Computation of Topological Indices of Triglyceride

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Abstract
In this paper, we compute $ABC$ index, Randic connectivity index, Sum connectivity index, $GA$ index, Harmonic index, General Randic index of Triglyceride.

AMS subject classification:
Keywords: $ABC$ index, Randic connectivity index, Sum connectivity index, $GA$ index, Harmonic index, General Randic index and Triglyceride.

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 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.

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. 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 $E$. 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 $uv$. Recently Sridhar and his co-authors [13] determined $ABC$ index, $ABC_4$ index, Randic connectivity index, Sum connectivity index, $GA_1$ index and $GA_5$ index of Graphene.

The $ABC$ index is one of the degree based molecular descriptor, which was introduced by Estrada et al. [8] in late 1990’s and it can be used for modelling thermodynamic properties of organic chemical compounds, it is also used as a tool for explaining the stability of branched alkanes [9]. For further results on $ABC$ index see the papers [3, 4, 5, 6, 10, 11, 17, 18, 19] 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,

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

The first and oldest degree based topological index is Randic index [12] denoted by $\chi(G)$ and was introduced by Milan Randic in 1975. It provides a quantitative assessment of branching of molecules.

**Definition 1.2.** Randic index was defined as follows

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$
Sum connectivity index belongs to a family of Randic like indices and it was introduced by Zhou and Trinajstic [21]. Further studies on Sum connectivity index can be found in [22, 23].

**Definition 1.3.** 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 $GA$ index of $G$ was introduced by D. Vukicevic et al. [14]. Further studies on $GA$ index can be found in [2, 7, 16].

**Definition 1.4.** Let $G$ be a graph and $e = uv$ be an edge of $G$ then,

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

The Harmonic index was introduced by Zhong [20]. It has been found that the harmonic index correlates well with the Randic index and with the $\pi$-electronic energy of benzenoid hydrocarbons.

**Definition 1.5.** 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 [15, 22].

There are several degree based indices introduced to test the properties of compounds and drugs, which have been widely used in chemical and pharmacy engineering. Bollobas and Erdos [1] introduced the General Randic index.

**Definition 1.6.** Let $G = (V, E)$ be a graph and $d_u$ be the degree of a vertex $u$ then the General Randic index is defined as

$$R_k(G) = \sum_{e=uv \in E(G)} (d_ud_v)^k.$$ 

where $k$ is a real number.

## 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. \therefore Triglyceride contains $|E_{2,2}| = 41$, $|E_{2,3}| = 9$, $|E_{1,3}| = 3$ and $|E_{2,1}| = 3$ edges.

**Theorem 2.1.** The atom bond connectivity index of triglyceride is given by, $ABC(G) = 39.926149$.

**Proof.** The atom-bond connectivity index of triglyceride is

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

$$= |E_{2,2}| \sqrt{\frac{2 + 2 - 2}{2.2}} + |E_{2,3}| \sqrt{\frac{2 + 3 - 2}{2.3}} + |E_{1,3}| \sqrt{\frac{1 + 3 - 2}{1.3}}$$

$$+ |E_{2,1}| \sqrt{\frac{2 + 1 - 2}{2.1}}.$$

$$= |E_{2,2}| \frac{1}{\sqrt{2}} + |E_{2,3}| \frac{1}{\sqrt{2}} + |E_{1,3}| \sqrt{\frac{2}{3}} + |E_{2,1}| \frac{1}{\sqrt{2}}$$

$$= 41 \frac{1}{\sqrt{2}} + 9 \frac{1}{\sqrt{2}} + 3 \sqrt{\frac{2}{3}} + 3 \frac{1}{\sqrt{2}}$$

$$ABC(G) = 39.926149.$$
Theorem 2.2. The randic connectivity index of triglyceride is given by, $\chi(G) = 28.02760577$.

Proof. The randic connectivity index of triglyceride is

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

$$
= |E_{2,2}| \frac{1}{\sqrt{2 \cdot 2}} + |E_{2,3}| \frac{1}{\sqrt{2 \cdot 3}} + |E_{1,3}| \frac{1}{\sqrt{1 \cdot 3}} + |E_{2,1}| \frac{1}{\sqrt{2 \cdot 1}}.
$$

$$
= |E_{2,2}| \frac{1}{\sqrt{4}} + |E_{2,3}| \frac{1}{\sqrt{6}} + |E_{1,3}| \frac{1}{\sqrt{3}} + |E_{2,1}| \frac{1}{\sqrt{2}}.
$$

$$
= 41 \frac{1}{2} + 9 \frac{1}{\sqrt{6}} + 3 \frac{1}{\sqrt{3}} + 3 \frac{1}{\sqrt{2}}.
$$

$$
\chi(G) = 28.02760577.
$$

Theorem 2.3. The sum connectivity index of triglyceride is given by, $S(G) = 27.75697317$.

