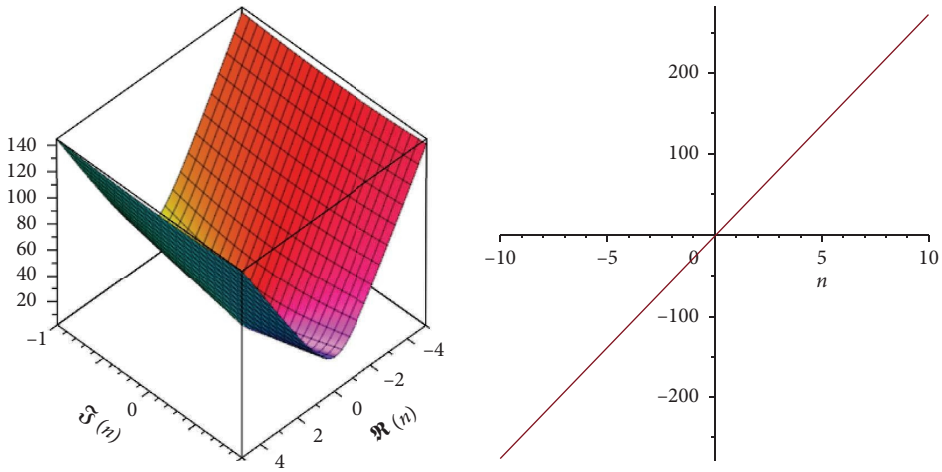

Figure 4: 2-D and 3-D structure of third Zagreb index.

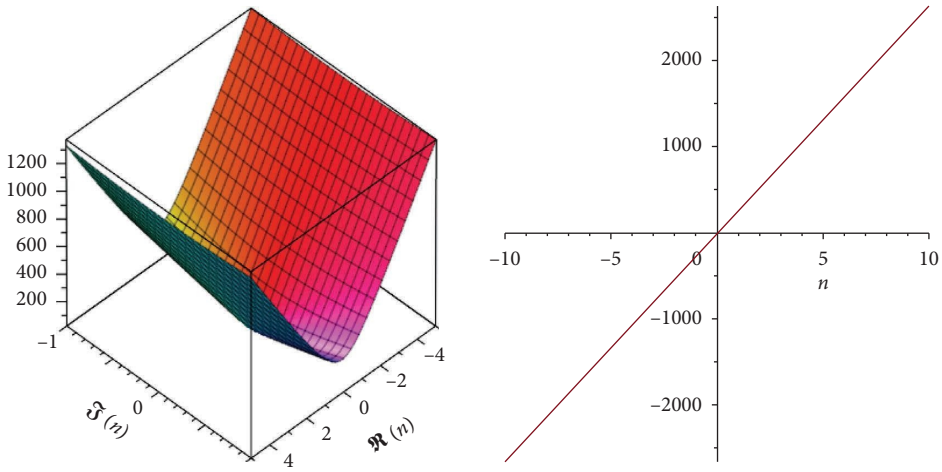

Figure 5: 2-D and 3-D structure of modified first Zagreb index.

Theorem 5. *Let "G" be the graph, then the "hyper 2nd Zagreb index" is*

$$mHM_2(G) = 1188n - 281. \tag{22}$$

Proof

$$\begin{aligned} M(G;x,y) &= (3n+2)xy^3 + 2nxy^4 + (3n+1)x^2y^2 + (13n-2)x^2y^3 + nx^2y^4 + (5n-3)x^3y^3 \\ &\quad + nx^3y^4, \\ D_x^2D_y^2M(G;x,y) &= 9(3n+2)xy^3 + 16.2nxy^4 + 16(3n+1)x^2y^2 + 36(13n-2)x^2y^3 + 64nx^2y^4 \\ &\quad + 81(5n-3)x^3y^3 + 144nx^3y^4, \\ D_x^2D_y^2M(G;x,y)|_{x=y=1} &= 1188n - 281. \end{aligned} \tag{23}$$

The modified hyper second Zagreb index is plotted in 2D and 3D in Figure 6, which reveals how it depends on the relevant parameters. The graph's behavior in the *xy*-plane vertically upward changed when we increased the value of *n*. □

