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STUDIES ON TOPOLOGICAL INDICES OF TRIGLYCERIDE

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Abstract: In this paper, we compute First Zagreb index, Second Zagreb index, First Multiple Zagreb index, Second Multiple Zagreb index, Re-defined version of Zagreb index and , Hyper Zagreb index, Forgotten topological index, Augmented Zagreb index, Arithmetic-Geometric index, SK index, SK_1 index and SK_2 index of Triglyceride.

AMS Subject Classification: 05C12, 05C90
Key Words: ABC index, ABC_4 index, Sum connectivity index, Randic connectivity index, GA index and GA_5 index

1. Introduction

A triglyceride is an ester formed by three fatty acids to a single glycerol molecule. Triglycerides are mainly circulated in the body to provide cells for energy, it is the main constituents of body fat in humans and animals, as well as vegetable fat. After the body consumes a meal with fats, the unused portions are transported to fat cells and stored as triglycerides. Triglycerides are fats, and they are used to produce the energy currency of a cell called adenosine triphosphate (ATP). When energy is required by cells, the fat is removed and

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sent to cells via cholesterol transport. Triglycerides are also used in the cell membrane to control permeability of the cell. It is the most common form of fat in foods and in the body and it is needed for good health and they are a rich energy source, as they provide more than twice as much energy for the body as carbohydrates and protein. However, high triglyceride levels increase the risk of heart disease, according to the American Heart Association. Triglyceride fatty acid tails can be saturated or unsaturated. Saturated fatty acid tails are all single bond carbons. This means that for each carbon, there are two hydrogens and two carbons attached. There are no double bonds in a saturated molecule. Unsaturated fatty acids have at least one double bond. Single bond molecules are called monosaturated. A molecule that contains more double bonds is called polyunsaturated. Here we consider carbon atoms of saturated fatty acid.The vertices represents the carbon atoms and the edges represents the bonds between the corresponding atoms and their molecular graphs represent the carbon skeleton of the molecule [5, 23].

Topological indices are the molecular descriptors that describe the structures of chemical compounds and they help us to predict certain physicochemical properties like boiling point, enthalpy of vaporization, stability, etc. Topological indices are introduced to test the medicinal properties of new drugs which is widely welcomed in developing areas. All molecular graphs considered in this paper are finite, connected, loopless, and without multiple edges. Let $G = (V, E)$ be a graph with vertex set V and edge set E. Recently Sridhar and his co-authors [19] determined ABC index, ABC_4 index, Randic connectivity index, Sum connectivity index, GA index and GA_5 index of Graphene. 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 [15], and also V. S. Shigehalli and Rachanna Kanabur [18] determined the four new topological indices on Graphene. For further results on Topological indices see the papers [2, 3, 4, 6, 25] and the references cited there in.

A pair of molecular descriptors (or topological index), known as the First Zagreb index $M_1(G)$ and the Second Zagreb index $M_2(G)$, first appeared in the topological formula for the total π-energy of conjugated molecules that has been derived in 1972 by I. Gutman and N.Trinajstic[11]. 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, CERIUS, TAM, DISSI. $M_1(G)$ and $M_2(G)$ were recognize

as measures of the branching of the carbonatom molecular skeleton [14], and since then these are frequently used for structureproperty modeling. Details on the chemical applications of the two Zagreb indices can be found in the books [21, 22]. Further studies on Zagreb indices can be found in [1, 12, 26, 27, 28].

Definition 1.1. For a simple connected graph G, the first and second zagreb indices were defined as follows

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v), \qquad M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

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

In 2012, M. Ghorbani and N. Azimi [10] defined the Multiple Zagreb topological indices of a graph G, based on degree of vertices of G.

Definition 1.2. For a simple connected graph G, the first and second multiple Zagreb indices were defined as follows

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

Properties of the first and second Multiple Zagreb indices may be found in [7, 13] .

As degree-based topological indices, the Re-defined version of Zagreb indices of a graph G introduced by Ranjini et al., [17], and Usha et al., [24].

