

## Topological 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  $G$ ,  $Top(H) = Top(G)$ . In this paper, we compute ABC index,  $ABC_4$  index, Randic index, sum connectivity index, GA index,  $GA_5$  index, first Zagreb index, second Zagreb index, first multiple Zagreb index, second multiple Zagreb index, augmented Zagreb index, harmonic index and hyper Zagreb index, first Zagreb polynomial, second Zagreb polynomial, third Zagreb polynomial, forgotten topological index, forgotten polynomial and symmetric division index of Cetirizine.

**Keywords:** ABC index,  $ABC_4$  index, Randic connectivity index, Sum connectivity index, GA index,  $GA_5$  index, First Zagreb index, Second Zagreb index, First Multiple Zagreb index, Second Multiple Zagreb index, Augmented Zagreb index, Harmonic index, Hyper Zagreb index, First Zagreb polynomial, Second Zagreb polynomial, Third Zagreb polynomial, Forgotten topological index, Forgotten polynomial, Symmetric division index and Cetirizine.

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### I. INTRODUCTION

Ceterizine 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  $C_{21}H_{25}ClN_2O_3$ .

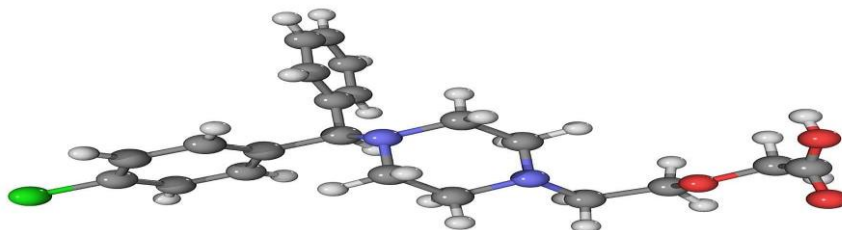


Figure 1 - Cetirizine

Topological indices are the molecular descriptors that describe the structures of chemical compounds and they help us to predict certain physic-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  $u \in E(G)$  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 atom-bond connectivity index, ABC index is one of the degree based molecular descriptor, which was introduced by Estrada et al. [7] in late 1990's and it can be used for modeling thermodynamic properties of organic chemical compounds, it is also used as a tool for explaining the stability of branched alkenes [8]. Some upper bounds for the atom-bond connectivity index of graphs can be found in [3]. The atom-bond connectivity index of chemical bicyclic graphs, connected graphs can be seen in [4, 30]. For further results on ABC index of trees see the papers [11, 21, 29, 31] and the references cited there in.

**Definition.1.1.** Let  $G = (V, E)$  be a molecular graph and  $d_u$  is the degree of the vertex  $u$ , then ABC index of  $G$  is defined as,

$$ABC(G) = \sum_{uv \in E} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

The fourth atom bond connectivity index,  $ABC_4(G)$  index was introduced by M.Ghorbaniet al. [15] in 2010. Further studies on  $ABC_4(G)$  index can be found in [9, 10].

**Definition.1.2.** Let  $G$  be a graph, then its fourth ABC index is defined as,

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{s_u + s_v - 2}{s_u s_v}},$$

where  $S_u$  is sum of degrees of all neighbors of vertex  $u$  in  $G$ . In other words  $s_u = \sum_{uv \in E(G)} d_v$ , similarly  $S_v$ . The first and oldest degree based topological index is Randic index [23] denoted by  $\chi(G)$  and was introduced by Milan Randic in 1975. It provides a quantitative assessment of branching of molecules.

**Definition.1.3.** For the graph  $G$  Randic index is defined as,

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

Sum connectivity index belongs to a family of Randic like indices and it was introduced by Zhou and N. Trinajstić[33]. Further studies on Sum connectivity index can be found in [34, 35].

**Definition.1.4.** For a simple connected graph  $G$ , its sum connectivity index  $S(G)$  is defined as,

$$S(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}$$

The geometric-arithmetric index,  $GA(G)$  index of a graph  $G$  was introduced by D. Vukicević et al.[27]. Further studies on  $GA$  index can be found in [2, 5, 32].

**Definition.1.5.** Let  $G$  be a graph and  $e = uv$  be an edge of  $G$  then

$$GA(G) = \sum_{e=uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

The fifth geometric-arithmetric index,  $GA_5(G)$  was introduced by A.Graovac et al [16] in 2011.

**Definition.1.6.** For a Graph  $G$ , the fifth Geometric-arithmetric index is defined as,

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{s_u s_v}}{s_u + s_v},$$

where  $S_u$  is the sum of the degrees of all neighbors of the vertex  $u$  in  $G$ , similarly  $S_v$ .