Theorem 6. *Let "G" be the graph, then the "SK" index is*

$$mSK(G) = 71n - 8. \tag{24}$$

Proof

$$\begin{aligned} M(G;x,y) &= (3n+2)xy^3 + 2nxy^4 + (3n+1)x^2y^2 + (13n-2)x^2y^3 + nx^2y^4 \\ &\quad + (5n-3)x^3y^3 + nx^3y^4, \\ \frac{1}{2}D_xJM(G;x,y) &= 2.(3n+2)x^4 + 5nx^5 + 2(3n+1)x^4 + \frac{5}{2}(13n-2)x^5 + 3nx^6 \\ &\quad + 3(5n-3)x^6 + \frac{7}{2}nx^7, \\ \frac{1}{2}D_xJM(G;x,y)|_{x=1} &= 71n - 8. \end{aligned} \tag{25}$$

The SK index is plotted in 2D and 3D in Figure 7, which reveals how it depends on the relevant parameters. The graph's behavior in the *xy*-plane vertically upward changed when we increased the value of *n*. □

Theorem 7. *Let "G" be the graph, then the "SK_1 index" is*

$$mSK_1(G) = 86n - 14.5. \tag{26}$$

Proof

$$\begin{aligned} M(G;x,y) &= (3n+2)xy^3 + 2nxy^4 + (3n+1)x^2y^2 + (13n-2)x^2y^3 + nx^2y^4 \\ &\quad + (5n-3)x^3y^3 + nx^3y^4, \\ \frac{D_xD_y}{2}M(G;x,y) &= \frac{3}{2}(3n+2) + \frac{4}{2}.2n + \frac{4}{2}(3n+1) + \frac{6}{2}(13n-2) + \frac{8}{2}n + \frac{9}{2}(5n-3) + \frac{12}{2}n, \\ \frac{D_xD_y}{2}M(G;x,y)|_{x=y=1} &= M(G) = 86n - 14.5. \end{aligned} \tag{27}$$

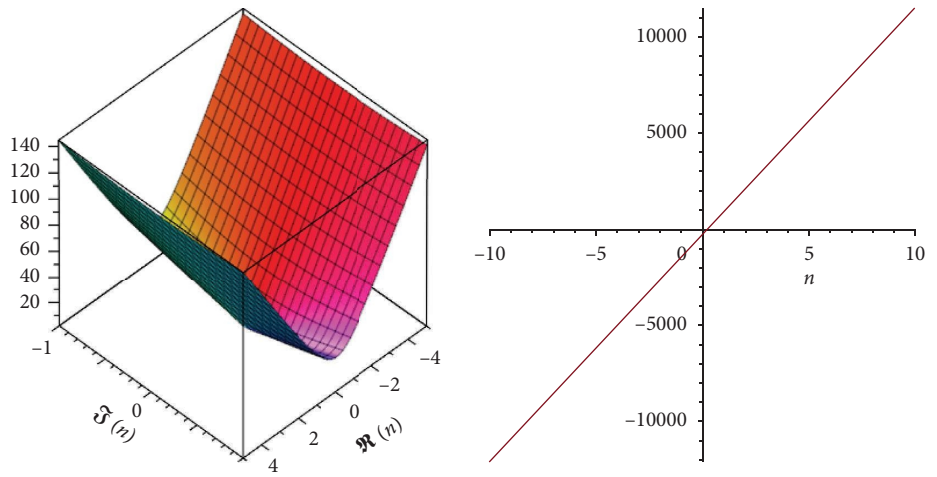

Figure 6: 2-D and 3-D structure of modified hyper second Zagreb index.

