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Computation of Certain Degree-based Topological Indices of Propranolol ($C_{16}H_{21}NO_2$)

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Abstract

Chemists now have access to several valuable tools, such as topological indices. Topological indices are numerical invariants that are related to a chemical graph and can be used to predict biological activity and physiochemical characteristics. These indices are researched and used in chemical graph theory, medicine and other disciplines of science. In this research work, we will compute the topological indices likegeometric arithmeticindex, atom bond connectivity index, forgotten index, randic connectivity index, harmonic index, sombor index,fifth geometric arithmetic index, sanskruti Index of the Propranolol ($C_{16}H_{21}NO_2$).

Keywords: Topological Indices; Hand-shaking Lemma; Propranolol ($C_{16}H_{21}NO_2$).

1. Introduction and Preliminaries

Assume that $G = (V, E)$ is a simple and without loops molecular graph. The vertices $V(G)$represent the atoms of the molecule, while the edges$E(G)$indicate chemical bonds. The edges in the graph (G) that connect to a vertex is referred to as vertex degree. A degree vertex is represented by$d_w\{w \in V(G)\}$and $S_w = \sum_{x \in N_G(w)} d_x$, where $N_G(w) = \{x \in V(G) \mid wx \in E(G)\}$.

For unspecified terminologies and notations we recommended[1]. In graph $(G)$to find the total number of edges hand-shaking lemmais very useful[2].

IfG is a graph of size n, then

$$\sum_{w \in V(G)} \deg(w) = 2n.$$

Propranolol is a medication of beta-blocker used to treat high blood pressure, irregular heartbeats, trembling, hypertension, and other diseases [3]. It is widely known as Inderal, used to enhance the chances of survival, reduce migraine and chest pain. The molecular formula of propranolol is $(C_{16}H_{21}NO_2)$ and its chemical structure is depicted inFigure 1.

Chemical graph theory that applies graph theory to the mathematical modeling of chemical comounds. This idea had a significant impact on the improvement of the chemical sciences. The graph-theoretic approach may be used to model molecular compounds. Topological descriptors improve understanding and prediction of bioactivities and chemical characteristics of compounds. A topological index is a numerical number that provides relevant information about a chemical structure or molecule. Topological indices are utilized in the QSAR/QSPR studies to predict chemical characteristics and physical characteristics of a molecular compound.Different types of topological indices exists such asdistance-based,eccentric-based and degree-basedindices[4][5]etc.

The Wiener index is defined in [6] as follows:

$$W(G) = \frac{1}{2}\sum_{(w,x)} d(w,x).$$

Where (w,x) is order pair of vertices in G and $d(w,x)$ is the distance of vertex $w - x$ in$G$.

The geometric-arithmetic index (GA)[7] of graph $G$is defined as:

$$GA(G) = \sum_{\mathrm{wx} \in E(G)} \frac{2\sqrt{d_w d_x}}{d_w + d_x}. \qquad (1)$$

The atomic bond connectivity index$(ABC)$of graph $G$is defined [8]as:

$$ABC(G) = \sum_{\mathrm{wx} \in E(G)} \sqrt{\frac{d_w + d_x - 2}{d_w d_x}}. \qquad (2)$$

The forgotten index$(F)$is defined[9] as:

$$F(G) = \sum_{wx \in E(G)} (d_w^2 + d_x^2). \quad (3)$$

Let G be molecular graph, then Randic connectivity index is defined[10] as:

$$RC(G) = \sum_{wx \in E(G)} \frac{1}{\sqrt{d_w d_x}}. \quad (4)$$

The Harmonic index is defined [11] as:

$$H(G) = \sum_{wx \in E(G)} \frac{2}{(d_w + d_x)}. \quad (5)$$

The Sombor index is defined [12] as:

$$SO(G) = \sum_{wx \in E(G)} \sqrt{d_w^2 + d_x^2}. \quad (6)$$

The $GA_5(G)$index is defined [13] as:

$$GA_5(G) = \sum_{wx \in E(G)} \frac{2\sqrt{S_w \times S_x}}{S_w + S_x}. \quad (7)$$

TheSanskruti Index$S(G)$is defined [14] as:

$$S(G) = \sum_{wx \in E(G)} \left(\frac{S_w S_x}{S_w + S_x - 2}\right)^3. \quad (8)$$

For more detail, we mention the readers to follow the following research articles [15][16][17].

