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On P_3-degree Based Topological Indices of Fenofibrate Graph

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Abstract

Topological indices are numerical descriptors of molecular structures, extensively used in chem-informatics, drug design, and material science to study molecular properties and predict biological activities. Fenofibrate, a clinically important lipid-lowering drug, is a molicule of significant interest in quantitative structure-activity relationship (QSAR) studies. This study focuses on computing degree-based topological indices of fenofibrate molecular graph. These indices, derived from the degree of vertices in the molecular structure, include: Zagreb Indices,Randic Index, Atom-bond connectivity, Geometric-Arithmetic Index,Harmonic Index. These are some Topological indices based on P_3-degrees.

Keywords: P3-degree; fenofibrate; Atom bond connectivity; Atom bond sum connectivity; Augmented Zagreb index; Sum Augmented Zagreb index; Harmonic index Arithmetic-geometric index; Geometric-arithmetic index.

2020 Mathematics Subject Classification: 05C15, 97K30, 05C07, 05C09, 05C92.

1. Introduction

Topological indices are numerical descriptors of molecular structures that play a crucial role in quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) studies. Among these, P_3- degree-based topological indices are derived from the graph representation of chemical compounds, where atoms are treated as vertices and chemical bonds as edges. These indices emphasize the P_3 path degree, a concept reflecting the degree of vertices within the context of three-vertex paths in a molecular graph. Fenofibrate, a widely used hypolipidemic agent, has a complex molecular structure that can be effectively studied using graph-theoretic methods. By representing fenofibrate as a molecular graph, where its atoms and bonds correspond to vertices and edges, P_3-degree-based topological indices provide insights into its structural and chemical properties. These indices are particularly useful in predicting biological activities, optimizing drug design, and analyzing molecular stability.

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This paper focuses on the computation and analysis of P_3- degree-based topological indices for fenofibrate. These indices, such as the Zagreb indices, Randic index, and atom-bond connectivity (ABC) index, are extended to include P_3- degree contributions. The study aims to explore how the P_3- degree influences the structural interpretation of fenofibrate and its potential correlations with pharmacological properties. The graph $G = (V, E)$ where $V = V(G)$ be the vertex set and $E = E(G)$ be the edge set, $d(r)$ be the degree vertex (r).

Definition 1.1. *I. B. Furtula, A. Graovac, D. Vuki ˇcevi ´c [4], introduced the Atom-bond connectivity index of tree in 2009 as follows:*

$$ABC^{P_3}(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_{P_3}(u) + d_{P_3}(v) - 2}{d_{P_3}(u)d_{P_3}(v)}}$$

Definition 1.2. *In 2022, A. Ali, B. Furtula,I. Rečzepović [1] defined the Atom-bond sum connectivity index of a graph G as follows:*

$$ABS^{P_3}(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_{P_3}(u) + d_{P_3}(v) - 2}{d_{P_3}(u) + d_{P_3}(v)}}$$

Definition 1.3. *B. Furtula, A. Graovac, D. Vuki ˇcevi ´c, Augmented Zagreb index [5], and it is defined in 2010:*

$$AGI^{P_3}(G) = \sum_{uv\in E(G)} \left[\frac{d_{P_3}(u)d_{P_3}(v)}{d_{P_3}(u) + d_{P_3}(v) - 2}\right]^3$$

Definition 1.4. *V. R. Kulli [14], defined the Sum augmented and multiplicative sum augmented indices in 2023 as follows:*

$$SAI^{P_3}(G) = \sum_{uv\in E(G)} \left[\frac{d_{P_3}(u) + d_{P_3}(v)}{d_{P_3}(u) + d_{P_3}(v) - 2}\right]^3$$

Definition 1.5. *Yan Yuan, Bo Zhou, N. Trinajstic, [18] introduced the Geometric-arithmetic index defined in 2010.*

$$GAI^{P_3}(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_{P_3}(u)d_{P_3}(v)}}{d_{P_3}(u) + d_{P_3}(v)}$$

Definition 1.6. *Shegehall V. S, and Kanabur R. [16] introduced the Arithmetic-geometric index defined in 2015.*

$$AGI^{P_3}(G) = \sum_{uv\in E(G)} \frac{d_{P_3}(u) + d_{P_3}(v)}{2\sqrt{d_{P_3}(u)d_{P_3}(v)}}$$

Definition 1.7. *M. H. Khalifeha, H. Yousefi-Azari, A. R. Ashrafi, [8] introduced the First Zagreb index and Second Zagreb index in 2009 as follows:*

$$M_1^{P_3}(G) = \sum_{uv\in E(G)} [d_{P_3}(u) + d_{P_3}(v)], \text{ and } M_2^{P_3}(G) = \sum_{uv\in E(G)} d_{P_3}(u)d_{P_3}(v)$$