Definition 1.3. For a simple connected graph G, the Re-defined version of Zagreb indices are defined as follows

$$ReZG_1(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{d_u d_v}.$$

$$ReZG_2(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}.$$

$$ReZG_3(G) = \sum_{uv \in E(G)} (d_u d_v)(d_u + d_v).$$

G.H. Shirdel et.al[18] introduced a new distance-based of Zagreb indices of a graph G named Hyper-Zagreb index

Definition 1.4. The hyper Zagreb index is defined as,

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

The forgotten topological index was defined to be used in the analysis of drug molecular structures, which is quite helpful for pharmaceutical and medical scientists to grasp the biological and chemical characteristics of new drugs. Such tricks are popularly employed in developing countries where enough money is lacked to afford the relevant chemical reagents and equipment. Sun et al. (2014) [20] deduced some basic nature of forgotten topological index and reported that this index can reinforce the physico-chemical flexibility of Zagreb indices. Very recently, Gao et al. [9] manifested the forgotten topological index of some significant drug molecular structures.

Definition 1.5. Followed by the first and second Zagreb indices, Furtula and Gutman (2015) introduced forgotten topological index (also called F-index) which was defined as $F(G) = \sum_{uv \in E(G)} (d_u^2 + d_v^2)$.

The Augmented Zagreb index was introduced by Furtula et al [8]. This graph invariant has proven to be a valuable predictive index in the study of the heat of formation in octanes 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 1.6. Let $G = (V, E)$ be a graph and d_u be the degree of a vertex u, then augmented zagreb indexis denoted by $AZI(G)$ and is defined as $AZI(G)= \sum_{uv \in E(G)} \Big[\frac{d_u d_v}{d_u + d_v - 2}\Big]^3$.
Further studies can be found in [16] and the references cited there in.

Definition 1.7. Let $G=(V, E)$ be a molecular graph and d_u is the degree of the vertex u, then Arithmetic-Geometric index of G is defined as, $AG_1(G)= \sum_{uv \in E(G)} \Big(\frac{d_u + d_v}{2\sqrt{d_u d_v}}\Big)$.

Definition 1.8. For a simple connected graph G, SK index was defined as follows $SK(G)= \sum_{uv \in E(G)} \Big(\frac{d_u + d_v}{2}\Big)$.

Definition 1.9. For a simple connected graph G, its SK_1 index is defined as, $SK_1 = \sum_{uv \in E(G)} \Big(\frac{d_u . d_v}{2}\Big)$.

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Definition 1.10. Let G be a graph and e = uv be an edge of G then, $SK_2 = \sum_{uv \in E(G)} \left(\frac{d_u + d_v}{2}\right)^2$.

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2. Main results

Consider a two-dimensional structure of triglyceride as shown in the figure-1. Let $|E_{i,j}|$ denotes the number of edges connecting the vertices of degrees d_i and d_j. The figure-1 contains the edges of the type $E_{2,2}$, $E_{2,3}$, $E_{1,3}$ and $E_{2,1}$ which are colored in green, red, black and blue respectively. Triglyceride contains $|E_{2,2}|$=41, $|E_{2,3}|$=9, $|E_{1,3}|$=3 and $|E_{2,1}|$=3 edges.

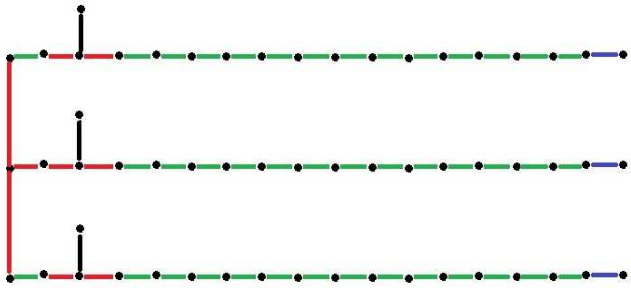
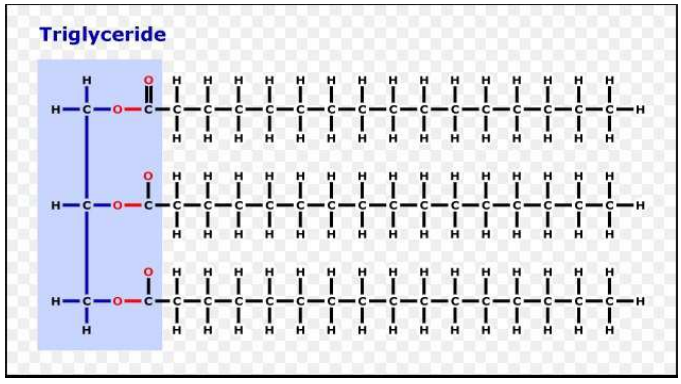