2. Methodology:

First we draw the structure of Propranolol ($C_{16}H_{21}NO_2$). We generalized vertices and the edges of the Propranolol ($C_{16}H_{21}NO_2$)by using hand-shaking lemma.

After generalization, we computed geometric arithmetic index, atom bond connectivity index, forgotten index, randic connectivity index, harmonic index, sombor index, fifth geometric arithmetic index, sanskruti Index of the Propranolol ($C_{16}H_{21}NO_2$).

3. Degree Based Topological Indices of thePropranolol $(C_{16}H_{21}NO_2)$

Theorem 3.1.

The geometric arithmetic index of the Propranolol $(C_{16}H_{21}NO_2)$ is

$$GA(C_{16}H_{21}NO_2) = 19.4364$$

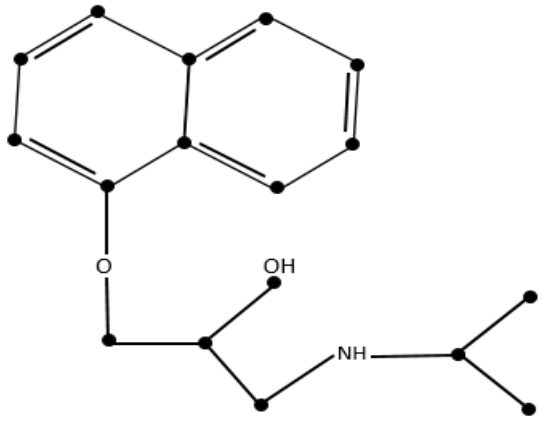

Figure 1.Chemical structure of propranolol $(C_{16}H_{21}NO_2)$.

Proof: Consider the propranolol$(C_{16}H_{21}NO_2)$. Let $E_{(w,x)}$ denote the edges connecting the vertices of degree d_w and d_x.Two dimensional structure ofpropranolol contain edges of the type$E_{(1,3)}$,$E_{(2,2)}$, $E_{(2,3)}$ and$E_{(3,3)}$as shown in Table 1.

Table 1. Partition of edges.

$E[d_w, d_x]$	$E_{(1,3)}$	$E_{(2,2)}$	$E_{(2,3)}$	$E_{(3,3)}$
Number of edges	3	7	8	2

By Equation *(1)* and the *Table 1*, we acquire the results, i.e.

$$GA(C_{16}H_{21}NO_2) = \sum_{wx \in E(G)} \frac{2\sqrt{d_w d_x}}{d_w + d_x}.$$

$$GA(C_{16}H_{21}NO_2) = |E_{(1,3)}| \sum_{wx \in E(C_{16}H_{21}NO_2)} \frac{2\sqrt{d_w d_x}}{d_w + d_x} + |E_{(2,2)}| \sum_{wx \in E(C_{16}H_{21}NO_2)} \frac{2\sqrt{d_w d_x}}{d_w + d_x}$$

$$+ |E_{(2,3)}| \sum_{wx \in E(C_{16}H_{21}NO_2)} \frac{2\sqrt{d_w d_x}}{d_w + d_x} + |E_{(3,3)}| \sum_{wx \in E(C_{16}H_{21}NO_2)} \frac{2\sqrt{d_w d_x}}{d_w + d_x}.$$

$$= 3\left(\frac{\sqrt{3}}{2}\right) + 7\left(\frac{2\sqrt{4}}{4}\right) + 8\left(\frac{2\sqrt{6}}{5}\right) + 2\left(\frac{2\sqrt{9}}{6}\right).$$

$$= 3\left(\frac{\sqrt{3}}{2}\right) + 7 + \frac{16\sqrt{6}}{5} + 2.$$

$$GA(C_{16}H_{21}NO_2) = 19.4364$$

Theorem3.2.