A pair of molecular descriptors (or topological index), known as the first Zagreb index  $Z_1(G)$  and second Zagreb index  $Z_2(G)$ , first appeared in the topological formula for the total  $\pi$ -energy of conjugated molecules that has been derived in 1972 by I. Gutman and N.Trinajstić[17]. Soon after these indices have been used as branching indices. Later the Zagreb indices found applications in QSPR and QSAR studies. Zagreb indices are included in a number of programs used for the routine computation of topological indices POLLY, DRAGON, CERUIUS, TAM, DISSI.  $Z_1(G)$  and  $Z_2(G)$  were recognize as measures of the branching of the carbon atom molecular skeleton [20], and since then these are frequently used for structure property modeling. Details on the chemical applications of the two Zagreb indices can be found in the books [25, 26]. Further studies on Zagreb indices can be found in [1, 18].

**Definition.1.7.** For a simple connected graph  $G$ , the first and second Zagreb indices were defined as follows,

$$Z_1(G) = \sum_{e=uv \in E(G)} (d_u + d_v), \quad Z_2(G) = \sum_{e=uv \in E(G)} (d_u d_v)$$

Where  $d_v$  denotes the degree (number of first neighbors) of vertex  $v$  in  $G$ .

In 2012, M. Ghorbani and N. Azimi [14] defined the Multiple Zagreb topological indices of a graph  $G$ , based on degree of vertices of  $G$ .

**Definition.1.8.** For a simple connected graph  $G$ , the first and second multiple Zagreb indices were defined as follows

$$PM_1(G) = \prod_{e=uv \in E(G)} (d_u + d_v), \quad PM_2(G) = \prod_{e=uv \in E(G)} (d_u d_v).$$

Properties of the first and second multiple Zagreb indices may be found in [6, 19].

The augmented Zagreb index was introduced by Furtula et al [12]. This graph invariant has proven to be a valuable predictive index in the study of the heat of formation in octane's and heptanes, is a novel topological index in chemical graph theory, whose prediction power is better than atom-bond connectivity index. Some basic investigation implied that AZI index has better correlation properties and structural sensitivity among the very well established degree based topological indices.

**Definition.1.9.** Let  $G = (V, E)$  be a graph and  $d_u$  be the degree of a vertex  $u$ , then augmented Zagreb index is denoted by  $AZI(G)$  and is defined as,

$$AZI(G) = \sum_{uv \in E} \left[ \frac{d_u d_v}{d_u + d_v - 2} \right]^3.$$

Further studies can be found in [22] and the references cited there in.

The harmonic index was introduced by Zhong[36]. It has been found that the harmonic index correlates well with the Randic index and with the  $\pi$ -electron energy of benzenoid hydro carbons.

**Definition.1.10.** Let  $G = (V, E)$  be a graph and  $d_u$  be the degree of a vertex  $u$  then harmonic index is defined as,

$$H(G) = \sum_{e=uv \in E(G)} \frac{2}{d_u + d_v}.$$

Further studies on  $H(G)$  can be found in [28, 34].

G.H. Shirdel et.al[24] introduced a new distance-based of Zagreb indices of a graph  $G$  named Hyper-Zagreb Index.

**Definition.1.11 .** The hyper Zagreb index is defined as,

$$HM(G) = \sum_{e=uv \in E(G)} (d_u + d_v)^2.$$

Fath-Tabar [37] introduced the third Zagreb index in 2011. which is defined by,

**Definition.1.12.** For a simple connected graph  $G$ , the third Zagreb index is defined as,

$$ZG_3(G) = \sum_{e=uv \in E(G)} |d_u - d_v|.$$

Again in 2011 Fath-Tabar [37] introduced the first, second and third Zagreb Polynomials as follows by,

**Definition.1.13.** The first, second and third Zagreb Polynomials for a simple connected graph  $G$  is defined as,

$$\begin{aligned} ZG_1(G, x) &= \sum_{e=uv \in E(G)} x^{d_u + d_v}, \\ ZG_2(G, x) &= \sum_{e=uv \in E(G)} x^{d_u d_v}, \\ ZG_3(G, x) &= \sum_{e=uv \in E(G)} x^{|d_u - d_v|}. \end{aligned}$$

**Definition.1.14.** The forgotten topological index is also a degree based topological index, denoted by  $F(G)$  for simple graph  $G$ . It was encountered in [13], defined as,

$$F(G) = \sum_{e=uv \in E(G)} [(d_u)^2 + (d_v)^2].$$

**Definition.1.15.** The forgotten topological polynomials for a graph  $G$  defined as,

$$F(G, x) = \sum_{e=uv \in E(G)} x^{[(d_u)^2 + (d_v)^2]}.$$

**Definition.1.16.** There are some new degrees based graph invariants, which plays an important role in chemical graph theory. These topological indices are quite useful for determining total surface area and heat formation of some chemical compounds. These graphs invariants are as follow symmetric division index,

$$SDD(G) = \sum_{e=uv} \left\{ \frac{\min(d_u, d_v)}{\max(d_u, d_v)} + \frac{\max(d_u, d_v)}{\min(d_u, d_v)} \right\}.$$

