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Topological Indices of Certain Derived Graphs of Triglycerides

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ABSTRACT: Topological graph indices are the bridge between structure and properties. These numerical descriptors, derived from the structural information of molecules represented as graphs, offer a powerful tool for predicting the physical, chemical, and biological properties of compounds without the need for extensive experimental trials. Triglycerides, a type of fat, are essential for energy storage and various metabolic processes. By representing triglyceride molecules as graphs and calculating their topological indices, scientists can potentially predict their physical and chemical properties, such as melting point and solubility. In this work, we determined nine specific topological indices for the total graph, the subdivision graph, the additional vertex subdivision graph, and the additional edge subdivision graph of the triglyceride graph. This information could be valuable for understanding the role of triglycerides in health and disease, as well as for developing new therapies and dietary strategies.

Key Words: Topological indices, molecular graph, triglyceride, derived graphs.

Contents

1. Introduction

Topological graph indices are graph invariants commonly used in quantitative structure-activity relationships (QSAR) and quantitative structure-property relationships (QSPR). These indices facilitate the prediction of a molecule's physical and chemical properties without relying on costly and time-consuming experimental methods. This process involves representing the molecule as a graph, where atoms are depicted as vertices and chemical bonds as edges. Once the molecule is modeled in this way, mathematical calculations can be applied to the graph to derive the required scientific information. The application of topological indices in the field of chemistry began in 1947, when chemist H. Wiener introduced the Wiener index, a fundamental topological descriptor. This index was initially employed to correlate the boiling points, a key physical property, of alkanes, which are a type of paraffin hydrocarbon [1]. Wiener's work laid the foundation for using mathematical representations of molecular structures to predict various chemical and physical properties, further advancing the field of chemical graph theory.

Triglycerides [2,3] are a form of lipid present in the bloodstream (Figure 1). Following a meal, the body transforms surplus calories, that are not immediately utilized, into triglycerides, which are then stored in adipose tissue. These lipids serve as an energy reservoir and contribute to the production of

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adenosine triphosphate (ATP), the molecule responsible for cellular energy. When cells require energy, triglycerides are mobilized and transported via cholesterol carriers to meet the demand.

Additionally, they play a role in maintaining cell membrane permeability. Consistently consuming more calories than expended, particularly carbohydrates and fats, can lead to elevated triglyceride levels, a condition known as hypertriglyceridemia. According to the American Heart Association, high triglyceride concentrations are associated with an increased risk of cardiovascular disease.

The fatty acid chains in triglycerides can be saturated or unsaturated. Saturated fatty acids are composed of carbon atoms linked by single bonds, where each carbon is bonded to two hydrogen atoms and one other carbon. This structure lacks any double bonds. On the other hand, unsaturated fatty acids contain at least one double bond between carbon atoms. Fatty acids with only one double bond are known as monounsaturated, while those with multiple double bonds are referred to as polyunsaturated. In this context, we focus on the carbon atoms found in saturated fatty acids.

We review the definitions and essential concepts of the total graph, the additional vertex subdivision graph, the additional edge subdivision graph, and the subdivision graph of a triglyceride graph.

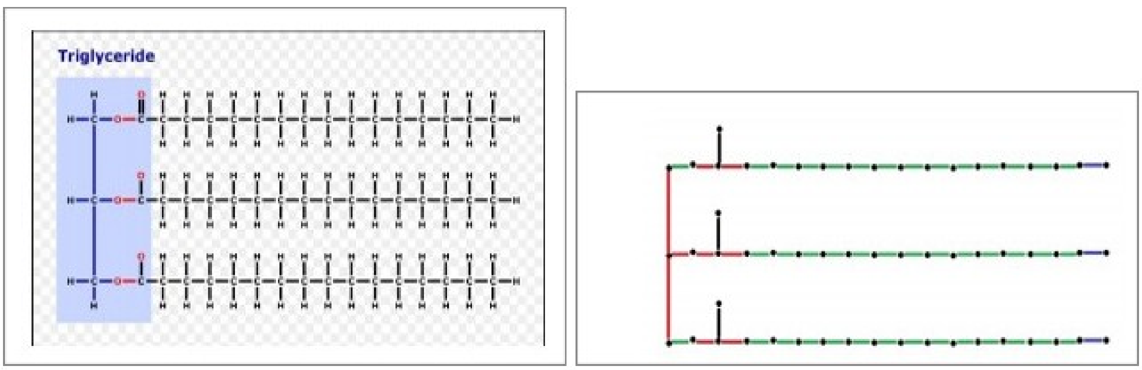

Figure 1: Triglyceride and molecular graph of triglyceride

1.1. Definitions

Let G be a graph with the vertex set V(G) and edge set E(G).

