Degree Based Topological Indices of Fenofibrate

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Abstract

Fenofibrate is a drug approved by U S Food and Drugs Administration used to reduce high cholesterol and triglycerides level in blood. Here we determined some degree based topological indices of Fenofibrate.

Keywords—*Fenofibrate, topological indices, QSAR.*

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1. INTRODUCTION

Topological indices are numerical values obtained from chemical structures. These topological indices are very useful for comparison of physico-chemical properties among them. This will reduce the cost of laboratory expenses.

Fenofibrate is a drug approved by U S Food and Drugs Administration used to reduce high cholesterol and triglycerides level in blood. It is very important to determine topological indices of this drug to compare physico-chemical properties using QSAR models.

Quantitative structure activity relationship (QSAR) is a computational modeling used to relate structural properties with biological properties of chemical structures.

The graph G=(V,E) where V=V(G) be the vertex set and E=E(G) be the edge set. dg(r) be the degree of vertex r.

Definition 1:ABC(atom bond connectivity) index of a graph *G* defined in [1] as,

$$ABC(G) = \sum_{rs\in E(G)} \sqrt{\frac{dg(r)+dg(s)-2}{dg(r)dg(s)}} \quad \text{.......}(1)$$

Definition 2:ABS(atom bond sum connectivity) index of a graph *G* defined in [2] as,

$$ABS(G) = \sum_{rs\in E(G)} \sqrt{\frac{dg(r)+dg(s)-2}{dg(r)+dg(s)}} \quad \text{.......}(2)$$

Definition 3:AZI (augmented Zagreb index) is defined in[3] as

$$AZI(G) = \sum_{rs\in E(G)} \left(\frac{dg(r)dg(s)}{dg(r)+dg(s)-2)}\right)^3 \quad \text{.......} (3)$$

Definition 4:SAI(sum augmented index)defined in [4] as,

$$SAI(G) = \sum_{rs\in E(G)} \left(\frac{dg(r)+dg(s)}{dg(r)+dg(s)-2)}\right)^3 \quad \text{.......}(4)$$

Definition 5: GA(geometric-arithmetic index)[5] of a graph *G* is defined as,

$$GA(G) = \sum_{rs\in E(G)} \frac{2\sqrt{dg(r)dg(s)}}{dg(r)+dg(s)} \quad \text{.......}(5)$$

Definition 6: AG(arithmetic-geometric index)of a graph *G* is defined [6]as,

$$AG(G) = \sum_{rs\in E(G)} \frac{dg(r)+dg(s)}{2\sqrt{dg(r)dg(s)}} \quad \text{.......}(6)$$

Definition 7: GO1(first Gourava index) and GO2 (second Gourava index) of a graph *G* are defined [7] as ,

$$GO_1(G) = \sum_{rs\in E(G)} \left[\left(dg(r)+dg(s)\right)+dg(r)dg(s)\right] \quad \text{.......}(7)$$

$$GO_2(G) = \sum_{rs\in E(G)} \left[\left(dg(r)+dg(s)\right)dg(r)dg(s)\right] \quad \text{.......}(8)$$

Definition8:HGO_1(first hyper Gourava and HGO_2 (second hyper Gourava index) of a graph *G* are defined in [8] as,

$$HGO_1(G) = \sum_{rs\in E(G)} [dg(r)+dg(s)+dg(r)dg(s)]^2 \quad \text{.......}(9)$$

$$HGO_2(G) = \sum_{rs\in E(G)} [(dg(r)+dg(s))dg(r)dg(s)]^2 \quad \text{.....}(10)$$

2. Results and Discussions

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

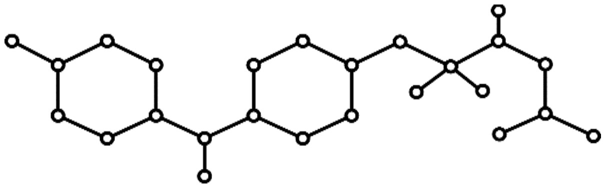

Figure 1: Chemical Structure of fenofibrate.