## II. MAIN RESULTS

**Theorem.2.1.** The atom bond connectivity index of Cetirizine is 20.712946.

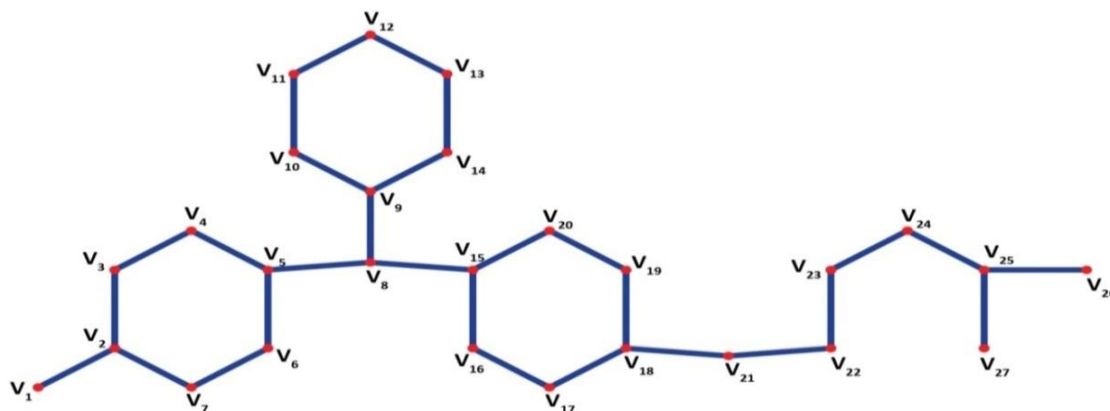


Figure 2.

**Proof:** Consider a molecular graph of Cetirizine ( $C_{21}H_{25}ClN_2O_3$ ). Let  $m_{ij}$  denotes edges connecting the vertices of degrees  $d_i$  and  $d_j$ . Two-dimensional structure of Cetirizine (as shown in the Figure-2) contains edges of the type  $m_{1,3}$ ,  $m_{2,2}$ ,  $m_{2,3}$  and  $m_{3,3}$ . From the figure-2, the number edges of these types are  $|m_{1,3}| = 3$ ,  $|m_{2,2}| = 11$ ,  $|m_{2,3}| = 12$  and  $|m_{3,3}| = 3$ .

∴ The atom-bond connectivity index of Cetirizine  $ABC(C_{21}H_{25}ClN_2O_3)$

$$\begin{aligned} &= \sum_{uv \in E} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\ &= |m_{1,3}| \sqrt{\frac{1+3-2}{1.3}} + |m_{2,2}| \sqrt{\frac{2+2-2}{2.2}} + |m_{2,3}| \sqrt{\frac{2+3-2}{2.3}} + |m_{3,3}| \sqrt{\frac{3+3-2}{3.3}} \\ &= 3 \times \sqrt{\frac{2}{3}} + 11 \times \sqrt{\frac{1}{2}} + 12 \times \sqrt{\frac{1}{2}} + 3 \times \frac{2}{3}. \end{aligned}$$

$$\therefore ABC(C_{21}H_{25}ClN_2O_3) = 20.712946.$$

**Theorem.2.2.** The fourth atom bond connectivity index of Cetirizine is 16.377236.

**Proof:** Let  $e_{ij}$  denotes the edges of Cetirizine with  $i = S_u$  and  $j = S_v$ . It is easy to see that the summation of degrees of edge end points of Cetirizine have eight edge types  $e_{3,4}$ ,  $e_{3,5}$ ,  $e_{4,4}$ ,  $e_{4,5}$ ,  $e_{5,5}$ ,  $e_{5,6}$ ,  $e_{5,7}$ , and  $e_{7,9}$  as shown in the following figure - 2. Clearly from the figure - 2,  $|e_{3,4}| = 2$ ,  $|e_{3,5}| = 1$ ,  $|e_{4,4}| = 3$ ,  $|e_{4,5}| = 5$ ,  $|e_{5,5}| = 6$ ,  $|e_{5,6}| = 3$ ,  $|e_{5,7}| = 6$  and  $|e_{7,9}| = 3$ .