1.1.1. [4] Total graph T(G). It is the graph whose vertex set is $V \cup E$, with two vertices of T(G) being adjacent if and only if the corresponding elements of G are adjacent or incident.

1.1.2. [5] Additional vertex subdivision graph R(G). It is defined as the graph obtained from G by adding a new vertex to V(G) for each edge of G and by joining such each new vertex to the end vertices of the edge corresponding to it.

1.1.3. [5] Additional edge subdivision graph Q(G). It is defined as the graph obtained from G by adding a new vertex to V(G) for each edge of G and by joining those pairs of new vertices which correspond to adjacent edges of G by a new edge.

1.1.4. [6] The subdivision graph S(G). It is obtained from G by adding a new vertex onto each edge of G. Another way of obtaining S(G) is replacing each edge of G by a path of length 2.

1.2. Lemma

[7] Let G be a graph with n vertices and m edges. Then R(G) has n + m vertices and 3m edges.

1.3. Topological indices

Let G be a graph and let d_u denote the degree of a vertex $u \in V(\mathrm{G})$. We review the definitions of the topological indices under consideration.

1.3.1 Geometric–Arithmetic Index [8]. It is denoted and defined as:

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u \cdot d_v}}{d_u + d_v} \tag{1.1}$$

It is commonly used to study molecular branching and stability in chemistry.

1.3.2 Randić Index [9]. Also known as the connectivity index, it is defined by:

$$RA(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u \cdot d_v}}. \tag{1.2}$$

It helps in predicting molecular properties like boiling points, stability, and bioactivity.

1.3.3 First Hyper-Zagreb Index [10,11]. It is denoted and defined by:

$$HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2 \tag{1.3}$$

It helps in characterizing molecular graphs, particularly in QSPR/QSAR studies.

1.3.4 Forgotten Topological Index [12,13]. It is denoted and defined by:

$$F(G) = \sum_{uv \in E(G)} \left(d_u^2 + d_v^2\right) \tag{1.4}$$

This index evaluates branching in molecular structures and correlates with physical properties.

1.3.5 Atom-Bond Connectivity Index [14]. It is defined as:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u \cdot d_v}} \tag{1.5}$$

It helps in understanding molecular stability and thermodynamic properties.

1.3.6 Redefined First Zagreb Index [15]. It is denoted and defined by:

$$ReZG_1(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{d_u \cdot d_v} \tag{1.6}$$

It is applied in QSPR/QSAR modeling to predict chemical and biological properties.

1.3.7 Redefined Third Zagreb Index [15]. A higher-order Zagreb index is used to capture graph invariants by redefined mathematical formulas involving degrees. It is defined by:

$$ReZG_3(G) = \sum_{uv \in E(G)} (d_u d_v)(d_u + d_v) \tag{1.7}$$

It enhances molecular descriptor calculations for complex graphs.

1.3.8 First Reformulated Zagreb Index [16,17]. By reformulating the classical Zagreb index, the First Reformulated Zagreb index is defined as:

$$EM_1(G) = \sum_{uv \in E(G)} (d_u + d_v - 2)^2 \tag{1.8}$$

It is used in modeling molecular structures and predicting chemical activity.

1.3.9 Veerabhadraiah Lokesha Index [18]. It is denoted and defined by:

$$VL(G) = \frac{1}{2} \sum_{uv \in E(G)} (d_u + d_v + d_u \cdot d_v) \tag{1.9}$$

It is used for analyzing molecular topology in specialized studies.

2. Main Results

The above-mentioned topological indices are computed for the total graph, the subdivision graph, and the additional vertex and additional edge subdivision graphs of the triglyceride graph.

Theorem 2.1 *Let G be the total graph of triglyceride. Then, the relevant indices are given by:*

$$\begin{array}{lll} GA(G) = 225.716838 & RA(G) = 56.106148 & HM(G) = 15724 \\ F(G) = 7942 & ABC(G) = 138.558361 & ReZG_1(G) = 113 \\ ReZG_3(G) = 33082 & EM_1(G) = 9128 & VL(G) = 2883.5 \end{array}$$

Proof: Let the graph G represent the total graph of triglyceride, which comprises nine distinct edge classifications. The specifics of these classifications are outlined in Table 1 [3].