The graph G of fenofibrate has 25 vertices and 26 edges are shown in the above graph.

$dg(r), dg(s): rs \in E(G)$	Number of edges
(1, 3)	5
(1, 4)	2
(2, 2)	4
(2, 3)	11
(2, 4)	1
(3, 3)	2
(3, 4)	1

Table1. Edge Partition of Fenofibrate

Theorem 1: ABC index of fenofibrate is $ABC(G) = 19.1070$.

Proof: From (1),

$$ABC(G) = \sum_{rs \in E(G)} \sqrt{\frac{dg(r) + dg(s) - 2}{dg(r)dg(s)}}$$

$$= 5\left(\sqrt{\frac{1+3-2}{1\times 3}}\right) + 2\left(\sqrt{\frac{1+4-2}{1\times 4}}\right) + 4\left(\sqrt{\frac{2+2-2}{2\times 2}}\right) + 11\left(\sqrt{\frac{2+3-2}{2\times 3}}\right) + 1\left(\sqrt{\frac{2+4-2}{2\times 4}}\right) + 2\left(\sqrt{\frac{3+3-2}{3\times 3}}\right) + 1\left(\sqrt{\frac{3+4-2}{3\times 4}}\right)$$

$=19.1070$

Theorem 2:. ABS index of fenofibrate is $ABS(G) = 19.7283$.

Proof: From (2),

$$ABS(G) = \sum_{rs \in E(G)} \sqrt{\frac{dg(r) + dg(s) - 2}{dg(r) + dg(s)}}$$

$$=5\left(\sqrt{\frac{1+3-2}{1+3}}\right) + 2\left(\sqrt{\frac{1+4-2}{1+4}}\right) + 4\left(\sqrt{\frac{2+2-2}{2+2}}\right) + 11\left(\sqrt{\frac{2+3-2}{2+3}}\right) + 1\left(\sqrt{\frac{2+4-2}{2+4}}\right) + 2\left(\sqrt{\frac{3+3-2}{3+3}}\right) + 1\left(\sqrt{\frac{3+4-2}{3+4}}\right)$$

=19.7283

Theorem 3:. AZI index of fenofibrate is $AZI(G)$ =186.2209.

Proof: From (3),

$$AZI(G) = \sum_{rs\in E(G)} \left(\frac{dg(r)dg(s)}{dg(r)+dg(s)-2)}\right)^3$$

$$= 5\left[\frac{1\times 3}{1+3-2}\right]^3 + 2\left[\frac{1\times 4}{1+4-2}\right]^3 + 4\left[\frac{2\times 2}{2+2-2}\right]^3 + 11\left[\frac{2\times 3}{2+3-2}\right]^3 + 1\left[\frac{2\times 4}{2+4-2}\right]^3 + 2\left[\frac{3\times 3}{3+3-2}\right]^3 + 1\left[\frac{3\times 4}{3+4-2}\right]^3$$

=186.2209

Theorem 4:. SAI index of fenofibrate is $SAI(G)$ =145.0541.

Proof: From (4),

$$SAI(G) = \sum_{rs\in E(G)} \left(\frac{dg(r)+dg(s)}{dg(r)+dg(s)-2)}\right)^3$$

$$= 5\left[\frac{1+3}{1+3-2}\right]^3 + 2\left[\frac{1+4}{1+4-2}\right]^3 + 4\left[\frac{2+2}{2+2-2}\right]^3 + 11\left[\frac{2+3}{2+3-2}\right]^3 + 1\left[\frac{2+4}{2+4-2}\right]^3 + 2\left[\frac{3+3}{3+3-2}\right]^3 + 1\left[\frac{3+4}{3+4-2}\right]^3$$

=145.0541

Theorem 5:. GA index of fenofibrate is $GA(G)$ =24.0547.