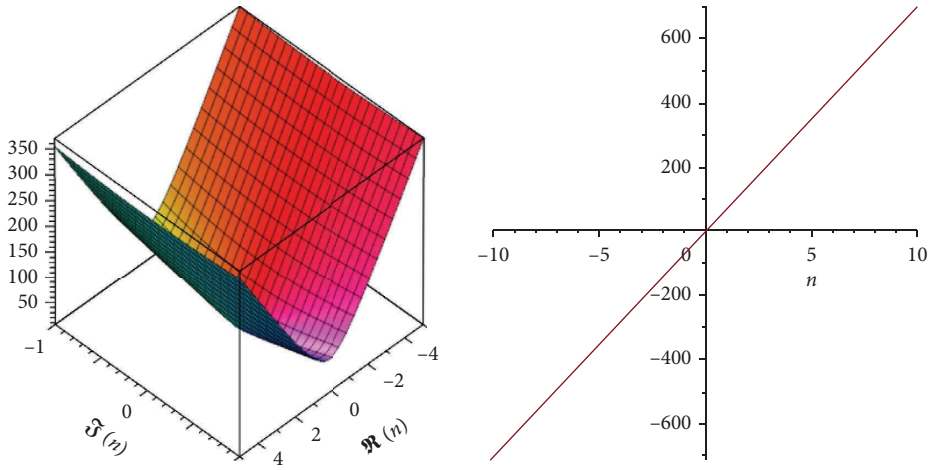

Figure 7: 2-D and 3-D structure of SK index.

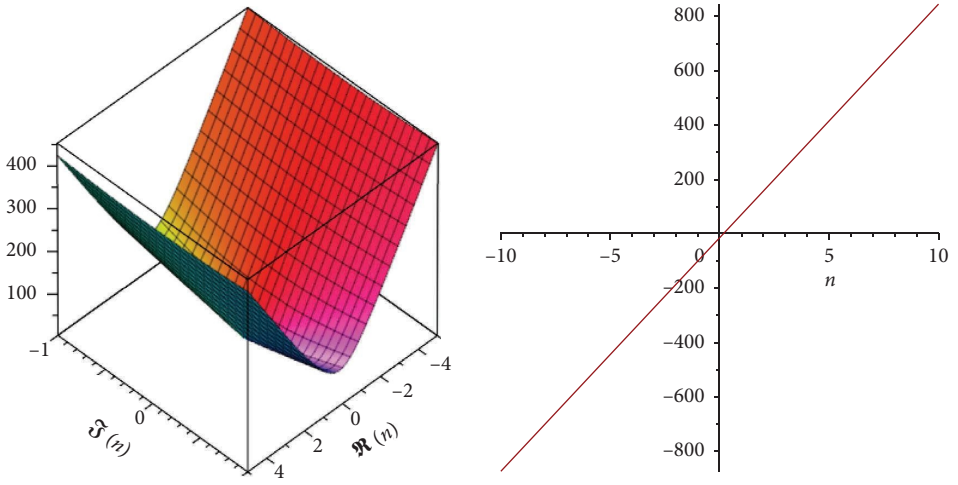

Figure 8: 2-D and 3-D structure of SK_1 index.

The SK_1 index is plotted in 2D and 3D in Figure 8, which reveals how it depends on the relevant parameters. The graph's behavior in the xy-plane vertically upward changed when we increased the value of n. □

Theorem 8. *Let "G" be the graph, then the "SK_2 index" is*

$$mSK_2(G) = 184n - 27.5. \tag{28}$$

Proof

$$\begin{aligned}
M(G;x,y) &= (3n+2)xy^3 + 2nxy^4 + (3n+1)x^2y^2 + (13n-2)x^2y^3 + nx^2y^4 \\
&\quad + (5n-3)x^3y^3 + nx^3y^4, \\
\frac{D_x^2}{4}M(G;x,y) &= \frac{(3n+2)}{4}xy^3 + \frac{n}{2}xy^4 + (3n+1)x^2y^2 + (13n-2)x^2y^3 \\
&\quad + nx^2y^4 + \frac{9(5n-3)}{4}x^3y^3 + \frac{9n}{4}x^3y^4, \\
\frac{D_x^2}{4}M(G;x,y)|_{x=y=1} &= 31.75n - 7.25, \\
\frac{D_y^2}{4}M(G;x,y) &= \frac{3^2(3n+2)}{4}xy^3 + \frac{4^2.2n}{4}xy^4 + (3n+1)x^2y^2 + \frac{9(13n-2)}{4}x^2y^3 + \frac{16n}{4}x^2y^4 \\
&\quad + \frac{9(5n-3)}{4}x^3y^3 + \frac{16n}{4}x^3y^4, \\
\frac{D_y^2}{4}M(G;x,y)|_{x=y=1} &= 66.25n - 5.75, \\
\frac{D_xD_y}{2}M(G;x,y) &= \frac{3}{2}(3n+2) + \frac{4}{2}.2n + \frac{4}{2}(3n+1) + \frac{6}{2}(13n-2) + \frac{8}{2}n + \frac{9}{2}(5n-3) + \frac{12}{2}n, \\
\frac{D_xD_y}{2}M(G;x,y)|_{x=y=1} &= M(G) = 86n - 14.5, \\
\left(\frac{D_x^2}{4} + \frac{D_y^2}{4} + \frac{D_xD_y}{2}\right)M(G;x,y)|_{x=y=1} &= 184n - 27.5.
\end{aligned} \tag{29}$$