Definition 1.8. *The Harmonic index was introduced by Zhong [19], and defined as follows:*

$$HI^{P_3}(G) = \sum_{uv \in E(G)} \frac{2}{d_{P_3}(u) + d_{P_3}(v)}$$

Definition 1.9. *G. H. Shirdel et al. [17] introduced the hyper Zagreb index and defined it as follows:*

$$HM^{P_3}(G) = \sum_{uv \in E(G)} [d_{P_3}(u) + d_{P_3}(v)]^2$$

Inspired by work on the P_3-degree of the graphs [3] and Fenofibrate graphs, we find the followings:

2. Main results and Discussions

The chemical structure of fenofibrate is shown in the below graph.

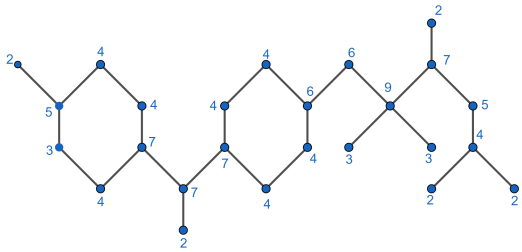

Figure 1: Chemical Structure of fenofibrate

In fenofibrate the chemical formal is $C_{20}H_{21}O_4Cl$ as a graph G. We partition the edges of graph G into edges of the type $E_{(d_{P_3}(u), d_{P_3}(v))}$.

$d_{P_3}(u), d_{P_3}(v) : uv \in E(G)$	Number of edges
(2,4)	2
(2,5)	1
(2,7)	2
(3,9)	2
(4,4)	4
(4,5)	3
(4,6)	2
(4,7)	4
(5,7)	1
(6,6)	1
(6,9)	1
(7,7)	2
(7,9)	1

Table 1: Degree of fenofibrate

Theorem 2.1. *The P_3-Atom bond connectivity index of fenofibrate is 15.4128661804.*

Proof.

$$ABC^{P_3}(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_{P_3}(u) + d_{P_3}(v) - 2}{d_{P_3}(u) d_{P_3}(v)}}$$

$$\begin{aligned} ABC^{P_3}(G) = {} & 2\left[\sqrt{\frac{2+4-2}{2\times 4}}\right] + 1\left[\sqrt{\frac{2+5-2}{2\times 5}}\right] + 2\left[\sqrt{\frac{2+7-2}{2\times 7}}\right] + 2\left[\sqrt{\frac{2+9-2}{2\times 9}}\right] + 4\left[\sqrt{\frac{4+4-2}{4\times 4}}\right] \\ & + 3\left[\sqrt{\frac{4+5-2}{4\times 5}}\right] + 2\left[\sqrt{\frac{4+6-2}{4\times 6}}\right] + 4\left[\sqrt{\frac{4+7-2}{4\times 7}}\right] + 1\left[\sqrt{\frac{5+7-2}{5\times 7}}\right] + 1\left[\sqrt{\frac{6+6-2}{6\times 6}}\right] \\ & + 1\left[\sqrt{\frac{6+9-2}{6\times 9}}\right] + 2\left[\sqrt{\frac{7+7-2}{7\times 7}}\right] + 1\left[\sqrt{\frac{7+9-2}{7\times 9}}\right] \\ & = 15.4128661804 \end{aligned}$$

□

Theorem 2.2. *The P_3-Atom bond sum connectivity index of fenofibrate is 19.5101765314.*

Proof.

$$ABS^{P_3}(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_{P_3}(u) + d_{P_3}(v) - 2}{d_{P_3}(u) + d_{P_3}(v)}}$$

$$\begin{aligned} ABS^{P_3}(G) = {} & 2\left[\sqrt{\frac{2+4-2}{2+4}}\right] + 1\left[\sqrt{\frac{2+5-2}{2+5}}\right] + 2\left[\sqrt{\frac{2+7-2}{2+7}}\right] + 2\left[\sqrt{\frac{3+9-2}{3+9}}\right] + 4\left[\sqrt{\frac{4+4-2}{4+4}}\right] \\ & + 3\left[\sqrt{\frac{4+5-2}{4+5}}\right] + 2\left[\sqrt{\frac{4+6-2}{4+6}}\right] + 4\left[\sqrt{\frac{4+7-2}{4+7}}\right] + 1\left[\sqrt{\frac{5+7-2}{5+7}}\right] + 1\left[\sqrt{\frac{6+6-2}{6+6}}\right] \\ & + 1\left[\sqrt{\frac{6+9-2}{6+9}}\right] + 2\left[\sqrt{\frac{7+7-2}{7+7}}\right] + \left[\sqrt{\frac{7+9-2}{7+9}}\right] \\ & = 19.5101765314 \end{aligned}$$