FIG 1: TWO DIMENSIONAL STRUCTURE OF TRIGLYCERIDE



Theorem 2.1. *The First Zagreb index of Triglyceride is given by,* $M_1(G)$=230.

Proof. The First Zagreb index of Triglyceride is $M_1(G)$
$= \sum_{uv \in E(G)} (d_u + d_v).$
$=|E_{2,2}|(2+2) + |E_{2,3}|(2+3) + |E_{1,3}|(1+3) + |E_{2,1}|(2+1).$
$=|E_{2,2}|(4) + |E_{2,3}|(5) + |E_{1,3}|(4) + |E_{2,1}|(3).$
$=41(4) + 9(5) + 3(4) + 3(3).$
$M_1(G)=230.$ □

Theorem 2.2. *The Second Zagreb index of Triglyceride is given by,* $M_2(G)=233$

Proof. The Second Zagreb index of Triglyceride is $M_2(G)$
$= \sum_{uv \in E(G)} (d_u d_v).$
$=|E_{2,2}|(2.2) + |E_{2,3}|(2.3) + |E_{1,3}|(1.3) + |E_{2,1}|(2.1).$
$=41(4) + 9(6) + 3(3) + 3(2).$
$M_2(G)=233.$ □

Theorem 2.3. *The First Multiple Zagreb index of Triglyceride is given by,* $PM_1(G)=1.632049(10)^{34}$

Proof. The First Multiple Zagreb index of Triglyceride is $PM_1(G)$
$= \prod_{uv \in E(G)} (d_u + d_v).$
$= \prod_{uv \in |E_{2,2}|} (d_u + d_v). \prod_{uv \in |E_{2,2}|} (d_u + d_v). \prod_{uv \in |E_{2,3}|} (d_u + d_v).$
$\prod_{e=uv \in |E_{1,3}|} (d_u + d_v). \prod_{uv \in |E_{2,1}|} (d_u + d_v).$
$=4^{41}.5^9.4^3.3^3.$
$PM_1(G)=1.632049(10)^{34}.$ □

Theorem 2.4. *The Second Multiple Zagreb index of Triglyceride is given by,* $PM_2(G)=3.5526(10)^{34}$

Proof. The Second Multiple Zagreb index of Triglyceride is $PM_2(G)$
$= \prod_{uv \in E(G)} (d_u + d_v).$
$= \prod_{uv \in |E_{2,2}|} (d_u d_v). \prod_{e=uv \in |E_{2,2}|} (d_u d_v). \prod_{uv \in |E_{2,3}|} (d_u d_v). \prod_{uv \in |E_{1,3}|} (d_u d_v). \prod_{uv \in |E_{2,1}|} (d_u d_v).$

$=4^{41}.6^{9}.3^{3}.3^{3}$.
$PM_2(G)=3.5526(10)^{34}$. □

Theorem 2.5. *The Re-defined First version of Zagreb index of Triglyceride is given by,* $RezG_1(G)=57$

