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Computing Zagreb Indices For Propranolol

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Abstract

A chemical graph is a simple graph whose vertices relate to the atoms and edges relate to the chemical bonds in terms of graph theory. A topological index of a molecular structure is a numerical pattern which helps to understand the physical, chemical and biological properties of molecular structures. They are also significantly important in quantitative structure-property relationship and quantitative structure-activity relationship investigations. Mainly, topological indices are sorted based on distance, degree and spectrum. Among these, chemical graphs which are based on the degree assume a significant role in chemical graph theory. It is defined in terms of degrees of the vertices of a graph. The Zagreb indices is one among the degree-based topological indices which depends on the connection number to compute the total electron of the alternate hydrocarbon. In this paper, we have analysed certain types of Zagreb indices of Propranolol.

Keywords: Topological indices; Propranolol; Zagreb index.

INTRODUCTION

Graph theory is very much useful in chemistry mainly in modelling molecular structures. The properties which are computable for graphs lay the groundwork to identify the relationships between molecular structure and biological activity of the compounds under study [1, 2]. Topological indices are numerical value associated to molecular graph. Several indices have been identified and used for correlation analysis [3].

The most widely used topological index is the Wiener index used by Harold Wiener in 1947, which depends on the topological distance of vertices in the graph. It is utilized to compare the physical properties of alkane isomers [4].

The first and the second Zagreb indices are the earliest degree based topological indices presented by Gutman, N. Trinajstic in the year 1972 [5]. The formulae of these indices for the graphs like path, cycle, star and complete graphs were computed in the year 2012 [6]. The lower and the upper bounds of these two indices were discussed in the year 2017 [7]. The Zagreb and multiplicative Zagreb indices of Eulerian graphs, double graphs, subdivision graphs, double graphs of the subdivision graphs and subdivision graphs of the double graphs of G were also calculated [8, 9]. In the series of papers [10 – 14] Zagreb and multiplicative Zagreb indices of Molecular Structures were computed.

The theoretical analysis of topological indices like Zagreb indices for the molecular structures gives an important application prospect in chemical and pharmacy engineering. They are utilized to test the medication and pharmacology attributes of medications. Zagreb index (1st, 2nd, 3rd, multiplicative, redefined) and polynomial of Dox-loaded micelle helps in anticancer drug study [15]. For the purpose of examining drug structures, the modified first Zagreb connection number index is described[16]. Zagreb indices are analyzed using multi-order polynomials are clearing the new way for new medication innovation for AIDS [17]. Few Zagreb indices on the well – know biodegradable dendrimers such as fourth-generation poly(amidoamine) dendrimer and the dendrimer based on glycerol and succinic acid are used in cancer therapy [18].

Propranolol is a beta - blocker, which is utilized to treat angina, heart cadence issues and other heart or circulatory circumstances [19]. It additionally assists with treating coronary failure, and to decrease the seriousness and recurrence of headache migraines. This drug reduces the activity of certain naturally occurring synthetic substances in our bodies, such as epinephrine, which relaxes veins and slows down the heartbeat to increase blood flow and reduce circulatory strain. It also helps to reduce our symptoms if we have too much thyroid hormone in our body.

The molecular formula of Propranolol is $C_{16}H_{21}NO_2$ and its molecular structure is shown in Figure 1. For Propranolol, the degree based topological indices like geometric arithmetic index, atom bond connectivity index, forgotten index, randic connectivity index, harmonic index, sombor index, fifth geometric arithmetic index, sanskruti index were calculated [20].

In this paper, we have worked out Zagreb indices, Multiplicative Zagreb indices, Redefined Zagreb indices and Hyper Zagreb index for Propranolol.

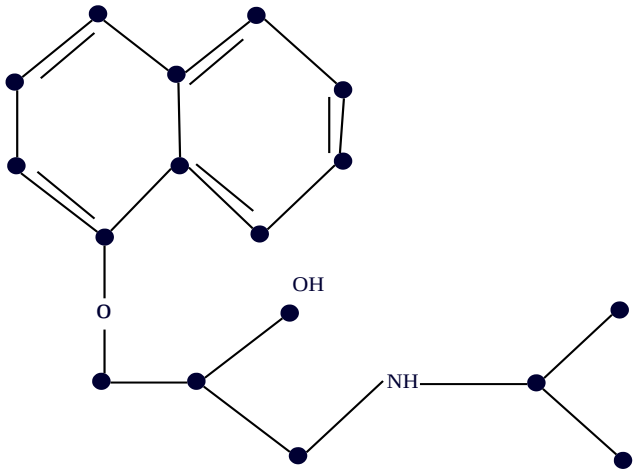

Figure 1 Chemical Structure of Propranolol ($C_{16}H_{21}NO_2$)

BASIC CONCEPTS AND TERMINOLOGY

Let G be a simple chemical graph, where the atoms of the molecule are represented by the vertex set $V(G)$ and the chemical bonds are represented the edge set $E(G)$. The number of edges that are incident with a certain vertex is used to calculate the vertex's degree and it is represented by d_p where $p \in V(G)$.