The SK_2 index is plotted in 2D and 3D in Figure 9, which reveals how it depends on the relevant parameters. The graph's behavior in the xy-plane vertically upward changed when we increased the value of n. □

Theorem 9. *Let "G" be the graph, then the "hyper 1st Zagreb index" is*

$$mHM_1(G) = 736n - 110. \tag{30}$$

Proof

$$\begin{aligned}
M(G;x,y) &= (3n+2)xy^3 + 2nxy^4 + (3n+1)x^2y^2 + (13n-2)x^2y^3 + nx^2y^4 + (5n-3)x^3y^3 \\
&\quad + nx^3y^4, \\
\left(D_y^2 + D_x^2 + 2D_xD_y\right)M(G;x,y) &= 16(3n+2)xy^3 + 25.2nxy^4 + 16(3n+1)x^2y^2 \\
&\quad + 25(13n-2)x^2y^3 + 36nx^2y^4 + 36(5n-3)x^3y^3 \\
&\quad + 49nx^3y^4, \\
\left(D_y^2 + D_x^2 + 2D_xD_y\right)M(G;x,y)|_{x=y=1} &= 736n - 110.
\end{aligned} \tag{31}$$

□

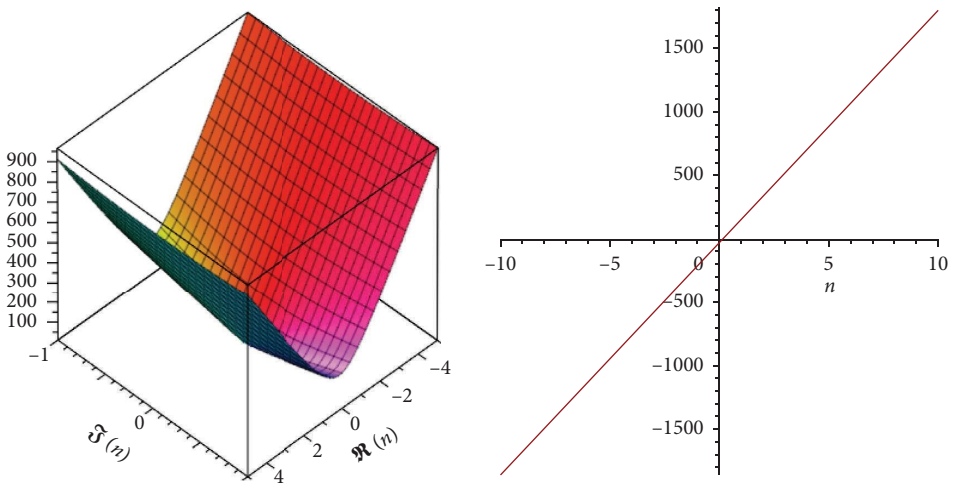

Figure 9: 2-D and 3-D structure of SK_2 index.

The hyper Zagreb index is plotted in 2D and 3D in Figure 10, which reveals how it depends on the relevant parameters. The graph's behavior in the xy-plane vertically upward changed when we increased the value of n.

Theorem 10. *Let "G" be the graph, then the "redefined 1st Zagreb index" is*

$$mRM_1(G) = 25n. \tag{32}$$

Proof

$$M(G;x,y) = (3n+2)xy^3 + 2nxy^4 + (3n+1)x^2y^2 + (13n-2)x^2y^3 + nx^2y^4 + (5n-3)x^3y^3 + nx^3y^4,$$

$$\begin{aligned}\left(S_x + S_y\right)M(G;x,y) &= \frac{4}{3}(3n+2)xy^3 + \frac{10}{4}nxy^4 + \frac{2(3n+1)}{2}x^2y^2 + \frac{5(13n-2)}{6}x^2y^3 + \frac{3n}{4}x^2y^4 \\ &\quad + \frac{2(5n-3)}{3}x^3y^3 + \frac{2n}{4}x^3y^4,\end{aligned} \tag{33}$$

$$\left(S_x + S_y\right)M(G;x,y)|_{x=y=1} = 25n.$$

The redefined first Zagreb index is plotted in 2D and 3D in Figure 11, which reveals how it depends on the relevant parameters. The graph's behavior in the xy-plane vertically upward changed when we increased the value of n. □