X	(2,3)	(2,4)	(2,6)	(3,4)	(4,4)	(4,5)	(4,6)	(5,5)	(5,6)
Y	3	6	3	6	159	22	12	7	9

Table 1: The edge partition of the total graph of triglyceride where X signifies the classification of edges (d_u, d_v) with $uv \in E(G)$ and Y represents the number of edges.

By employing these, the relevant indices are obtained as follows:

$$GA(G) = 3\left(\frac{2\sqrt{2\cdot 3}}{2+3}\right) + 6\left(\frac{2\sqrt{2\cdot 4}}{2+4}\right) + 3\left(\frac{2\sqrt{2\cdot 6}}{2+6}\right) + 6\left(\frac{2\sqrt{3\cdot 4}}{3+4}\right) + 159\left(\frac{2\sqrt{4\cdot 4}}{4+4}\right)$$

$$+22\left(\frac{2\sqrt{4\cdot 5}}{4+5}\right) + 12\left(\frac{2\sqrt{4\cdot 6}}{4+6}\right) + 7\left(\frac{2\sqrt{5\cdot 5}}{5+5}\right) + 9\left(\frac{2\sqrt{5\cdot 6}}{5+6}\right) = 225.716838$$

$$RA(G) = 3\left(\frac{1}{\sqrt{2\cdot 3}}\right) + 6\left(\frac{1}{\sqrt{2\cdot 4}}\right) + 3\left(\frac{1}{\sqrt{2\cdot 6}}\right) + 6\left(\frac{1}{\sqrt{3\cdot 4}}\right) + 159\left(\frac{1}{\sqrt{4\cdot 4}}\right)$$

$$+22\left(\frac{1}{\sqrt{4\cdot 5}}\right) + 12\left(\frac{1}{\sqrt{4\cdot 6}}\right) + 7\left(\frac{1}{\sqrt{5\cdot 5}}\right) + 9\left(\frac{1}{\sqrt{5\cdot 6}}\right) = 56.106148$$

$$HM(G) = 3(2+3)^2 + 6(2+4)^2 + 3(2+6)^2 + 6(3+4)^2 + 159(4+4)^2 + 22(4+5)^2$$

$$+12(4+6)^2 + 7(5+5)^2 + 9(5+6)^2 = 15724$$

$$F(G) = 3(2^2+3^2) + 6(2^2+4^2) + 3(2^2+6^2) + 6(3^2+4^2) + 159(4^2+4^2) + 22(4^2+5^2)$$

$$+12(4^2+6^2) + 7(5^2+5^2) + 9(5^2+6^2) = 7942$$

$$ABC(G) = 3\sqrt{\frac{2+3-2}{2\cdot 3}} + 6\sqrt{\frac{2+4-2}{2\cdot 4}} + 3\sqrt{\frac{2+6-2}{2\cdot 6}} + 6\sqrt{\frac{3+4-2}{3\cdot 4}} + 159\sqrt{\frac{4+4-2}{4\cdot 4}}$$

$$+22\sqrt{\frac{4+5-2}{4\cdot 5}}+12\sqrt{\frac{4+6-2}{4\cdot 6}}+7\sqrt{\frac{5+5-2}{5\cdot 5}}+9\sqrt{\frac{5+6-2}{5\cdot 6}}=138.558361$$

$$ReZG_1(G)=3\left(\frac{2+3}{2\cdot 3}\right)+6\left(\frac{2+4}{2\cdot 4}\right)+3\left(\frac{2+6}{2\cdot 6}\right)+6\left(\frac{3+4}{3\cdot 4}\right)+159\left(\frac{4+4}{4\cdot 4}\right)$$

$$+22\left(\frac{4+5}{4\cdot 5}\right)+12\left(\frac{4+6}{4\cdot 6}\right)+7\left(\frac{5+5}{5\cdot 5}\right)+9\left(\frac{5+6}{5\cdot 6}\right)=113$$

$$ReZG_3(G)=3\big[(2\cdot 3)(2+3)\big]+6\big[(2\cdot 4)(2+4)\big]+3\big[(2\cdot 6)(2+6)\big]+6\big[(3\cdot 4)(3+4)\big]$$