The atom bond connectivity index of the propranolol $(C_{16}H_{21}NO_2)$ is

$$ABC(C_{16}H_{21}NO_2) = 14.889$$

Proof: By Equation *(2)* and the *Table 1*, we acquire the results, i.e.

$$ABC(G) = \sum_{wx \in E(G)} \sqrt{\frac{d_w + d_x - 2}{d_w d_x}}.$$

$$ABC(C_{16}H_{21}NO_2) = \left|E_{(1,3)}\right| \sum_{wx \in E(C_{16}H_{21}NO_2)} \sqrt{\frac{d_w + d_x - 2}{d_w d_x}} + \left|E_{(2,2)}\right| \sum_{wx \in E(C_{16}H_{21}NO_2)} \sqrt{\frac{d_w + d_x - 2}{d_w d_x}}$$

$$+\left|E_{(2,3)}\right| \sum_{wx \in E(C_{16}H_{21}NO_2)} \sqrt{\frac{d_w + d_x - 2}{d_w d_x}} + \left|E_{(3,3)}\right| \sum_{wx \in E(C_{16}H_{21}NO_2)} \sqrt{\frac{d_w + d_x - 2}{d_w d_x}}$$

$$= 3\sqrt{\frac{1+3-2}{(1)(3)}} + 7\sqrt{\frac{2+2-2}{(2)(2)}} + 8\sqrt{\frac{2+3-2}{(2)(3)}} + 2\sqrt{\frac{3+3-2}{(3)(3)}}$$

$$= 3\sqrt{\frac{2}{3}} + 7\sqrt{\frac{1}{2}} + 8\sqrt{\frac{1}{2}} + 2\sqrt{\frac{2}{3}}$$

$$ABC(C_{16}H_{21}NO_2) = 14.6890$$

Theorem3.3.

The forgotten index ofthr propranolol $(C_{16}H_{21}NO_2)$ is

$$F(C_{16}H_{21}NO_2) = 226.0000$$

Proof: By Equation *(3)* and the *Table 1*, we acquire the results, i.e.

$$F(C_{16}H_{21}NO_2) = \sum_{wx \in E(G)} (d_w^2 + d_x^2).$$

$$F(C_{16}H_{21}NO_2) = \left|E_{(1,3)}\right| \sum_{wx \in E(C_{16}H_{21}NO_2)} (d_w^2 + d_x^2) + \left|E_{(2,2)}\right| \sum_{wx \in E(C_{16}H_{21}NO_2)} (d_w^2 + d_x^2)$$

$$+\left|\mathrm{E}_{(2,3)}\right| \sum_{\mathrm{wx}\in E(C_{16}H_{21}NO_2)} (d_w^2 + d_x^2) + \left|\mathrm{E}_{(3,3)}\right| \sum_{\mathrm{wx}\in E(C_{16}H_{21}NO_2)} (d_w^2 + d_x^2).$$

$$= 3(1+9) + 7(4+4) + 8(4+9) + 2(9+9).$$

$$= 30 + 56 + 104 + 36.$$

$$F(C_{16}H_{21}NO_2) = 226.$$

Theorem3.4.