The fourth atom-bond connectivity index of Cetirizine  $ABC_4(C_{21}H_{25}ClN_2O_3)$

$$\begin{aligned} &= \sum_{uv \in E(G)} \sqrt{\frac{s_u + s_v - 2}{s_u s_v}} \\ &= |m_{3,4}| \left( \sqrt{\frac{3+4-2}{3.4}} \right) + |m_{3,5}| \left( \sqrt{\frac{3+5-2}{3.5}} \right) + |m_{4,4}| \left( \sqrt{\frac{4+4-2}{4.4}} \right) + |m_{4,5}| \left( \sqrt{\frac{4+5-2}{4.5}} \right) + |m_{5,5}| \left( \sqrt{\frac{5+5-2}{5.5}} \right) + \\ &\quad |m_{5,6}| \left( \sqrt{\frac{5+6-2}{5.6}} \right) + |m_{5,7}| \left( \sqrt{\frac{5+7-2}{5.7}} \right) + |m_{7,9}| \left( \sqrt{\frac{7+9-2}{7.9}} \right) \\ &= 2 \times \sqrt{\frac{5}{12}} + 1 \times \sqrt{\frac{6}{15}} + 3 \times \sqrt{\frac{6}{16}} + 5 \times \sqrt{\frac{7}{20}} + 6 \times \sqrt{\frac{8}{25}} + 3 \times \sqrt{\frac{9}{30}} + 6 \times \sqrt{\frac{10}{35}} + 3 \times \sqrt{\frac{14}{63}}. \end{aligned}$$

$$\therefore ABC_4(C_{21}H_{25}ClN_2O_3) = 16.377236.$$

**Theorem.2.3.** The Randic connectivity index of Cetirizine is 13.13103.

**Proof:** Randic connectivity index of Cetirizine  $\chi(C_{21}H_{25}ClN_2O_3)$

$$\begin{aligned} &= \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \\ &= |m_{1,3}| \left(\frac{1}{\sqrt{1.3}}\right) + |m_{2,2}| \left(\frac{1}{\sqrt{2.2}}\right) + |m_{2,3}| \left(\frac{1}{\sqrt{2.3}}\right) + |m_{3,3}| \left(\frac{1}{\sqrt{3.3}}\right). \\ &= 3 \times \left(\frac{1}{\sqrt{3}}\right) + 11 \times \left(\frac{1}{2}\right) + 12 \times \left(\frac{1}{\sqrt{6}}\right) + 3 \times \left(\frac{1}{3}\right). \end{aligned}$$

$$\therefore \chi(C_{21}H_{25}ClN_2O_3) = 13.13103.$$

**Theorem.2.4.** The sum connectivity index of Cetirizine is 13.591308.

**Proof:** Consider the sum connectivity index of Cetirizine  $S(C_{21}H_{25}ClN_2O_3)$

$$\begin{aligned} &= \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}} \\ &= |m_{1,3}| \left(\frac{1}{\sqrt{1+3}}\right) + |m_{2,2}| \left(\frac{1}{\sqrt{2+2}}\right) + |m_{2,3}| \left(\frac{1}{\sqrt{2+3}}\right) + |m_{3,3}| \left(\frac{1}{\sqrt{3+3}}\right). \\ &= 3 \times \left(\frac{1}{2}\right) + 11 \times \left(\frac{1}{2}\right) + 12 \times \left(\frac{1}{\sqrt{5}}\right) + 3 \times \left(\frac{1}{\sqrt{6}}\right). \end{aligned}$$

$$\therefore S(C_{21}H_{25}ClN_2O_3) = 13.591308.$$

**Theorem.2.5.** The geometric-arithmic index of Cetirizine is 28.355627.

**Proof:** The geometric-arithmic index of Cetirizine  $GA(C_{21}H_{25}ClN_2O_3)$

$$\begin{aligned} &= \sum_{e=uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\ &= |m_{1,3}| \left(\frac{2\sqrt{1.3}}{1+3}\right) + |m_{2,2}| \left(\frac{2\sqrt{2.2}}{2+2}\right) + |m_{2,3}| \left(\frac{2\sqrt{2.3}}{2+3}\right) + |m_{3,3}| \left(\frac{2\sqrt{3.3}}{3+3}\right). \\ &= 3 \times \left(\frac{2\sqrt{3}}{4}\right) + 11 \times \left(\frac{2\sqrt{4}}{4}\right) + 12 \times \left(\frac{2\sqrt{6}}{5}\right) + 3 \times \left(\frac{2\sqrt{9}}{6}\right). \end{aligned}$$

$$\therefore GA(C_{21}H_{25}ClN_2O_3) = 28.355627.$$

**Theorem.2.6.** The fifth geometric-arithmic index of Cetirizine is 28.7969.

**Proof:** The fifth geometric-arithmic index of Cetirizine  $GA_5(C_{21}H_{25}ClN_2O_3) = \sum_{uv \in E(G)} \frac{2\sqrt{s_u s_v}}{s_u + s_v}$

