

# LEAP ZAGREB INDICES OF CETIRIZINE

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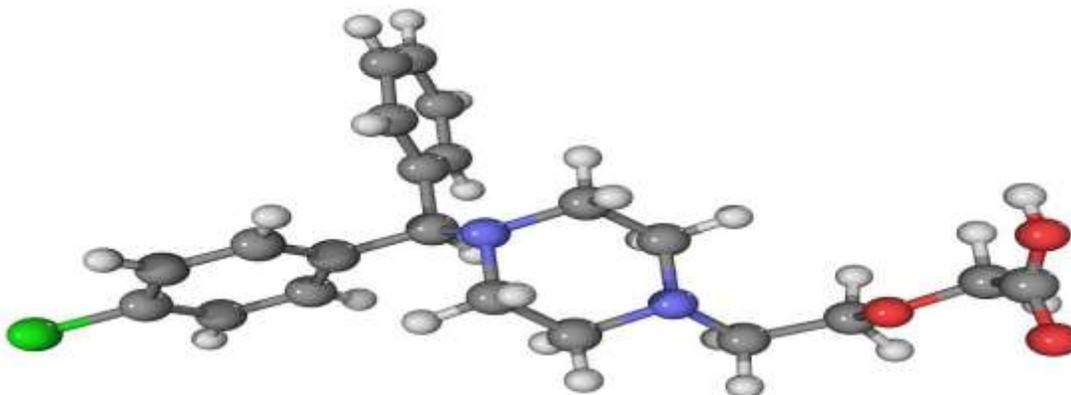
**Abstract:** Graph theory has provided chemists with a variety of useful tools, such as topological indices. A topological index  $Top(G)$  of a graph  $G$  is a number with the property that for every graph  $H$  isomorphic to  $G$ ,  $Top(H) = Top(G)$ . Based on second distance degrees of the vertices, A.M. Naji et al. defined a topological index called Leap Zagreb indices of Graphs. In this article, we have computed first, second and third Leap Zagreb indices of Cetirizine.

**Mathematics Subject Classification :** Primary 05C50,05C69.

**Keywords:** Topological index, Zagreb index First leap Zagreb index , second leap Zagreb index and third leap Zagreb index, Cetirizine.

## I. INTRODUCTION

Cetirizine was discovered in Belgium by a multinational biopharmaceutical company, Union Chimique Belge(UCB) during 1980's. This drug came into medical use in the year 1987. It is used to treat the symptoms of allergic reaction like watery eyes, a runny nose, sneezing, itchy eyes and throat etc. Its molecular formula is  $C_{21}H_{25}ClN_2O_3$ .



**Figure 1 - Structural graph of Cetirizine**

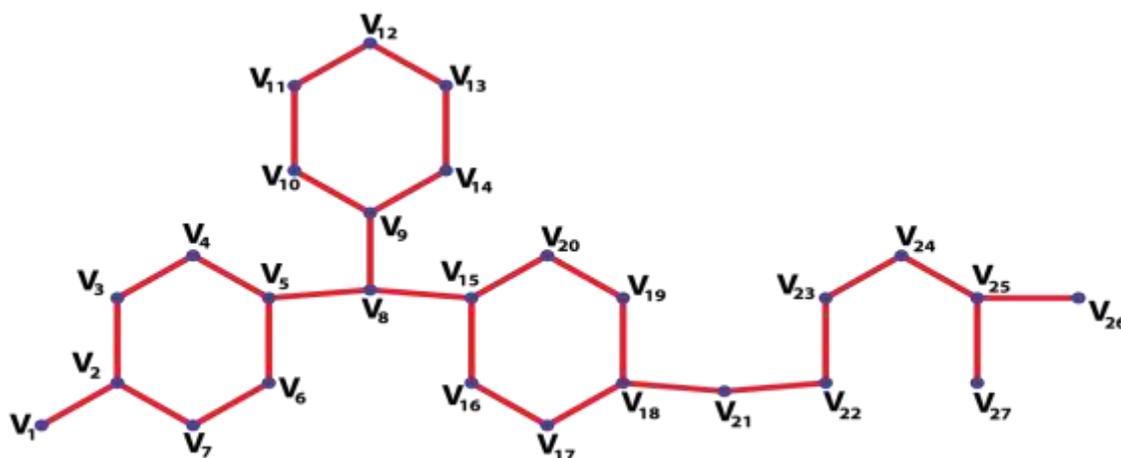


Figure - Molecular graph of Cetirizine

Topological indices are the molecular descriptors that describe the structures of chemical compounds and they help us to predict certain physico-chemical properties like boiling point, enthalpy of vaporization, stability, etc. Molecules and molecular compounds are often modeled by molecular graph. A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. Note that hydrogen atoms are often omitted. All molecular graphs considered in this paper are finite, connected, loop less and without multiple edges.

Let  $G = (V, E)$  be a graph with vertex set  $V$  and edge set  $E$ . The degree of a vertex  $u \in V(G)$  is denoted by  $d_u$  and is the number of vertices that are adjacent to  $u$ . The edge connecting the vertices  $u$  and  $v$  is denoted by  $uv$ .

The Zagreb indices were first introduced in [1] where the authors examined the dependence of total pi-electron energy of molecular structures. For a molecular graph, the first Zagreb index  $M_1(G)$  and the second Zagreb index  $M_2(G)$  are defined, respectively, as follows.