$$+159\big[(4\cdot 4)(4+4)\big]+22\big[(4\cdot 5)(4+5)\big]+12\big[(4\cdot 6)(4+6)\big]$$

$$+7\big[(5\cdot 5)(5+5)\big]+9\big[(5\cdot 6)(5+6)\big]=33082$$

$$EM_1(G)=3(2+3-2)^2+6(2+4-2)^2+3(2+6-2)^2+6(3+4-2)^2+159(4+4-2)^2+22(4+5-2)^2$$

$$+12(4+6-2)^2+7(5+5-2)^2+9(5+6-2)^2=9128$$

$$VL(G)=\tfrac{1}{2}\Big[3(2+3+2\cdot 3)+6(2+4+2\cdot 4)+3(2+6+2\cdot 6)+6(3+4+3\cdot 4)+159(4+4+4\cdot 4)$$

$$+22(4+5+4\cdot 5)+12(4+6+4\cdot 6)+7(5+5+5\cdot 5)+9(5+6+5\cdot 6)\Big]=2883.5$$

Thus, the result follows. □

Theorem 2.2 *Let G be the additional vertex subdivision graph of triglyceride. Then,*

$GA(G)=111.414405$	$RA(G)=56.141620$	$HM(G)=1858$
$F(G)=938$	$ABC(G)=79.195959$	$ReZG_1(G)=113$
$ReZG_3(G)=1900$	$EM_1(G)=490$	$VL(G)=457$

Proof: Let the graph G represent the additional vertex subdivision graph of triglyceride, which comprises nine distinct edge classifications. The specifics of these classifications are outlined in Table 2 [3].

X	(1,2)	(2,2)	(2,3)
Y	6	94	12

Table 2: The edge partition of the additional vertex subdivision graph of triglyceride where X signifies the classification of edges (d_u, d_v) with $uv \in E(G)$ and Y represents the number of edges.

By employing data from Table 2, the relevant indices are derived as follows:

$$GA(G)=6\left(\frac{2\sqrt{1\cdot 2}}{1+2}\right)+94\left(\frac{2\sqrt{2\cdot 2}}{2+2}\right)+12\left(\frac{2\sqrt{2\cdot 3}}{2+3}\right)=111.414405$$

$$RA(G)=6\left(\frac{1}{\sqrt{1\cdot 2}}\right)+94\left(\frac{1}{\sqrt{2\cdot 2}}\right)+12\left(\frac{1}{\sqrt{2\cdot 3}}\right)=56.141620$$

$$HM(G) = 6(1+2)^2 + 94(2+2)^2 + 12(2+3)^2 = 1858$$

$$F(G) = 6(1^2+2^2) + 94(2^2+2^2) + 12(2^2+3^2) = 938$$

$$ABC(G) = 6\sqrt{\frac{1+2-2}{1\cdot 2}} + 94\sqrt{\frac{2+2-2}{2\cdot 2}} + 12\sqrt{\frac{2+3-2}{2\cdot 3}} = 79.195959$$

$$ReZG_1(G) = 6\left(\frac{1+2}{1\cdot 2}\right) + 94\left(\frac{2+2}{2\cdot 2}\right) + 12\left(\frac{2+3}{2\cdot 3}\right) = 113$$

$$ReZG_3(G) = 6\big[(1\cdot 2)(1+2)\big] + 94\big[(2\cdot 2)(2+2)\big] + 12\big[(2\cdot 3)(2+3)\big] = 1900$$

$$EM_1(G) = 6(1+2-2)^2 + 94(2+2-2)^2 + 12(2+3-2)^2 = 490$$

$$VL(G) = \tfrac{1}{2}\Big[6(1+2+1\cdot 2) + 94(2+2+2\cdot 2) + 12(2+3+2\cdot 3)\Big] = 457$$

Thus, the result follows. □

Theorem 2.3 *Let G be the additional edge subdivision graph of triglyceride. Then,*

$GA(G) = 160.261021$	$RA(G) = 53.711923$	$HM(G) = 8072$
$F(G) = 4368$	$ABC(G) = 113.742022$	$ReZG_1(G) = 113$
$ReZG_3(G) = 13600$	$EM_1(G) = 4168$	$VL(G) = 1498$

Proof: Let the graph G represent the additional edge subdivision graph of triglyceride, which comprises nine distinct edge classifications. The specifics of these classifications are outlined in Table 3 [3].