Theorem 11. *Let "G" be the graph, then the "modified Albertson index" is*

$$mMA(G) = 138n + 6. \tag{34}$$

Proof

$$\begin{aligned}M(G;x,y) &= (3n+2)xy^3 + 2nxy^4 + (3n+1)x^2y^2 + (13n-2)x^2y^3 + nx^2y^4 + (5n-3)x^3y^3 \\ &\quad + nx^3y^4, \\ \left(D_y^2 - D_x^2\right)M(G;x,y) &= 8(3n+2)xy^3 + 15.2nxy^4 + 0.(3n+1)x^2y^2 + 5(13n-2)x^2y^3 \\ &\quad + 12nx^2y^4 + 0(5n-3)x^3y^3 + 7nx^3y^4, \\ \left(D_y^2 - D_x^2\right)M(G;x,y)|_{x=y=1} &= 138n + 6.\end{aligned} \tag{35}$$

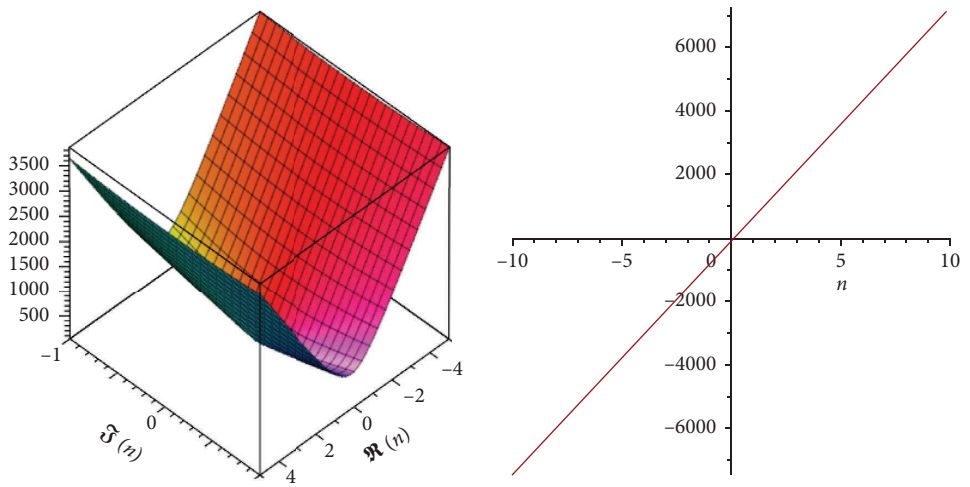

Figure 10: 2-D and 3-D structure of hyper Zagreb index.

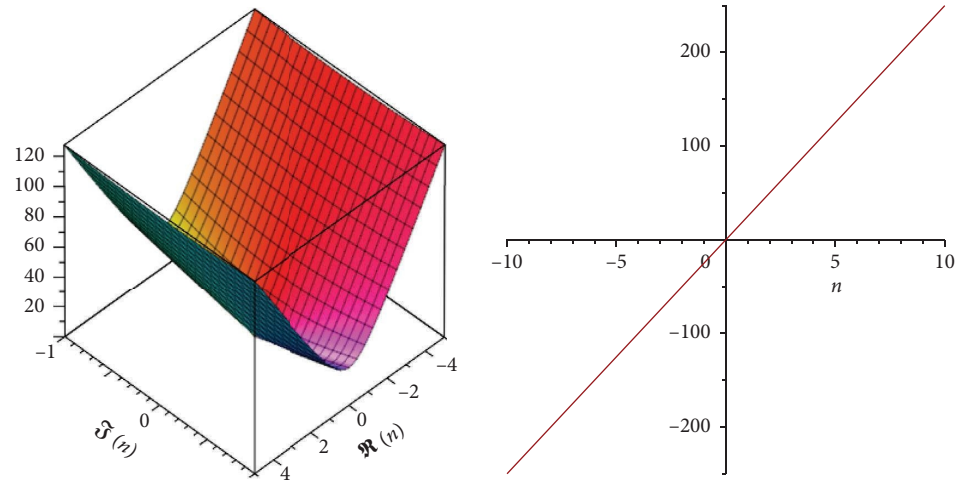

Figure 11: 2-D and 3-D structure of redefined 1st Zagreb index.