The fundamental definitions required for the study are covered in this section.

Definition .1. [21] The first Zagreb index of a graph G is defined as

$$M_1(G) = \sum_{p \in V(G)} d^2(p).$$

Definition .2. [22] The second Zagreb index of a graph G is defined as

$$M_2(G) = \sum_{pq \in E(G)} d_p d_q.$$

Definition .3. [23] The third Zagreb index of a graph G is defined as

$$M_3(G) = \sum_{pq \in E(G)} |d_p - d_q|.$$

Definition .4. [24] The first multiplicative Zagreb index of a graph G is defined as

$$PM_1(G) = \prod_{pq \in E(G)} [d_p + d_q].$$

Definition .5. [25, 26] The second multiplicative Zagreb index of a graph G is defined as

$$PM_2(G) = \prod_{pq \in E(G)} [d_p d_q].$$

Definition .6. [27] The redefined first Zagreb index for a graph G is defined as

$$ReZG_1(G) = \sum_{pq \in E(G)} \frac{d_p + d_q}{d_p d_q}.$$

Definition .7. [28] The redefined second Zagreb index for a graph G is defined as

$$ReZG_2(G) = \sum_{pq \in E(G)} \frac{d_p d_q}{d_p + d_q}.$$

Definition .8. [28] The redefined third Zagreb index for a graph G is defined as

$$ReZG_3(G) = \sum_{pq \in E(G)} [d_p d_q][d_p + d_q].$$

Definition .9. [29] The hyper Zagreb index for a graph G is defined as

$$HM(G) = \sum_{pq \in E(G)} [d_p + d_q]^2.$$

TOPOLOGICAL INDICES OF THE PROPRANOLOL BASED ON DEGREE

Theorem. 1. The first Zagreb index of the Propranolol $(C_{16}H_{21}NO_2)$ is $M_1(C_{16}H_{21}NO_2) = 92$.

Proof: Let G be the graph of the Propranolol $(C_{16}H_{21}NO_2)$. Let V_p denote the vertices of degrees d_p and $E_{(p,q)}$ denote the edges which connects the vertices of degrees d_p and d_q. The vertex set and edge set of propranolol $(C_{16}H_{21}NO_2)$ has the following partition as shown in Tables 1 & 2.

TABLE .1. *Partition of vertices*

$V(d_p)$	V_1	V_2	V_3
Number of vertices	3	11	5

TABLE .2. *Partition of edges*

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

By definition 1 and Table 1, we get the results, i.e.

$M_1(C_{16}H_{21}NO_2) = \sum_{p \in V(G)} d_p^2$. (1)

$$M_1(C_{16}H_{21}NO_2) = |V_1| \sum_{p \in V(C_{16}H_{21}NO_2)} d_p^2 + |V_2| \sum_{p \in V(C_{16}H_{21}NO_2)} d_p^2 + |V_3| \sum_{p \in V(C_{16}H_{21}NO_2)} d_p^2$$
$$= 3(1^2) + 11(2^2) + 5(3^2)$$

Therefore, $M_1(C_{16}H_{21}NO_2) = 92$.

Theorem .2. The second Zagreb index of the Propranolol $(C_{16}H_{21}NO_2)$ is $M_2(C_{16}H_{21}NO_2) = 103$.

Proof: By definition 2 and Table 2, we get the results, i.e.

$M_2(C_{16}H_{21}NO_2) = \sum_{pq \in E(G)} d_p d_q$ (2)

$$M_2(C_{16}H_{21}NO_2)$$
$$= |E_{(1,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} d_p d_q + |E_{(2,2)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} d_p d_q$$
$$+ |E_{(2,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} d_p d_q + |E_{(3,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} d_p d_q$$
$$= 3(1\times 3) + 7(2\times 2) + 8(2\times 3) + 2(3\times 3)$$
$$= 3(3) + 7(4) + 8(6) + 2(9)$$

Therefore, $M_2(C_{16}H_{21}NO_2) = 103$.