The randic connectivity index of the propranolol $(C_{16}H_{21}NO_2)$ is

$$RC(C_{16}H_{21}NO_2) = 9.1647$$

Proof: By Equation *(4)* and the *Table 1*, we acquire the results, i.e.

$$RC(C_{16}H_{21}NO_2) = \sum_{\mathrm{wx}\in E(G)} \frac{1}{\sqrt{d_w d_x}}.$$

$$RC(C_{16}H_{21}NO_2) = \left|\mathrm{E}_{(1,3)}\right| \sum_{\mathrm{wx}\in E(C_{16}H_{21}NO_2)} \frac{1}{\sqrt{d_w d_x}} + \left|\mathrm{E}_{(2,2)}\right| \sum_{\mathrm{wx}\in E(C_{16}H_{21}NO_2)} \frac{1}{\sqrt{d_w d_x}}$$

$$+\left|\mathrm{E}_{(2,3)}\right| \sum_{\mathrm{wx}\in E(C_{16}H_{21}NO_2)} \frac{1}{\sqrt{d_w d_x}} + \left|\mathrm{E}_{(3,3)}\right| \sum_{\mathrm{wx}\in E(C_{16}H_{21}NO_2)} \frac{1}{\sqrt{d_w d_x}}.$$

$$= 3\frac{1}{\sqrt{3}} + 7\frac{1}{\sqrt{4}} + 8\frac{1}{\sqrt{6}} + 2\frac{1}{\sqrt{9}}.$$

$$= \sqrt{3} + \frac{7}{\sqrt{4}} + \frac{8}{\sqrt{6}} + \frac{2}{3}.$$

$$RC(C_{16}H_{21}NO_2) = 9.1647$$

Theorem3.5.

The harmonic index of the propranolol $(C_{16}H_{21}NO_2)$ is

$$H(C_{16}H_{21}NO_2) = 9.7000$$

Proof: By Equation *(5)* and the *Table 1*, we acquire the results, i.e.

$$H(C_{16}H_{21}NO_2) = \sum_{\mathrm{wx}\in E(G)} \frac{2}{(d_w + d_x)}.$$

$$H(C_{16}H_{21}NO_2) = \left|\mathrm{E}_{(1,3)}\right| \sum_{\mathrm{wx}\in E(C_{16}H_{21}NO_2)} \frac{2}{(d_w + d_x)} + \left|\mathrm{E}_{(2,2)}\right| \sum_{\mathrm{wx}\in E(C_{16}H_{21}NO_2)} \frac{2}{(d_w + d_x)}$$

$$+\left|\mathrm{E}_{(2,3)}\right| \sum_{\mathrm{wx}\in E(C_{16}H_{21}NO_2)} \frac{2}{(d_w + d_x)} + \left|\mathrm{E}_{(3,3)}\right| \sum_{\mathrm{wx}\in E(C_{16}H_{21}NO_2)} \frac{2}{(d_w + d_x)}.$$

$$= 3\frac{2}{(4)} + 7\frac{2}{(4)} + 8\frac{2}{(5)} + 2\frac{2}{(6)}.$$

$$= \frac{3}{(2)} + \frac{7}{(2)} + \frac{16}{(5)} + \frac{2}{(3)}.$$

$$H(C_{16}H_{21}NO_2) = 9.7000$$

Theorem3.6.

The Sombor index of the propranolol $(C_{16}H_{21}NO_2)$ is

$$SO(C_{16}H_{21}NO_2) = 66.6155$$

Proof: By Equation *(6)* and the *Table 1*, we acquire the results, i.e.

$$SO(\mathrm{G}) = \sum_{wx \in E(\mathrm{G})} \sqrt{d_w^2 + d_x^2}.$$

$$SO(C_{16}H_{21}NO_2) = \left|\mathrm{E}_{(1,3)}\right| \sum_{\mathrm{wx} \in E(C_{16}H_{21}NO_2)} \sqrt{d_w^2 + d_x^2} + \left|\mathrm{E}_{(2,2)}\right| \sum_{\mathrm{wx} \in E(C_{16}H_{21}NO_2)} \sqrt{d_w^2 + d_x^2}$$

$$+\left|\mathrm{E}_{(2,3)}\right| \sum_{\mathrm{wx} \in E(C_{16}H_{21}NO_2)} \sqrt{d_w^2 + d_x^2} + \left|\mathrm{E}_{(3,3)}\right| \sum_{\mathrm{wx} \in E(C_{16}H_{21}NO_2)} \sqrt{d_w^2 + d_x^2}.$$

$$= 3\left(\sqrt{10}\right) + 7\left(\sqrt{8}\right) + 8\left(\sqrt{13}\right) + 2\left(\sqrt{18}\right).$$

$$SO(C_{16}H_{21}NO_2) = 66.6155$$

Theorem3.7.