X	(2,2)	(2,4)	(2,6)	(4,4)	(4,6)
Y	6	97	15	41	9

Table 3: The edge partition of the additional edge subdivision graph of triglyceride where X signifies the classification of edges (d_u, d_v) with $uv \in E(G)$ and Y represents the number of edges.

By employing Table 3, the relevant indices are obtained as follows:

$$GA(G) = 6\left(\frac{2\sqrt{2\cdot 2}}{2+2}\right) + 97\left(\frac{2\sqrt{2\cdot 4}}{2+4}\right) + 15\left(\frac{2\sqrt{2\cdot 6}}{2+6}\right) + 41\left(\frac{2\sqrt{4\cdot 4}}{4+4}\right) + 9\left(\frac{2\sqrt{4\cdot 6}}{4+6}\right) = 160.261021$$

$$RA(G) = 6\left(\frac{1}{\sqrt{2\cdot 2}}\right) + 97\left(\frac{1}{\sqrt{2\cdot 4}}\right) + 15\left(\frac{1}{\sqrt{2\cdot 6}}\right) + 41\left(\frac{1}{\sqrt{4\cdot 4}}\right) + 9\left(\frac{1}{\sqrt{4\cdot 6}}\right) = 53.711923$$

$$HM(G) = 6(2+2)^2 + 97(2+4)^2 + 15(2+6)^2 + 41(4+4)^2 + 9(4+6)^2 = 8072$$

$$F(G) = 6(2^2+2^2) + 97(2^2+4^2) + 15(2^2+6^2) + 41(4^2+4^2) + 9(4^2+6^2) = 4368$$

$$ABC(G) = 6\sqrt{\frac{2+2-2}{2\cdot 2}} + 97\sqrt{\frac{2+4-2}{2\cdot 4}} + 15\sqrt{\frac{2+6-2}{2\cdot 6}} + 41\sqrt{\frac{4+4-2}{4\cdot 4}} + 9\sqrt{\frac{4+6-2}{4\cdot 6}} = 113.742022$$

$$ReZG_1(G) = 6\left[\frac{1+2}{1\cdot 2}\right] + 94\left[\frac{2+2}{2\cdot 2}\right] + 12\left[\frac{2+3}{2\cdot 3}\right] = 113$$

$$ReZG_3(G) = 6[(1\cdot 2)(1+2)] + 94[(2\cdot 2)(2+2)] + 12[(2\cdot 3)(2+3)] = 1900$$

$$EM_1(G) = 6[(1+2-2)^2] + 94[(2+2-2)^2] + 12[(2+3-2)^2] = 490$$

$$VL(G) = \tfrac{1}{2}\Big[6(1+2+1\cdot 2) + 94(2+2+2\cdot 2) + 12(2+3+2\cdot 3)\Big] = 457$$

Thus, the result follows. □

Theorem 2.4 *Let G be the subdivision graph of triglyceride. Then,*

$$\begin{array}{lll} GA(G) = 163.073150 & RA(G) = 53.69255653 & HM(G) = 8290 \\ F(G) = 4390 & ABC(G) = 114.330568 & ReZG_1(G) = 113 \\ ReZG_3(G) = 14424 & EM_1(G) = 4298 & VL(G) = 1559 \end{array}$$

Proof: Let the graph G represent the subdivision graph of triglyceride, which comprises nine distinct edge classifications. The specifics of these classifications are outlined in Table 4 [3].

X	(1,3)	(1,4)	(2,3)	(2,4)	(2,5)	(3,4)	(3,5)	(4,4)	(4,5)	(5,5)
Y	3	3	3	84	7	8	7	38	13	4

Table 4: The subdivision graph of triglyceride where X denotes the type of edges (d_u, d_v) with $uv \in E(G)$ and Y is the number of edges.