Proof. The sum connectivity index of triglyceride is

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

$$
= |E_{2,2}| \frac{1}{\sqrt{2 + 2}} + |E_{2,3}| \frac{1}{\sqrt{2 + 3}} + |E_{1,3}| \frac{1}{\sqrt{1 + 3}} + |E_{2,1}| \frac{1}{\sqrt{2 + 1}}.
$$

$$
= |E_{2,2}| \frac{1}{\sqrt{4}} + |E_{2,3}| \frac{1}{\sqrt{5}} + |E_{1,3}| \frac{1}{\sqrt{4}} + |E_{2,1}| \frac{1}{\sqrt{3}}.
$$

$$
= 41 \frac{1}{2} + 9 \frac{1}{\sqrt{5}} + 3 \frac{1}{2} + 3 \frac{1}{\sqrt{3}}.
$$

$$
S(G) = 27.75697317.
$$

Theorem 2.4. The geometric-arithmetic index of triglyceride is given by, $GA(G) = 28.24466641$. 

Proof. The geometric-arithmetic index of triglyceride is

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

\[ = |E_{2,2}|(2\sqrt{\frac{2}{2+2} + |E_{2,3}|(2\sqrt{\frac{2}{2+3} + |E_{1,3}|(2\sqrt{\frac{2}{1+3} + |E_{2,1}|(2\sqrt{\frac{2}{2+1}}).} \]

\[ = |E_{2,2}|(2\sqrt{\frac{2}{2+2} + |E_{2,3}|(2\sqrt{\frac{2}{2+3} + |E_{1,3}|(2\sqrt{\frac{2}{1+3} + |E_{2,1}|(2\sqrt{\frac{2}{2+1}}.} \]

\[ = 41 + 9(2\sqrt{\frac{2}{2+2} + 3\sqrt{\frac{2}{2+3} + 3(2\sqrt{\frac{2}{2+1}}.} \]

\[ GA(G) = 28.24466641. \]

Theorem 2.5. The harmonic index of triglyceride is given by, \( H(G) = 27.6. \)

Proof. The harmonic index of triglyceride is

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

\[ = |E_{2,2}|(\frac{2}{2+2} + |E_{2,3}|(\frac{2}{2+3} + |E_{1,3}|(\frac{2}{1+3} + |E_{2,1}|(\frac{2}{2+1}). \]

\[ = |E_{2,2}|(\frac{2}{2+2} + |E_{2,3}|(\frac{2}{2+3} + |E_{1,3}|(\frac{2}{1+3} + |E_{2,1}|(\frac{2}{2+1}). \]

\[ = 41 + 9(\frac{2}{2+2} + 3(\frac{2}{2+3} + 3(\frac{2}{2+1}). \]

\[ H(G) = 27.6. \]

Theorem 2.6. The general randic index of triglyceride is given by, \( R_k(G) = 41(2^k + 9(3^k)(2^k) + 3(3^k) + 3(2^k). \)

Proof. The general randic index of triglyceride is

\[ R_k(G) = \sum_{e=uv \in E(G)} (d_ud_v)^k. \]

\[ = |E_{2,2}|(2^k + |E_{2,3}|(2.3)^k + |E_{1,3}|(1.3)^k + |E_{2,1}|(2.1)^k. \]

\[ = |E_{2,2}|(4^k + |E_{2,3}|(6^k + |E_{1,3}|(3^k + |E_{2,1}|(2^k). \]

\[ = 41(4^k) + 9(6^k) + 3(3^k) + 3(2^k). \]

\[ R_k(G) = 41(2^k) + 9(3^k)(2^k) + 3(3^k) + 3(2^k). \]
3. Conclusion

The problem of finding the general formula for $ABC$ index, Randic connectivity index, Sum connectivity index, $GA$ index, Harmonic index, General Randic index of triglyceride is solved here analytically without using computers.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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