The fifth geometric arithmetic index of the propranolol $(C_{16}H_{21}NO_2)$ is

$$GA_5(C_{16}H_{21}NO_2) = 18.3589$$

Proof: Consider the propranolol$(C_{16}H_{21}NO_2)$.Let $E_{(w,x)}$ denote the edges connecting the vertices of degree S_w and S_x.Two dimensional structure of propranolol contain edges of the type$E_{(3,4)}$,$E_{(3,5)}, E_{(4,4)}, E_{(4,5)}, E_{(5,5)}, E_{(7,5)}, E_{(8,5)}$ and$E_{(7,8)}$.as in Table 2.

Table 2. Partition of edges.

$E[S_w, S_x]$	$E_{(3,4)}$	$E_{(3,5)}$	$E_{(4,4)}$	$E_{(4,5)}$	$E_{(5,5)}$	$E_{(7,5)}$	$E_{(8,5)}$	$E_{(7,8)}$
Number of edges	2	1	1	5	4	4	1	2

By Equation *(7)* and *Table* 2, we acquire the results, i.e.

$$GA_5(G) = \sum_{wx \in E(G)} \frac{2\sqrt{S_w \times S_x}}{S_w + S_x}.$$

$$GA_5(C_{16}H_{21}NO_2) = |E_{(3,4)}| \sum_{wx \in E(C_{16}H_{21}NO_2)} \frac{2\sqrt{S_w \times S_x}}{S_w + S_x} + |E_{(3,5)}| \sum_{wx \in E(C_{16}H_{21}NO_2)} \frac{2\sqrt{S_w \times S_x}}{S_w + S_x}$$

$$+|E_{(4,4)}| \sum_{wx \in E(C_{16}H_{21}NO_2)} \frac{2\sqrt{S_w \times S_x}}{S_w + S_x} + |E_{(4,5)}| \sum_{wx \in E(C_{16}H_{21}NO_2)} \frac{2\sqrt{S_w \times S_x}}{S_w + S_x}$$

$$+ |E_{(5,5)}| \sum_{wx \in E(C_{16}H_{21}NO_2)} \frac{2\sqrt{S_w \times S_x}}{S_w + S_x} + |E_{(7,5)}| \sum_{wx \in E(C_{16}H_{21}NO_2)} \frac{2\sqrt{S_w \times S_x}}{S_w + S_x}$$

$$+ |E_{(8,5)}| \sum_{wx \in E(C_{16}H_{21}NO_2)} \frac{2\sqrt{S_w \times S_x}}{S_w + S_x} + |E_{(7,8)}| \sum_{wx \in E(C_{16}H_{21}NO_2)} \frac{2\sqrt{S_w \times S_x}}{S_w + S_x}.$$

$$= (2)\frac{2\sqrt{3 \times 4}}{3+4} + (1)\frac{2\sqrt{3 \times 5}}{3+5} + (1)\frac{2\sqrt{4 \times 4}}{4+4} + (5)\frac{2\sqrt{4 \times 5}}{4+5} + (4)\frac{2\sqrt{5 \times 5}}{5+5} + (4)\frac{2\sqrt{7 \times 5}}{7+5}$$

$$+ (1)\frac{2\sqrt{8 \times 5}}{8+5} + (2)\frac{2\sqrt{7 \times 8}}{7+8}$$

$$GA_5(C_{16}H_{21}NO_2) = \frac{8\sqrt{3}}{7} + \frac{\sqrt{15}}{4} + 1 + \frac{10\sqrt{20}}{9} + \frac{4\sqrt{10}}{5} + \frac{2\sqrt{35}}{3} + \frac{2\sqrt{40}}{13} + \frac{4\sqrt{56}}{15}$$

$$GA_5(C_{16}H_{21}NO_2) = 18.3589$$

Theorem3.8.