By employing Table 4, the relevant indices are obtained as follows:

$$GA(G) = 3\left(\frac{2\sqrt{1\cdot 3}}{1+3}\right) + 3\left(\frac{2\sqrt{1\cdot 4}}{1+4}\right) + 3\left(\frac{2\sqrt{2\cdot 3}}{2+3}\right) + 84\left(\frac{2\sqrt{2\cdot 4}}{2+4}\right)$$

$$+7\left(\frac{2\sqrt{2\cdot 5}}{2+5}\right) + 8\left(\frac{2\sqrt{3\cdot 4}}{3+4}\right) + 7\left(\frac{2\sqrt{3\cdot 5}}{3+5}\right) + 38\left(\frac{2\sqrt{4\cdot 4}}{4+4}\right)$$

$$+13\left(\frac{2\sqrt{4\cdot 5}}{4+5}\right) + 4\left(\frac{2\sqrt{5\cdot 5}}{5+5}\right) = 163.073150$$

$$RA(G) = 3\left(\frac{1}{\sqrt{1\cdot 3}}\right) + 3\left(\frac{1}{\sqrt{1\cdot 4}}\right) + 3\left(\frac{1}{\sqrt{2\cdot 3}}\right) + 84\left(\frac{1}{\sqrt{2\cdot 4}}\right) + 7\left(\frac{1}{\sqrt{2\cdot 5}}\right)$$

$$+8\left(\frac{1}{\sqrt{3\cdot 4}}\right) + 7\left(\frac{1}{\sqrt{3\cdot 5}}\right) + 38\left(\frac{1}{\sqrt{4\cdot 4}}\right) + 13\left(\frac{1}{\sqrt{4\cdot 5}}\right) + 4\left(\frac{1}{\sqrt{5\cdot 5}}\right) = 53.69255653$$

$$HM(G) = 3(1+3)^2 + 3(1+4)^2 + 3(2+3)^2 + 84(2+4)^2 + 7(2+5)^2$$

$$+8(3+4)^2 + 7(3+5)^2 + 38(4+4)^2 + 13(4+5)^2 + 4(5+5)^2 = 8290$$

$$F(G) = 3(1^2+3^2) + 3(1^2+4^2) + 3(2^2+3^2) + 84(2^2+4^2) + 7(2^2+5^2)$$

$$+8(3^2+4^2)+7(3^2+5^2)+38(4^2+4^2)+13(4^2+5^2)+4(5^2+5^2)=4390$$

$$ABC(G)=3\sqrt{\frac{1+3-2}{1\cdot 3}}+3\sqrt{\frac{1+4-2}{1\cdot 4}}+3\sqrt{\frac{2+3-2}{2\cdot 3}}+84\sqrt{\frac{2+4-2}{2\cdot 4}}+7\sqrt{\frac{2+5-2}{2\cdot 5}}$$

$$+8\sqrt{\frac{3+4-2}{3\cdot 4}}+7\sqrt{\frac{3+5-2}{3\cdot 5}}+38\sqrt{\frac{4+4-2}{4\cdot 4}}+13\sqrt{\frac{4+5-2}{4\cdot 5}}+4\sqrt{\frac{5+5-2}{5\cdot 5}}=114.330568$$

$$ReZG_1(G)=3\left(\frac{1+3}{1\cdot 3}\right)+3\left(\frac{1+4}{1\cdot 4}\right)+3\left(\frac{2+3}{2\cdot 3}\right)+84\left(\frac{2+4}{2\cdot 4}\right)+7\left(\frac{2+5}{2\cdot 5}\right)$$

$$+8\left(\frac{3+4}{3\cdot 4}\right)+7\left(\frac{3+5}{3\cdot 5}\right)+38\left(\frac{4+4}{4\cdot 4}\right)+13\left(\frac{4+5}{4\cdot 5}\right)+4\left(\frac{5+5}{5\cdot 5}\right)=113$$

$$ReZG_3(G)=3(1\cdot 3)(1+3)+3(1\cdot 4)(1+4)+3(2\cdot 3)(2+3)+84(2\cdot 4)(2+4)+7(2\cdot 5)(2+5)$$

$$+8(3\cdot 4)(3+4)+7(3\cdot 5)(3+5)+38(4\cdot 4)(4+4)$$

$$+13(4\cdot 5)(4+5)+4(5\cdot 5)(5+5)=14424$$

$$EM_1(G)=3(1+3-2)^2+3(1+4-2)^2+3(2+3-2)^2+84(2+4-2)^2$$

$$+7(2+5-2)^2+8(3+4-2)^2+7(3+5-2)^2+38(4+4-2)^2+13(4+5-2)^2+4(5+5-2)^2=4298$$

$$VL(G)=\tfrac{1}{2}\Big[3(1+3+1\cdot 3)+3(1+4+1\cdot 4)+3(2+3+2\cdot 3)+84(2+4+2\cdot 4)$$

$$+7(2+5+2\cdot 5)+8(3+4+3\cdot 4)+7(3+5+3\cdot 5)+38(4+4+4\cdot 4)$$

$$+13(4+5+4\cdot 5)+4(5+5+5\cdot 5)\Big]=1559$$

Thus, the result follows. □

3. Discussion

Topological indices quantitatively relate a molecule's structural topology to its physicochemical properties. For triglycerides, which serve as vital energy-storage molecules, these indices help explain how structural connectivity influences thermodynamic, transport, and biological properties.