□

Theorem 2.3. *The P_3-Augmented Zagreb index of fenofibrate is 803.4583483625.*

Proof.

$$AGI^{P_3}(G) = \sum_{uv \in E(G)} \left[\frac{d_{P_3}(u) d_{P_3}(v)}{d_{P_3}(u) + d_{P_3}(v) - 2}\right]^3$$

$$\begin{aligned} AGI^{P_3}(G) = {} & 2\left[\frac{2\times 4}{2+4-2}\right]^3 + 1\left[\frac{2\times 5}{2+5-2}\right]^3 + 2\left[\frac{2\times 7}{2+7-2}\right]^3 + 2\left[\frac{3\times 9}{3+9-2}\right]^3 + 4\left[\frac{4\times 4}{4+4-2}\right]^3 \\ & + 3\left[\frac{4\times 5}{4+5-2}\right]^3 + 2\left[\frac{4\times 6}{4+6-2}\right]^3 + 4\left[\frac{4\times 7}{4+7-2}\right]^3 + 1\left[\frac{5\times 7}{5+7-2}\right]^3 + 1\left[\frac{6\times 6}{6+6-2}\right]^3 \\ & + 1\left[\frac{6\times 9}{6+9-2}\right]^3 + 2\left[\frac{7\times 7}{7+7-2}\right]^3 + 1\left[\frac{7\times 9}{7+9-2}\right]^3 \\ & = 803.4583483625 \end{aligned}$$

□

Theorem 2.4. *The P_3-Sum Augmented Zagreb index of fenofibrate is 53.5461920958.*

Proof.

$$SAI^{P_3}(G) = \sum_{uv\in E(G)} \left[\frac{d_{P_3}(u)+d_{P_3}(v)}{d_{P_3}(u)+d_{P_3}(v)-2}\right]^3$$

$$\begin{aligned} AGI^{P_3}(G) &= 2\left[\frac{2+4}{2+4-2}\right]^3 + 1\left[\frac{2+5}{2+5-2}\right]^3 + 2\left[\frac{2+7}{2+7-2}\right]^3 + 2\left[\frac{3+9}{3+9-2}\right]^3 + 4\left[\frac{4+4}{4+4-2}\right]^3 \\ &+ 3\left[\frac{4+5}{4+5-2}\right]^3 + 2\left[\frac{4+6}{4+6-2}\right]^3 + 4\left[\frac{4+7}{4+7-2}\right]^3 + 1\left[\frac{5+7}{5+7-2}\right]^3 + 1\left[\frac{6+6}{6+6-2}\right]^3 \\ &+ 1\left[\frac{6+9}{6+9-2}\right]^3 + 2\left[\frac{7+7}{7+7-2}\right]^3 + 1\left[\frac{7+9}{7+9-2}\right]^3 \\ &= 53.5461920958 \end{aligned}$$

□

Theorem 2.5. *The P_3-Geometric-arithmetic index of fenofibrate is 23.9454695786.*

Proof.

$$GAI^{P_3}(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_{P_3}(u)d_{P_3}(v)}}{d_{P_3}(u)+d_{P_3}(v)}$$

$$\begin{aligned} GAI^{P_3}(G) &= 2\left[\frac{2\sqrt{2\times 4}}{2+4}\right] + 1\left[\frac{2\sqrt{2\times 5}}{2+5}\right] + 2\left[\frac{2\sqrt{2\times 7}}{2+7}\right] + 2\left[\frac{2\sqrt{3\times 9}}{3+9}\right] + 4\left[\frac{2\sqrt{4\times 4}}{4+4}\right] + 3\left[\frac{2\sqrt{4\times 5}}{4+5}\right] \\ &+ 2\left[\frac{2\sqrt{4\times 6}}{4+6}\right] + 4\left[\frac{2\sqrt{4\times 7}}{4+7}\right] + 1\left[\frac{2\sqrt{5\times 7}}{5+7}\right] + 1\left[\frac{2\sqrt{6\times 6}}{6+6}\right] + 1\left[\frac{2\sqrt{6\times 9}}{6+9}\right] + 2\left[\frac{2\sqrt{7\times 7}}{7+7}\right] \\ &+ 1\left[\frac{2\sqrt{7\times 9}}{7+9}\right] \\ &= 23.9454695786 \end{aligned}$$