The Sanskruti Index of the propranolol ($C_{16}H_{21}NO_2$) is

$$S(C_{16}H_{21}NO_2) = 680.3774$$

Proof: By Equation *(8)* and *Table* 2, we acquire the results, i.e.

$$S(G) = \sum_{wx \in E(G)} \left(\frac{S_w S_x}{S_w + S_x - 2}\right)^3.$$

$$S(C_{16}H_{21}NO_2) = |E_{(3,4)}| \sum_{wx \in E(C_{16}H_{21}NO_2)} \left(\frac{S_w S_x}{S_w + S_x - 2}\right)^3$$

$$+\left|E_{(3,5)}\right| \sum_{wx \in E(C_{16}H_{21}NO_2)} \left(\frac{S_w S_x}{S_w + S_x - 2}\right)^3 + \left|E_{(4,4)}\right| \sum_{wx \in E(C_{16}H_{21}NO_2)} \left(\frac{S_w S_x}{S_w + S_x - 2}\right)^3$$

$$+ \left|E_{(4,5)}\right| \sum_{wx \in E(C_{16}H_{21}NO_2)} \left(\frac{S_w S_x}{S_w + S_x - 2}\right)^3 + \left|E_{(5,5)}\right| \sum_{wx \in E(C_{16}H_{21}NO_2)} \left(\frac{S_w S_x}{S_w + S_x - 2}\right)^3$$

$$+ \left|E_{(7,5)}\right| \sum_{wx \in E(C_{16}H_{21}NO_2)} \left(\frac{S_w S_x}{S_w + S_x - 2}\right)^3 + \left|E_{(8,5)}\right| \sum_{wx \in E(C_{16}H_{21}NO_2)} \left(\frac{S_w S_x}{S_w + S_x - 2}\right)^3$$

$$+ \left|E_{(7,8)}\right| \sum_{wx \in E(C_{16}H_{21}NO_2)} \left(\frac{S_w S_x}{S_w + S_x - 2}\right)^3.$$

$$= (2)\left(\frac{12}{3+4-2}\right)^3 + (1)\left(\frac{15}{3+5-2}\right)^3 + (1)\left(\frac{16}{4+4-2}\right)^3 + (5)\left(\frac{20}{4+5-2}\right)^3$$

$$+ (4)\left(\frac{25}{5+5-2}\right)^3 + (4)\left(\frac{35}{7+5-2}\right)^3 + (1)\left(\frac{40}{8+5-2}\right)^3 + (2)\left(\frac{56}{7+8-2}\right)^3.$$

$$= 2\left(\frac{12}{5}\right)^3 + \left(\frac{5}{2}\right)^3 + \left(\frac{8}{3}\right)^3 + 5\left(\frac{20}{7}\right)^3 + 4\left(\frac{25}{8}\right)^3 + 4\left(\frac{7}{2}\right)^3 + \left(\frac{40}{11}\right)^3 + 2\left(\frac{56}{13}\right)^3.$$

$$S(C_{16}H_{21}NO_2) = 680.3774$$

4.Conclusion:

Topological indices give critical information on the chemical structure and activity of a molecule. There are about 148 topological indices, computation of topological indices are very helpful to predict several characteristics of chemical structure without having to travel to the wet lab. In this research workwe computed geometric arithmeticindex, atom bond connectivity index, forgotten index, randic connectivity index, harmonic index, sombor index, fifth geometric arithmetic index, sanskruti Index of the Propranolol ($C_{16}H_{21}NO_2$).

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