Proof. The Re-defined First version of Zagreb index of Triglyceride is $RezG_1(G)$
$= \sum_{uv\in E(G)} \frac{d_u+d_v}{d_u d_v}$.
$=|E_{2,2}|\left(\frac{4}{4}\right)+|E_{2,3}|\left(\frac{5}{6}\right)+|E_{1,3}|\left(\frac{4}{3}\right)+|E_{2,1}|\left(\frac{3}{2}\right)$.
$=41(1)+9(\frac{5}{6})+3\left(\frac{4}{3}\right)+3(\frac{3}{2})$.
$RezG_1(G)=57$. □

Theorem 2.6. *The Re-defined Second version of Zagreb index of Triglyceride is given by,* $RezG_2(G)=56.05$

Proof. The Re-defined Second version of Zagreb index of Triglyceride is $RezG_2(G)$
$= \sum_{uv\in E(G)} \frac{d_u d_v}{d_u+d_v}$.
$=|E_{2,2}|\left(\frac{4}{4}\right)+|E_{2,3}|\left(\frac{6}{5}\right)+|E_{1,3}|\left(\frac{3}{4}\right)+|E_{2,1}|\left(\frac{2}{3}\right)$.
$=41(1)+9(\frac{6}{5})+3\left(\frac{3}{4}\right)+3(\frac{2}{3})$.
$RezG_2(G)=56.05$. □

Theorem 2.7. *The Re-defined third version of Zagreb index of Triglyceride is given by,* $RezG_3(G)=365$

Proof. The Re-defined third version of Zagreb index of Triglyceride is $RezG_3(G)$
$= \sum_{uv\in E(G)} (d_u d_v)(d_u+d_v)$.
$=|E_{2,2}|(4)(4)+|E_{2,3}|(6)(5)+|E_{1,3}|(3)(4)+|E_{2,1}|(2)(3)$.
$=41(1)+9(6)(5)+3(3)(4)+3(2)(3)$.
$RezG_3(G)=365$.

□

Theorem 2.8. *The Hyper Zagreb index of Triglyceride is given by,* $HM(G)=956$

Proof. The Hyper Zagreb index of Triglyceride is $HM(G)$
$= \sum_{uv \in E(G)} (d_u + d_v)^2.$
$=|E_{2,2}|\Big(4^2\Big) + |E_{2,3}|\Big(5^2\Big) + |E_{1,3}|\Big(4^2\Big) + |E_{2,1}|\Big(3^2\Big)$
$=41\Big(16\Big) + 9\Big(25\Big) + 3\Big(16\Big) + 3\Big(9\Big)$
$HM(G)$=956. □

Theorem 2.9. *The Forgotten topological index of Triglyceride is given by,* $F(G)$=490.

Proof. The Forgotten topological index of Triglyceride is $F(G)$
$= \sum_{uv \in E(G)} (d_u^2 + d_v^2).$
$=|E_{2,2}|(8) + |E_{2,3}|(13) + ||E_{1,3}||(10) + |E_{2,1}|(5)$
$=41(8) + 9(13) + 3(10) + 3(5)$
$F(G)$=490. □

Theorem 2.10. *The Augmented Zagreb index of Triglyceride is given by,* $AZI(G)$=434.125

Proof. The Augmented Zagreb index of Triglyceride is $AZI(G)$
$= \sum_{uv \in E(G)} \Big[\frac{d_u d_v}{d_u + d_v - 2}\Big]^3.$
$=|E_{2,2}|\Big(\frac{4}{2}\Big)^3 + |E_{2,3}|\Big(\frac{6}{3}\Big)^3 + |E_{1,3}|\Big(\frac{3}{2}\Big)^3 + |E_{2,1}|\Big(\frac{2}{1}\Big)^3$
$=41(8) + 9(8) + 3\Big(\frac{27}{8}\Big) + 3(8)$
$AZI(G)$=434.125. □

Theorem 2.11. *The Arithmetic-Geometric index of triglyceride is given by,* $AG_1(G)$= 56.83166867