$$\begin{aligned} &= |e_{3,4}| \left(\frac{2\sqrt{3.4}}{3+4}\right) + |e_{3,5}| \left(\frac{2\sqrt{3.5}}{3+5}\right) + |e_{4,4}| \left(\frac{2\sqrt{4.4}}{4+4}\right) + |e_{4,5}| \left(\frac{2\sqrt{4.5}}{4+5}\right) + |e_{5,5}| \left(\frac{2\sqrt{5.5}}{5+5}\right) + |e_{5,6}| \left(\frac{2\sqrt{5.6}}{5+6}\right) + \\ &|e_{5,7}| \left(\frac{2\sqrt{5.7}}{5+7}\right) + |e_{7,9}| \left(\frac{2\sqrt{7.9}}{7+9}\right) \\ &= 2 \times \left(\frac{2\sqrt{12}}{7}\right) + 1 \times \left(\frac{2\sqrt{15}}{8}\right) + 3 \times \left(\frac{2\sqrt{16}}{8}\right) + 5 \times \left(\frac{2\sqrt{20}}{9}\right) + 6 \times \left(\frac{2\sqrt{25}}{10}\right) + 3 \times \left(\frac{2\sqrt{30}}{11}\right) + \\ &6 \times \left(\frac{2\sqrt{35}}{12}\right) + 3 \times \left(\frac{2\sqrt{63}}{16}\right) \end{aligned}$$

$$\therefore GA_5(C_{21}H_{25}ClN_2O_3) = 28.7969.$$

**Theorem.2.7.** The first Zagreb index of Cetirizine is 134.

**Proof:** First Zagreb index of Cetirizine  $Z_1(C_{21}H_{25}ClN_2O_3)$

$$\begin{aligned} &= \sum_{e=uv \in E(G)} (d_u + d_v) \\ &= |m_{1,3}|(1 + 3) + |m_{2,2}|(2 + 2) + |m_{2,3}|(2 + 3) + |m_{3,3}|(3 + 3) \\ &= 3 \times (1 + 3) + 11 \times (2 + 2) + 12 \times (2 + 3) + 3 \times (3 + 3) \\ &= 3 \times 4 + 11 \times 4 + 12 \times 5 + 3 \times 6. \end{aligned}$$

$$\therefore Z_1(C_{21}H_{25}ClN_2O_3) = 134.$$

**Theorem.2.8.** The second Zagreb index of Cetirizine is 152.

**Proof:** The Second Zagreb index of Cetirizine  $Z_2(C_{21}H_{25}ClN_2O_3)$

$$\begin{aligned} &= \sum_{e=uv \in E(G)} (d_u \cdot d_v) \\ &= |m_{1,3}|(1.3) + |m_{2,2}|(2.2) + |m_{2,3}|(2.3) + |m_{3,3}|(3.3). \\ &= 3(3) + 11(4) + 12(6) + 3(9). \end{aligned}$$

$$\therefore Z_2(C_{21}H_{25}ClN_2O_3) = 152.$$

**Theorem.2.9.** The first multiple Zagreb index of Cetirizine is  $1.416 \times 10^{19}$ .

**Proof:** The first multiple Zagreb index of Cetirizine  $PM_1(C_{21}H_{25}ClN_2O_3)$

$$\begin{aligned}
 &= \prod_{e=uv \in E(G)} (d_u + d_v) \\
 &= \prod_{e=uv \in 1,3} (d_u + d_v) \prod_{e=uv \in 2,2} (d_u + d_v) \prod_{e=uv \in 2,3} (d_u + d_v) \prod_{e=uv \in 3,3} (d_u + d_v) \\
 &= 4^3 \times 4^{11} \times 5^{12} \times 6^3. \\
 \therefore PM_1(C_{21}H_{25}ClN_2O_3) &= 1.416 \times 10^{19}.
 \end{aligned}$$

**Theorem.2.10.** The second multiple Zagreb index of Cetirizine is  $1.797 \times 10^{20}$ .

**Proof:** The second multiple Zagreb index of Cetirizine  $PM_1(C_{21}H_{25}ClN_2O_3)$

$$\begin{aligned}
 &= \prod_{e=uv \in E(G)} (d_u \cdot d_v) \\
 &= \prod_{e=uv \in 1,3} (d_u \cdot d_v) \prod_{e=uv \in 2,2} (d_u \cdot d_v) \prod_{e=uv \in 2,3} (d_u \cdot d_v) \prod_{e=uv \in 3,3} (d_u \cdot d_v). \\
 &= 3^3 \times 4^{11} \times 6^{12} \times 9^3. \\
 \therefore PM_1(C_{21}H_{25}ClN_2O_3) &= 1.797 \times 10^{20}.
 \end{aligned}$$