Theorem .3. The third Zagreb index of the Propranolol $(C_{16}H_{21}NO_2)$ is $M_3(C_{16}H_{21}NO_2) = 14$.

Proof: By definition 3 and Table 2, we get the results, i.e.

$M_3(C_{16}H_{21}NO_2) = \sum_{pq\in E(G)} |d_p - d_q|$ (3)

$$M_3(C_{16}H_{21}NO_2) = |E_{(1,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} |d_p - d_q| + |E_{(2,2)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} |d_p - d_q|$$
$$+ |E_{(2,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} |d_p - d_q| + |E_{(3,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} |d_p - d_q|$$
$$= 3|1-3| + 7|2-2| + 8|2-3| + 2|3-3|$$
$$= 3(2) + 7(0) + 8(1) + 2(0)$$

Therefore, $M_3(C_{16}H_{21}NO_2) = 14$.

Theorem .4. The first multiplicative Zagreb index of the Propranolol $(C_{16}H_{21}NO_2)$ is $PM_1(C_{16}H_{21}NO_2) = 1{,}47{,}456 \times 10^8$.

Proof: By definition 4 and Table 2, we get the results, i.e.

$PM_1(C_{16}H_{21}NO_2) = \prod_{pq\in E(G)} [d_p + d_q]$ (4)

$$PM_1(C_{16}H_{21}NO_2) = \left(\prod_{pq\in E(C_{16}H_{21}NO_2)} [d_p + d_q]\right)^{|E_{(1,3)}|} \times \left(\prod_{pq\in E(C_{16}H_{21}NO_2)} [d_p + d_q]\right)^{|E_{(2,2)}|}$$
$$\times \left(\prod_{pq\in E(C_{16}H_{21}NO_2)} [d_p + d_q]\right)^{|E_{(2,3)}|} \times \left(\prod_{pq\in E(C_{16}H_{21}NO_2)} [d_p + d_q]\right)^{|E_{(3,3)}|}$$
$$= 4^3 \times 4^7 \times 5^8 \times 6^2$$

Therefore, $PM_1(C_{16}H_{21}NO_2) = 1{,}47{,}456 \times 10^8$.

Theorem .5. The second multiplicative Zagreb index of the Propranolol $(C_{16}H_{21}NO_2)$ is $PM_2(C_{16}H_{21}NO_2) = 60{,}183{,}678{,}025{,}728$.

Proof: By definition 5 and Table 2, we get the results, i.e.

$PM_2(C_{16}H_{21}NO_2) = \prod_{pq\in E(G)} [d_p d_q]$ (5)

$$PM_2(C_{16}H_{21}NO_2) = \left(\prod_{pq\in E(C_{16}H_{21}NO_2)} [d_p d_q]\right)^{|E_{(1,3)}|} \times \left(\prod_{pq\in E(C_{16}H_{21}NO_2)} [d_p d_q]\right)^{|E_{(2,2)}|}$$
$$\times \left(\prod_{pq\in E(C_{16}H_{21}NO_2)} [d_p d_q]\right)^{|E_{(2,3)}|} \times \left(\prod_{pq\in E(C_{16}H_{21}NO_2)} [d_p d_q]\right)^{|E_{(3,3)}|}$$
$$= 3^3 \times 4^7 \times 6^8 \times 9^2$$

Therefore, $PM_2(C_{16}H_{21}NO_2) = 60{,}183{,}678{,}025{,}728$.

Theorem .6. The redefined first Zagreb index of the Propranolol $C_{16}H_{21}NO_2$ is not a topological index.

Proof: By definition 6 and Table 2, we get the results, i.e.

$ReZG_1(C_{16}H_{21}NO_2) = \sum_{pq\in E(G)} \frac{d_p + d_q}{d_p d_q}$ (6)

$$ReZG_1(C_{16}H_{21}NO_2) = |E_{(1,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} \frac{d_p+d_q}{d_p d_q} + |E_{(2,2)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} \frac{d_p+d_q}{d_p d_q}$$
$$+|E_{(2,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} \frac{d_p+d_q}{d_p d_q} + |E_{(3,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} \frac{d_p+d_q}{d_p d_q}$$
$$= 3\left(\frac{1+3}{1\times 3}\right) + 7\left(\frac{2+2}{2\times 2}\right) + 8\left(\frac{2+3}{2\times 3}\right) + 2\left(\frac{3+3}{3\times 3}\right)$$
$$= 3\left(\frac{4}{3}\right) + 7\left(\frac{4}{4}\right) + 8\left(\frac{5}{6}\right) + 2\left(\frac{6}{9}\right)$$

Therefore, $ReZG_1(C_{16}H_{21}NO_2) = 19$.
Since, [29] $ReZG_1(C_{16}H_{21}NO_2)$ = Number of vertices of Propranolol, then the redefined first Zagreb index is not a topological index.