Proof. The Arithmetic-Geometric index index of triglyceride is $AG_1(G)$
$= \sum_{uv \in E(G)} \Big(\frac{d_u + d_v}{2\sqrt{d_u d_v}}\Big).$
$= |E_{2,2}|\Big(\frac{2+2}{2\sqrt{2.2}}\Big) + |E_{2,3}|\Big(\frac{2+3}{2\sqrt{2.3}}\Big) + |E_{1,3}|\Big(\frac{1+3}{2\sqrt{1.3}}\Big) + |E_{2,1}|\Big(\frac{2+1}{2\sqrt{2.1}}\Big).$
$=41\Big(\frac{4}{2\sqrt{4}}\Big) + 9\Big(\frac{5}{2\sqrt{6}}\Big) + 3\Big(\frac{4}{2\sqrt{3}}\Big) + 3\Big(\frac{3}{2\sqrt{2}}\Big).$
$= 41(1) + \Big(\frac{45}{2\sqrt{6}}\Big) + (2\sqrt{3}) + \Big(\frac{9}{2\sqrt{2}}\Big).$

$AG_1(G)$= 56.83166867.

□

Theorem 2.12. *The SKindex of triglyceride is given by,* $SK(G) = 115$

Proof. The SK index of triglyceride is $SK(G) = \sum_{uv\in E(G)} \Big(\frac{d_u + d_v}{2}\Big)$.

$=|E_{2,2}|\Big(\frac{2+2}{2}\Big) + |E_{2,3}|\Big(\frac{2+3}{2}\Big) + |E_{1,3}|\Big(\frac{1+3}{2}\Big) + |E_{2,1}|\Big(\frac{2+1}{2}\Big)$.

$=41\Big(\frac{4}{2}\Big) + 9\Big(\frac{5}{2}\Big) + 3\Big(\frac{4}{2}\Big) + 3\Big(\frac{3}{2}\Big)$.

$=41(2) + 9\Big(\frac{5}{2}\Big) + 3(2) + 3\Big(\frac{3}{2}\Big)$.

$SK(G) = 115$.

□

Theorem 2.13. *The SK_1 index of triglyceride is given by,* $SK_1(G)$= 116.5

Proof. The sum connectivity index of triglyceride is $SK_1(G)$

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

$=|E_{2,2}|\Big(\frac{2.2}{2}\Big) + |E_{2,3}|\Big(\frac{2.3}{2}\Big) + |E_{1,3}|\Big(\frac{1.3}{2}\Big) + |E_{2,1}|\Big(\frac{2.1}{2}\Big)$.

$=41\Big(\frac{4}{2}\Big) + 9\Big(\frac{6}{2}\Big) + 3\Big(\frac{3}{2}\Big) + 3\Big(\frac{2}{2}\Big)$.

$=41(2) + 9(3) + 3\Big(\frac{3}{2}\Big) + 3(1)$.

$SK_1(G)$= 116.5. □

Theorem 2.14. *The SK_2 index of triglyceride is given by,* $SK_2(G)$= 239

Proof. The SK_2 index of triglyceride is $SK_2(G)$

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

$=|E_{2,2}|\Big(\frac{2+2}{2}\Big)^2 + |E_{2,3}|\Big(\frac{2+3}{2}\Big)^2 + |E_{1,3}|\Big(\frac{1+3}{2}\Big)^2 + |E_{2,1}|\Big(\frac{2+1}{2}\Big)^2$.

$=41\Big(\frac{4}{2}\Big)^2 + 9\Big(\frac{5}{2}\Big)^2 + 3\Big(\frac{4}{2}\Big)^2 + 3\Big(\frac{3}{2}\Big)^2$.

$=41(2)^2 + 9\Big(\frac{5}{2}\Big)^2 + 3(2)^2 + 3\Big(\frac{3}{2}\Big)^2$.

$SK_2(G)$= 239 □

3. Conclusion

The problem of finding the general formula for First Zagreb index, Second Zagreb index, First Multiple Zagreb index, Second Multiple Zagreb index, Redefined version of Zagreb index, Hyper Zagreb index, Forgotten topological index, Augmented Zagreb index, Arithmetic-Geometric index, SK index, SK_1 index and SK_2 index of Triglyceride is solved here analytically without using computers.

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