**Theorem.2.11.** The augmented Zagreb index of Cetirizine is 228.29688.

**Proof:** The augmented Zagreb index of Cetirizine  $AZI(G) (C_{21}H_{25}ClN_2O_3)$

$$\begin{aligned}
 &= \sum_{uv \in E} \left[ \frac{d_u d_v}{d_u + d_v - 2} \right]^3. \\
 &= |m_{1,3}| \left[ \frac{1.3}{1+3-2} \right]^3 + |m_{2,2}| \left[ \frac{2.2}{2+2-2} \right]^3 + |m_{2,3}| \left[ \frac{2.3}{2+3-2} \right]^3 + |m_{3,3}| \left[ \frac{3.3}{3+3-2} \right]^3. \\
 &= 3 \times \left(\frac{3}{2}\right)^3 + 11 \times \left(\frac{4}{2}\right)^3 + 12 \times \left(\frac{6}{3}\right)^3 + 3 \times \left(\frac{9}{4}\right)^3. \\
 \therefore AZI(G) (C_{21}H_{25}ClN_2O_3) &= 228.29688.
 \end{aligned}$$

**Theorem.2.12.** The harmonic index of Cetirizine is 12.8.

**Proof:** The harmonic index of Cetirizine  $H(C_{21}H_{25}ClN_2O_3)$

$$\begin{aligned}
 &= \sum_{e=uv \in E(G)} \frac{2}{d_u + d_v}. \\
 &= |m_{1,3}| \left(\frac{2}{1+3}\right) + |m_{2,2}| \left(\frac{2}{2+2}\right) + |m_{2,3}| \left(\frac{2}{2+3}\right) + |m_{3,3}| \left(\frac{2}{3+3}\right). \\
 &= 3 \times \left(\frac{2}{4}\right) + 11 \times \left(\frac{2}{4}\right) + 12 \times \left(\frac{2}{5}\right) + 3 \times \left(\frac{2}{6}\right). \\
 \therefore H(C_{21}H_{25}ClN_2O_3) &= 12.8.
 \end{aligned}$$

**Theorem.2.13.** The hyper Zagreb index of Cetirizine is 632.

**Proof:** The hyper Zagreb index of Cetirizine  $HZ(C_{21}H_{25}ClN_2O_3)$

$$\begin{aligned}
 &= \sum_{e=uv \in E(G)} (d_u + d_v)^2. \\
 &= |m_{1,3}|(1+3)^2 + |m_{2,2}|(2+2)^2 + |m_{2,3}|(2+3)^2 + |m_{3,3}|(3+3)^2. \\
 &= 3 \times 4^2 + 11 \times 4^2 + 12 \times 5^2 + 3 \times 6^2. \\
 \therefore HZ(C_{21}H_{25}ClN_2O_3) &= 632.
 \end{aligned}$$

**Theorem.2.14.** The first Zagreb polynomial of Cetirizine is  $3x^6 + 12x^5 + 14x^4$ .

**Proof:** First Zagreb polynomials of Cetirizine  $ZG_1(C_{21}H_{25}ClN_2O_3)$

$$\begin{aligned}
 &= \sum_{e=uv \in E(G)} x^{d_u + d_v}. \\
 &= |m_{1,3}|x^{(1+3)} + |m_{2,2}|x^{(2+2)} + |m_{2,3}|x^{(2+3)} + |m_{3,3}|x^{(3+3)}. \\
 &= 3 \times x^4 + 11 \times x^4 + 12 \times x^5 + 3 \times x^6. \\
 \therefore ZG_1(C_{21}H_{25}ClN_2O_3, x) &= 3x^6 + 12x^5 + 14x^4.
 \end{aligned}$$

**Theorem.2.15.** The second Zagreb polynomials of Cetirizine is  $3x^9 + 12x^6 + 11x^4 + 3x^3$ .

**Proof:** Second Zagreb polynomials of Cetirizine  $ZG_2(C_{21}H_{25}ClN_2O_3, x)$

$$\begin{aligned}
 &= \sum_{e=uv \in E(G)} x^{d_u d_v}. \\
 &= |m_{1,3}|x^{(1.3)} + |m_{2,2}|x^{(2.2)} + |m_{2,3}|x^{(2.3)} + |m_{3,3}|x^{(3.3)}. \\
 &= 3 \times x^3 + 11 \times x^4 + 12 \times x^6 + 3 \times x^9.
 \end{aligned}$$

$$\therefore ZG_2(C_{21}H_{25}ClN_2O_3, x) = 3x^9 + 12x^6 + 11x^4 + 3x^3.$$

**Theorem.2.16.** The third Zagreb polynomials of Cetirizine is  $3x^2 + 12x + 14$ .

**Proof:** Third Zagreb polynomials of Cetirizine  $ZG_3(C_{21}H_{25}ClN_2O_3, x)$

$$\begin{aligned} &= \sum_{e=uv \in E(G)} x^{|d_u - d_v|} \\ &= |m_{1,3}|x^{|1-3|} + |m_{2,2}|x^{|2-2|} + |m_{2,3}|x^{|2-3|} + |m_{3,3}|x^{|3-3|}. \\ &= 3 \times x^2 + 11 \times x^0 + 12 \times x^1 + 3 \times x^0. \end{aligned}$$