□

Theorem 2.6. *The P_3-Arithmetic Geometric index of fenofibrate is 712.3678963134.*

Proof.

$$AGI^{P_3}(G) = \sum_{uv\in E(G)} \frac{d_{P_3}(u)+d_{P_3}(v)}{2\sqrt{d_{P_3}(u)d_{P_3}(v)}}$$

$$\begin{aligned} AGI^{P_3}(G) &= 2\left[\frac{2+4}{2\sqrt{2\times 4}}\right] + 1\left[\frac{2+5}{2\sqrt{2\times 5}}\right] + 2\left[\frac{2+7}{2\sqrt{2\times 7}}\right] + 2\left[\frac{3+9}{2\sqrt{3\times 9}}\right] + 4\left[\frac{4+4}{2\sqrt{4\times 4}}\right] + 3\left[\frac{4+5}{2\sqrt{4\times 5}}\right] \\ &+ 2\left[\frac{4+6}{2\sqrt{4\times 6}}\right] + 4\left[\frac{4+7}{2\sqrt{4\times 7}}\right] + 1\left[\frac{5+7}{2\sqrt{5\times 7}}\right] + 1\left[\frac{6+6}{2\sqrt{6\times 6}}\right] + 1\left[\frac{6+9}{2\sqrt{6\times 9}}\right] + 2\left[\frac{7+7}{2\sqrt{7\times 7}}\right] \\ &+ 1\left[\frac{7+9}{2\sqrt{7\times 9}}\right] \end{aligned}$$

$$= 712.3678963134$$

□

Theorem 2.7. *The P_3-First Zagreb index of fenofibrate is 263.*

Proof. For P_3-degree

$$M_1^{P_3}(G) = \sum_{uv \in E(G)} [d_{P_3}(u) + d_{P_3}(v)]$$

$$M_1^{P_3}(G) = 2(2+4) + 1(2+5) + 2(2+7) + 2(3+7) + 4(4+4) + 3(4+5) + 2(4+6) + 4(4+7) + 1(5+7) + 1(6+6) + 1(6+9) + 2(7+7) + 1(7+9) = 263$$

□

Theorem 2.8. *The P_3-Second Zagreb index of fenofibrate is 686.*

Proof. for P_3-degree

$$M_2^{P_3}(G) = \sum_{uv \in E(G)} [d_{P_3}(u) d_{P_3}(v)],$$

$$M_2^{P_3}(G) = 2(2\times 4) + 1(2\times 5) + 2(2\times 7) + 2(3\times 7) + 4(4\times 4) + 3(4\times 5) + 2(4\times 6) + 4(4\times 7) + 1(5\times 7) + 1(6\times 6) + 1(6\times 9) + 2(7\times 7) + 1(7\times 9) = 686$$

□

Theorem 2.9. *The P_3-harmonic index of fenofibrate is 6.8014790765.*

Proof. For P_3-degree

$$HI^{P_3}(G) = \sum_{uv \in E(G)} \frac{2}{d_{P_3}(u) + d_{P_3}(v)}$$

$$HI^{P_3}(G) = 2\left(\frac{2}{2+4}\right) + 1\left(\frac{2}{2+5}\right) + 2\left(\frac{2}{2+7}\right) + 2\left(\frac{2}{3+9}\right) + 4\left(\frac{2}{4+4}\right) + 3\left(\frac{2}{4+5}\right) + 2\left(\frac{2}{4+6}\right) + 4\left(\frac{2}{4+7}\right) + 1\left(\frac{2}{5+7}\right) + 1\left(\frac{2}{6+6}\right) + 1\left(\frac{2}{6+9}\right) + 2\left(\frac{2}{7+7}\right) + 1\left(\frac{2}{7+9}\right)$$

$$= 6.8014790765$$

□

Theorem 2.10. *The P_3-Hyper index of fenofibrate is 3227.*

Proof. For P_3-degree

$$HM^{P_3}(G) = \sum_{uv \in E(G)} [d_{P_3}(u) + d_{P_3}(v)]^2$$

$$\begin{aligned} HM^{P_3}(G) &= 2(2+4)^2 + 1(2+5)^2 + 2(2+7)^2 + 2(3+9)^2 + 4(4+4)^2 + 3(4+5)^2 + 2(4+6)^2 \\ &+ 4(4+7)^2 + 1(5+7)^2 + 1(6+6)^2 + 1(6+9)^2 + 2(7+7)^2 + 1(7+9)^2 \\ &= 3227 \end{aligned}$$

□

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