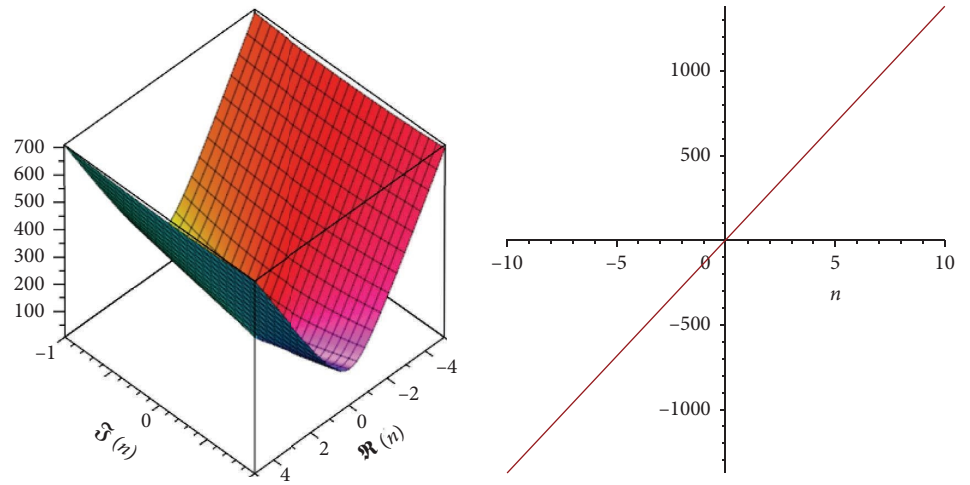

Figure 12: 2-D and 3-D structure of modified Albertson index.

Table 2: Comparison table of the topological indices.

n	$mM_1(G)$	$mM_2(G)$	$mM_3(G)$	$mMM_1(G)$	$mHM_2(G)$	mSK (G)	$mSK_1(G)$	$mSK_2(G)$	$mHM_1(G)$	$mRM_1(G)$	mMA (G)
1	126	143	30	242	907	63	71.5	156.5	626	25	144
2	268	315	58	507	2095	134	157.5	340.5	1362	50	282
3	410	487	86	772	3283	205	243.5	524.5	2098	75	420
4	552	659	114	1037	4471	276	329.5	708.5	2834	100	558
5	694	831	142	1302	5659	347	415.5	892.5	3570	125	696
6	836	1003	170	1567	6847	418	501.5	1076.5	4306	150	834
7	978	1175	198	1832	8035	489	587.5	1260.5	5042	175	972
8	1120	1347	226	2097	9223	560	673.5	1444.5	5778	200	1110
9	1262	1519	254	2362	10411	631	759.5	1628.5	6514	225	1248
10	1404	1691	282	2627	11599	702	845.5	1812.5	7250	250	1386