$$\therefore ZG_3(C_{21}H_{25}ClN_2O_3, x) = 3x^2 + 12x + 14.$$

**Theorem.2.17.** The forgotten topological index of Cetirizine is 328.

**Proof:** Consider Forgotten topological index of Cetirizine  $F(C_{21}H_{25}ClN_2O_3)$

$$\begin{aligned} &= \sum_{e=uv \in E(G)} [(d_u)^2 + (d_v)^2] \\ &= |m_{1,3}|(1^2 + 3^2) + |m_{2,2}|(2^2 + 2^2) + |m_{2,3}|(2^2 + 3^2) + |m_{3,3}|(3^2 + 3^2). \\ &= 3 \times 10 + 11 \times 8 + 12 \times 13 + 3 \times 18. \end{aligned}$$

$$\therefore F(C_{21}H_{25}ClN_2O_3) = 328.$$

**Theorem.2.18.** The forgotten polynomials of Cetirizine is  $3x^{18} + 12x^{13} + 3x^{10} + 11x^8$ .

**Proof:** Consider forgotten polynomials of Cetirizine  $FP(C_{21}H_{25}ClN_2O_3, x)$

$$\begin{aligned} &= \sum_{e=uv \in E(G)} x^{[(d_u)^2 + (d_v)^2]} \\ &= |m_{1,3}|x^{(1^2+3^2)} + |m_{2,2}|x^{(2^2+2^2)} + |m_{2,3}|x^{(2^2+3^2)} + |m_{3,3}|x^{(3^2+3^2)}. \\ &= 3 \times x^{10} + 11 \times x^8 + 12 \times x^{13} + 3 \times x^{18}. \end{aligned}$$

$$\therefore FP(C_{21}H_{25}ClN_2O_3, x) = 3x^{18} + 12x^{13} + 3x^{10} + 11x^8.$$

**Theorem.2.19.** The symmetric division index of Cetirizine is 64.

**Proof:** Symmetric division index of Cetirizine  $SDI(C_{21}H_{25}ClN_2O_3)$

$$\begin{aligned} &= \sum_{e=uv \in E(G)} \left\{ \frac{\min(d_u, d_v)}{\max(d_u, d_v)} + \frac{\max(d_u, d_v)}{\min(d_u, d_v)} \right\} \\ &= |m_{1,3}| \left\{ \frac{\min(1.3)}{\max(1.3)} + \frac{\max(1.3)}{\min(1.3)} \right\} + |m_{2,2}| \left\{ \frac{\min(2.2)}{\max(2.2)} + \frac{\max(2.2)}{\min(2.2)} \right\} \\ &\quad + |m_{2,3}| \left\{ \frac{\min(2.3)}{\max(2.3)} + \frac{\max(2.3)}{\min(2.3)} \right\} + |m_{3,3}| \left\{ \frac{\min(3.3)}{\max(3.3)} + \frac{\max(3.3)}{\min(3.3)} \right\} \\ &= 3 \times \frac{10}{3} + 11 \times 2 + 12 \times \frac{13}{6} + 3 \times 2. \end{aligned}$$

$$\therefore SDI(C_{21}H_{25}ClN_2O_3) = 64.$$

### III. CONCLUSION

ABC index, ABC<sub>4</sub> index, Randic connectivity index, Sum connectivity index, GA index, GA<sub>5</sub> index, first Zagreb index, second Zagreb index, first multiple Zagreb index, second multiple Zagreb index, augmented Zagreb index, Harmonic index and hyper Zagreb index, first Zagreb polynomial, second Zagreb polynomial, Third Zagreb polynomial, Forgotten polynomial, Forgotten topological index and symmetric division index of Cetirizine was computed.

### REFERENCES

- [1]. J. Braun, A. Kerber, M. Meringer, C. Rucker, Similarity of molecular descriptors: the equivalence of Zagreb indices and walk counts, MATCH 54 (2005) 163-176.
- [2]. S. Chen, W. Liu, the geometric-arithmetic index of nano tubes, J. Comput.Theor.Nanosci.7(2010) 1993-1995.
- [3]. J. Chen, J. Liu, X. Guo, Some upper bounds for the atom-bond connectivity index of graphs, Appl. Math. Lett.25 (2012) 1077-1081.
- [4]. J. Chen, X. Guo, The atom-bond connectivity index of chemical bicyclic graphs, Appl. Math.j. Chinese Univ. 27 (2012) 243-252.