Theorem .7. The redefined second Zagreb index of the Propranolol $(C_{16}H_{21}NO_2)$ is $ReZG_2(C_{16}H_{21}NO_2) = 21.85$.
Proof: By definition 7 and Table 2, we get the results, i.e.
$ReZG_2(C_{16}H_{21}NO_2) = \sum_{pq\in E(G)} \frac{d_p d_q}{d_p+d_q}$. (7)

$$ReZG_2(C_{16}H_{21}NO_2) = |E_{(1,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} \frac{d_p d_q}{d_p+d_q} + |E_{(2,2)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} \frac{d_p d_q}{d_p+d_q}$$
$$+|E_{(2,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} \frac{d_p d_q}{d_p+d_q} + |E_{(3,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} \frac{d_p d_q}{d_p+d_q}$$
$$= 3\left(\frac{1\times 3}{1+3}\right) + 7\left(\frac{2\times 2}{2+2}\right) + 8\left(\frac{2\times 3}{2+3}\right) + 2\left(\frac{3\times 3}{3+3}\right)$$
$$= 3\left(\frac{3}{4}\right) + 7\left(\frac{4}{4}\right) + 8\left(\frac{6}{5}\right) + 2\left(\frac{9}{6}\right)$$

Therefore, $ReZG_2(C_{16}H_{21}NO_2) = 21.85$.

Theorem .8. The redefined third Zagreb index of the Propranolol $(C_{16}H_{21}NO_2)$ is $ReZG_3(C_{16}H_{21}NO_2) = 496$.
Proof: By definition 8 and Table 2, we get the results, i.e.
$ReZG_3(C_{16}H_{21}NO_2) = \sum_{pq\in E(G)} [d_p d_q][d_p+d_q]$. (8)

$$ReZG_3(C_{16}H_{21}NO_2) = |E_{(1,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} [d_p d_q][d_p+d_q] + |E_{(2,2)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} [d_p d_q][d_p+d_q]$$
$$+ |E_{(2,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} [d_p d_q][d_p+d_q] + |E_{(3,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} [d_p d_q][d_p+d_q]$$

$$= [3\times(1\times 3)\times(1+3)] + [7\times(2\times 2)\times(2+2)] + [8\times(2\times 3)\times(2+3)]$$
$$+ [2\times(3\times 3)\times(3+3)]$$
$$= [3\times 3\times 4] + [7\times 4\times 4] + [8\times 6\times 5] + [2\times 9\times 6]$$

Therefore, $ReZG_3(C_{16}H_{21}NO_2) = 496$.

Theorem .9. The hyper Zagreb index of the Propranolol $(C_{16}H_{21}NO_2)$ is $HM(C_{16}H_{21}NO_2) = 432$.
Proof: By definition 9 and Table 2, we get the results, i.e.
$HM(C_{16}H_{21}NO_2) = \sum_{pq\in E(G)} [d_p + d_q]^2$. (9)

$$HM(C_{16}H_{21}NO_2) = |E_{(1,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} [d_p + d_q]^2 + |E_{(2,2)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} [d_p + d_q]^2$$
$$+ |E_{(2,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} [d_p + d_q]^2 + |E_{(3,3)}| \sum_{pq\in E(C_{16}H_{21}NO_2)} [d_p + d_q]^2$$
$$= 3(1+3)^2 + 7(2+2)^2 + 8(2+3)^2 + 2(3+3)^2$$
$$= 3(16) + 7(16) + 8(25) + 2(36)$$

Therefore, $HM(C_{16}H_{21}NO_2) = 432$.

CONCLUSION

To analyse the molecular structures of chemical compounds, topological indices are useful. In this specific research, we looked at a few numerical graph invariants of a few molecular graphs and also got several various Zagreb indices, including multiplicative & redefined Zagreb indices and hyper-Zagreb indices for Propranolol.

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