Proof: From (5),

$$GA(G) = \sum_{rs\in E(G)} \frac{2\sqrt{dg(r)dg(s)}}{dg(r)+dg(s)}$$

$$= 5\left[\frac{2\sqrt{1\times 3}}{1+3}\right] + 2\left[\frac{2\sqrt{1\times 4}}{1+4}\right] + 4\left[\frac{2\sqrt{2\times 2}}{2+2}\right] + 11\left[\frac{2\sqrt{2\times 3}}{2+3}\right] + 1\left[\frac{2\sqrt{2\times 4}}{2+4}\right] + 2\left[\frac{2\sqrt{3\times 3}}{3+3}\right] + 1\left[\frac{2\sqrt{3\times 4}}{3+4}\right]$$

=24.0547

Theorem 6:AG index of fenofibrate is $AG(G)$ =27.5713.

Proof: From (6),

$$AG(G) = \sum_{rs\in E(G)} \frac{dg(r)+dg(s)}{2\sqrt{dg(r)dg(s)}}$$

$$= 5\left[\frac{1+3}{2\sqrt{1\times 3}}\right] + 2\left[\frac{1+4}{2\sqrt{1\times 4}}\right] + 4\left[\frac{2+2}{2\sqrt{2\times 2}}\right] + 11\left[\frac{2+3}{2\sqrt{2\times 3}}\right] + 1\left[\frac{2+4}{2\sqrt{2\times 4}}\right] + 2\left[\frac{3+3}{2\sqrt{3\times 3}}\right] + 1\left[\frac{3+4}{2\sqrt{3\times 4}}\right]$$

=27.5713

Theorem 7: GO1 index of fenofibrate is $GO_1(G)$ =269.

Proof: From (7),

$$GO_1(G) = \sum_{rs\in E(G)} \left[\left(dg(r) + dg(s)\right) + dg(r)dg(s)\right]$$

=5[1 + 3 + 1(3)]+2[1 + 4 + 1(4)]+4[2 + 2 + 2(2)] +11[2 + 3 + 2(3)]+ 1[2 + 4 + 2(4)]

+2[3 + 3 + 3(3)]+1[3 + 4 + 3(4)]

=269

Theorem 8:GO2 index of fenofibrate is $GO_2(G) = 734$.

Proof: From (8),

$$GO_2(G) = \sum_{rs\in E(G)} \left[\left(dg(r) + dg(s)\right)dg(r)dg(s)\right]$$

$= 5[(1+3)(1\times 3)]$+$2[(1+4)(1\times 4)]$+$4[(2+2)(2\times 2)]$+$11[(2+3)+(2\times 3)] + 1[(2+4) + (2\times 4)]$+$2[(3+3)+(3\times 3)] + 1[(3+4)+(3\times 4)]$

$= 734$

Theorem 9:HGO1 index of fenofibrate is $HGO_1(G)$ =3001.

Proof: From (9),

$$HGO_1(G) = \sum_{rs\in E(G)} [(dg(r) + dg(s)) + dg(r)dg(s)]^2$$

=$5[1+3+1(3)]^2 + 2[1+4+1(4)]^2$+$4[2+2+2(2)]^2$+$11[2+3+2(3)]^2$+
$1[2+4+2(4)]^2$+$2[3+3+3(3)]^2$+$1[3+4+3(4)]^2$

=3001

Theorem 10:HGO2 index of fenofibrate is $HGO_2(G)$ =27636.

Proof: From (10),

$$HGO_2(G) = \sum_{rs\in E(G)} [(dg(r) + dg(s))dg(r)dg(s)]^2$$

=$5[(1+3)(1\times 3)]^2$+$2[(1+4)(1\times 4)]^2$+$4[(2+2)(2\times 2)]^2$+$11[(2+3)(2\times 3)]^2$
+$1[(2+4)(2\times 4)]^2$+$2[(3+3)(3\times 3)]^2$+$1[(3+4)(3\times 4)]^2$

=27636

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