- [5]. K. C. Das, N. Trinajstić, Comparison between first geometric-arithmetic index and atom-bond connectivity index, *Chem. Phys. Lett.* 497 (2010) 149-151.
- [6]. Eliasi M, Iranmanesh A, Gutman I. Multiplicative versions of first Zagreb index. *MATCH* 2012; 68: 217-230.
- [7]. E. Estrada, L. Torres, L. Rodriguez, I. Gutman, An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes, *Indian J. Chem.* 37A (1998), 849-855.
- [8]. E. Estrada Atom-bond connectivity and the energetic of branched alkanes, *Chem. Phys. Lett.* 463(2008) 422-425.
- [9]. M. R. Farahani, Computing fourth atom-bond connectivity index of V-Phenylenic Nano tubes and Nanotori. *Acta Chimica Slovenica.* 60(2), (2013), 429-432.
- [10]. M. R. Farahani, On the Fourth atom-bond connectivity index of Armchair Polyhex Nanotube, *Proc. Rom. Acad., Series B*, 15(1), (2013), 3-6.
- [11]. B. Furtula, A. Graovac, D. Vukicević, Atom-bond connectivity index of trees, *Discrete Appl. Math.* 157 (2009) 2828-2835.
- [12]. B. Furtula, A. Graovac, D. Vukicević, Augmented Zagreb index, *J. Math. Chem.* 48 (2010) 370-380.
- [13]. B. Furtula and Gutman I., A forgotten topological index, *J. Math. Chem.* 53 (2015) 213 – 220.
- [14]. Ghorbani M, Azimi N. Note on multiple Zagreb indices. *Iranian Journal of Mathematical Chemistry.* 2012; 3(2): 137-143.
- [15]. M. Ghorbani, M. A. Hosseinzadeh, Computing  $ABC_4$  index of Nanostardendrimers. *Optoelectron. Adv. Mater-Rapid commun.* 4(9), (2010), 1419-1422.
- [16]. A. Graovac, M. Ghorbani, M. A. Hosseinzadeh, Computing Fifth Geometric-Arithmetic index for nanostar dendrimers, *J. Math. Nanosci.* , 1, (2011) 33-42.
- [17]. I. Gutman, N. Trinajstić, Graph theory and molecular orbitals, Total  $\Pi$ - electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* 17 (1972) 535-538.
- [18]. I. Gutman, K.C. Das, The first Zagreb index 30 years after, *MATCH* 50 (2004) 83-92.
- [19]. I. Gutman: Multiplicative Zagreb indices of trees. *Bull. Soc. Math. Banja Luka* 18, 17-23 (2011).
- [20]. I. Gutman, B. Ruscic and N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Chem. Phys.* 62 (1975) 3399 - 3405.
- [21]. I. Gutman, B. Furtula, M. Ivanovic, Notes on trees with minimal atom-bond connectivity index. *MATCH* 67, (2012) 467-482.
- [22]. Y. Hung, B. Liu and L. Gan, augmented Zagreb Index of connected graphs *MATCH* 67 (2012) 483-494.
- [23]. M. Randić, On Characterization of molecular branching, *J. Amer. Chem. Soc.*, 97, (1975), 6609-6615.
- [24]. Shirdel, G.H., RezaPour H., Sayadi. A.M. The Hyper-Zagreb Index of Graph Operations. *Iranian Journal of Mathematical Chemistry*, 4(2), (2013), 213-220.
- [25]. R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2000.
- [26]. R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley-VCH, Weinheim, 2009, Vols. I and II.
- [27]. D. Vukicević-B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem.*, 46, (2009) 1369-1376.
- [28]. R. Wu, Z. Tang, and H. Deng, A lower bound for the harmonic index of a graph with minimum degree at least two, *Filomat* 27 (2013) 51-55.
- [29]. R. Xing, B. Zhou, Z. Du, Further results on atom-bond connectivity index of trees, *Discr. Appl. Math.* 157 (2010) 1536-1545.
- [30]. R. Xing, B. Zhou, F. Dong, On atom-bond connectivity index of connected graphs, *Discr. Appl. Math.*, in press.
- [31]. R. Xing, B. Zhou, Extremal trees with fixed degree sequence for atom-bond connectivity index. *Filomat* 26, (2012) 683-688.
- [32]. L. Xiao, S. Chen, Z. Guo, Q. Chen, The geometric-arithmetic index of benzenoid systems and phenylenes, *Int. J. Contemp. Math. Sci.* 5 (2010) 2225-2230.
- [33]. B. Zhou, R. Xing, On atom-bond connectivity index, *Z. Naturforsch.* 66a, (2011), 61-66.
- [34]. B. Zhou and N. Trinajstić, On a novel connectivity index, *J. Math. Chem.* 46, (2009), 1252-1270.
- [35]. B. Zhou and N. Trinajstić, On general sum-connectivity index, *J. Math. Chem.* 47, (2010), 210-218.
- [36]. L. Zhong, The harmonic index on graphs, *Appl. Math. Lett.* 25 (2012), 561-566.
- [37]. Ali Astanesh-Asl and G. H Fath-Tabar, Computing the first and third Zagreb polynomials of curtained product of graphs, *Irsnisn Journal of Marhematical Chemistry.* 2-2 (2011), 73 - 78.