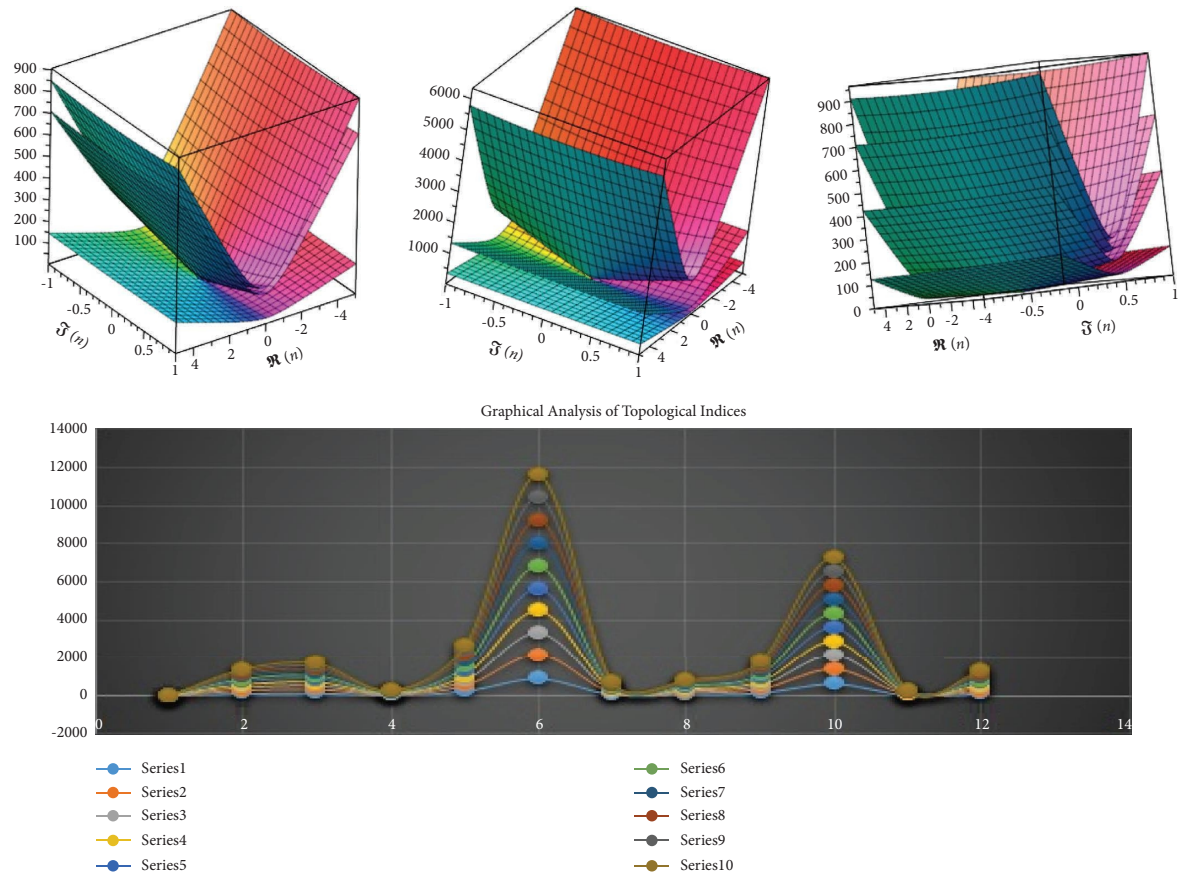

Figure 13: 2-D and 3-D graphical analysis of derived indices.

The modified Albertson index is plotted in 2D and 3D in Figure 12, which reveals how it depends on the relevant parameters. The graph's behavior in the xy-plane vertically upward changed when we increased the value of n. □

5. Comparison Analysis of Topological Indices via Graphical Representation

In this section, we computed the analysis of the topological indices in graphically which shows the 2D and 3D representing in assenting orders.

The Table 2 is calculated from the proof of the topological indices. These numerical values indicate the chemical structure properties.

The analysis of all topological indices is plotted in 2D and 3D in Figure 13, which reveals how it depends on the relevant parameters. The graph's behavior in the xy-plane vertically upward changed when we increased the value of n as mentioned in Table 2. In 2D graphs, we can observe that each index indicates its own behavior according to its property, which is helpful to find out the required value of the property that it shows.

6. Conclusion

The chemist now has access to a wide range of really helpful tools, thanks to graph theory. The goal of this study was to introduce the reader to one of these tools, specifically the novel degree-based topological indices that apply M-polynomials. The success of topological indices' extensive use in QSAR and QSPR investigations is proof that they carry important structural information. Topological indices are not a magic bullet though, and their users must be aware of both their drawbacks and potential hazards. In this work, we construct M-polynomials for the network of fenofibrate. We calculate the various degree-dependent topological indices shown in Table 1 using this polynomial. These topological invariants allow us to monitor the physical properties, biological activities, and chemical reactivity of a chemical molecule. We also chart the results. Using this graphical depiction of the topological indices, we can calculate the value of the topological indices for the fenofibrate network at various parameter values.

Data Availability

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

Conflicts of Interest

The authors declare that there are 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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