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

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

Motivated by this, in 2017, Naji et al., [2] have introduced a new distance-degree-based topological indices conceived depending on the second degrees of vertices, and are so-called leap Zagreb indices of a graph  $G$  and are defined as:

$$LM_1(G) = \sum_{v \in V(G)} d_2^2(v/G)$$

$$LM_2(G) = \sum_{uv \in E(G)} d_2(u/G) d_2(v/G)$$

$$LM_3(G) = \sum_{uv \in E(G)} (d_2(u/G) + d_2(v/G))$$

The leap Zagreb indices have several chemical applications. Surprisingly, the first leap Zagreb index has very good correlation with physical properties of chemical compound, like boiling point, entropy, DHVAP, HVAP and eccentric factor .

## II. Main Results and Discussion:

**Theorem 2.1:** First Leap Zagreb index of Cetirizine is 228.

**Proof:** Consider a molecular graph of Cetirizine . It contains 27 vertices and 29 edges. Cetirizine contains vertices of 2-degrees 1, 2, 3, 4 and 6 only and we can partition the vertices of cetirizine into five sets, viz.  $V_1$ ,  $V_2$ ,  $V_3$ ,  $V_4$  and  $V_6$ , where each set  $V_i$  represents the collection of all vertices with 2-degree  $i$ . The number of vertices of 2-degree 1, 2, 3, 4 and 6 are given in the following table-1.

Vertices of 2-degree $i$	$V_1(G)$	$V_2(G)$	$V_3(G)$	$V_4(G)$	$V_6(G)$
Frequency	1	11	11	3	1

TABLE - 1

Consider,

$$\begin{aligned}
 LM_1(G) &= \sum_{v \in V(G)} d_2^2(v/G) \\
 &= \sum_{v \in V_1(G)} d_2^2(v/G) + \sum_{v \in V_2(G)} d_2^2(v/G) + \sum_{v \in V_3(G)} d_2^2(v/G) + \sum_{v \in V_4(G)} d_2^2(v/G) + \sum_{v \in V_6(G)} d_2^2(v/G) \\
 &= 1(1)^2 + 11(2)^2 + 11(3)^2 + 3(4)^2 + 1(6)^2 \\
 &= 228.
 \end{aligned}$$

**Theorem 2.2:** Second Leap Zagreb index of cetirizine is 253.

**Proof:**

Cetirizine contains vertices of 2-degrees 1, 2, 3, 4 and 6 and edges of the type  $E_{1,2}$ ,  $E_{2,2}$ ,  $E_{2,3}$ ,  $E_{2,4}$ ,  $E_{3,1}$ ,  $E_{3,3}$ ,  $E_{3,4}$  and  $E_{4,6}$  respectively. The frequency of such edges are shown in the following table-5, where  $E_{i,j}$  is the collection of all edges joining the vertices of 2-degrees i and j in G.

Edge type	$E_{1,2}$	$E_{1,3}$	$E_{2,2}$	$E_{2,3}$	$E_{2,4}$	$E_{3,3}$	$E_{3,4}$	$E_{4,6}$
Frequency	2	1	5	6	2	6	4	3

**TABLE-2**

$$\begin{aligned}
 LM_2(G) &= \sum_{uv \in E(G)} d_2(u/G) d_2(v/G) \\
 &= \sum_{uv \in E_{1,2}(G)} d_2(u/G) d_2(v/G) + \sum_{uv \in E_{1,3}(G)} d_2(u/G) d_2(v/G) + \sum_{uv \in E_{2,2}(G)} d_2(u/G) d_2(v/G) \\
 &\quad + \sum_{uv \in E_{2,3}(G)} d_2(u/G) d_2(v/G) + \sum_{uv \in E_{2,4}(G)} d_2(u/G) d_2(v/G) + \sum_{uv \in E_{3,3}(G)} d_2(u/G) d_2(v/G) \\
 &\quad + \sum_{uv \in E_{3,4}(G)} d_2(u/G) d_2(v/G) + \sum_{uv \in E_{4,6}(G)} d_2(u/G) d_2(v/G) \\
 &= 2(1 \times 2) + 1(1 \times 3) + 5(2 \times 2) + 6(2 \times 3) + 2(2 \times 4) + 6(3 \times 3) + 4(3 \times 4) + 3(4 \times 6) \\
 \therefore LM_2(G) &= 253.
 \end{aligned}$$

**Theorem 2.3:** Third Leap Zagreb index of cetirizine is 166.

**Proof:** By definition of third Leap Zagreb index and by using table - 2 we have,

$$\begin{aligned}
 LM_3(G) &= \sum_{uv \in E(G)} d_2(u/G) + d_2(v/G) \\
 &= \sum_{uv \in E_{1,2}(G)} d_2(u/G) + d_2(v/G) + \sum_{uv \in E_{1,3}(G)} d_2(u/G) + d_2(v/G) + \sum_{uv \in E_{2,2}(G)} d_2(u/G) + d_2(v/G) \\
 &\quad + \sum_{uv \in E_{2,3}(G)} d_2(u/G) + d_2(v/G) + \sum_{uv \in E_{2,4}(G)} d_2(u/G) + d_2(v/G) + \sum_{uv \in E_{3,3}(G)} d_2(u/G) + d_2(v/G) \\
 &\quad + \sum_{uv \in E_{3,4}(G)} d_2(u/G) + d_2(v/G) + \sum_{uv \in E_{4,6}(G)} d_2(u/G) + d_2(v/G) \\
 &= 2(1+2) + 1(1+3) + 5(2+2) + 6(2+3) + 2(2+4) + 6(3+3) + 4(3+4) + 3(4+6)
 \end{aligned}$$

$$\therefore LM_3(G) = 166.$$

## CONCLUSIONS:

The first, second and third Leap Zagreb indices of Cetirizine are calculated without using computer.

## REFERENCES:

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