The Geometric–Arithmetic (GA) and Randić indices reflect the degree of branching and molecular compactness within the triglyceride structure. Higher values typically correspond to increased molecular stability and lower reactivity, suggesting that these indices can serve as indicators of the robustness of triglyceride bonds and their resistance to degradation.

The First Hyper-Zagreb and Forgotten indices capture nonlinear relationships among vertex degrees and thus describe the heterogeneity of atomic interactions within the molecule. They can be correlated with local electronic density and energy distribution, helping to predict how structural irregularities affect triglyceride reactivity and energy storage potential.

The Atom–Bond Connectivity (ABC) and Redefined First Zagreb ($ReZG_1$) indices reflect the strength of atomic and bond interactions. In triglycerides, they correspond to the saturation level of fatty acid chains, influencing melting points and solubility in lipid systems.

The Redefined Third Zagreb ($ReZG_3$) and First Reformulated Zagreb (EM_1) indices capture both local and global connectivity, linking bond multiplicity and molecular extension to mass and viscosity, while their correlation with the glycerol backbone aids in predicting molecular flexibility and energy.

The Veerabhadraiah–Lokesha (VL) index combines degree- and edge-based characteristics to represent overall molecular topology, serving as a stability descriptor through energy distribution across the molecular graph.

When compared with other lipid molecules such as fatty acids, diglycerides, and phospholipids, the observed topological behavior of triglycerides reveals both similarities and distinct characteristics. Degree-based indices like the Randić and GA indices show comparable patterns across lipid structures, indicating consistent connectivity among hydrocarbon chains. However, energy-related indices such as the Hyper-Zagreb, Forgotten, and Redefined Third Zagreb indices display higher magnitudes for triglycerides due to their larger molecular framework and greater bond density. In contrast, simpler lipids like diglycerides show lower index values because of fewer ester linkages and reduced branching. These comparative insights highlight that topological indices effectively distinguish triglycerides from other lipids in terms of structural compactness and energy potential, offering a theoretical foundation for modeling variations in lipid stability, reactivity, and biological functionality.

4. Conclusion

A comparative analysis of the specified topological indices was performed on triglyceride molecular graphs and their derived forms, namely the total graph $\mathrm{T}(G)$, the additional vertex subdivision graph $\mathrm{R}(G)$, the additional edge subdivision graph $\mathrm{Q}(G)$, and subdivision graph $\mathrm{S}(G)$. The corresponding results are illustrated in Figure 2. In these plots, *Array 1* represents the values of the nine topological indices for the original triglyceride molecule, whereas *Array 2* corresponds to the indices of $\mathrm{T}(G)$, $\mathrm{R}(G)$, $\mathrm{Q}(G)$, and $\mathrm{S}(G)$, respectively.

Across all modified triglyceride structures, a substantial increase was observed in the Redefined Third Zagreb Index, the First Hyper-Zagreb Index, the Forgotten Topological Index, and the First Reformulated Zagreb Index. Among these, the Redefined Third Zagreb Index exhibited the most pronounced variation, reflecting its high sensitivity to molecular transformations and connectivity changes. Additionally, the Veerabhadraiah-Lokesha Index showed a moderate increase, whereas the remaining indices displayed relatively consistent values compared with those of the original triglyceride molecule.

These observations underscore the distinctive responsiveness of certain indices, particularly the Redefined Third Zagreb Index, to specific structural modifications, suggesting their potential application in identifying and quantifying subtle topological variations within triglyceride molecules. This sensitivity is crucial for modeling the influence of molecular branching, connectivity, and complexity on the properties of triglycerides.

The integration of topological and chemical perspectives, as demonstrated in Figure 2, provides a deeper understanding of how graph-theoretical parameters correspond to real molecular characteristics. This framework enables more accurate predictions of structural behavior, molecular stability, and reactivity. These insights can be instrumental in advancing theoretical studies on lipid molecules, designing lipid-based materials, and exploring the roles of triglycerides in both biochemical and industrial contexts.

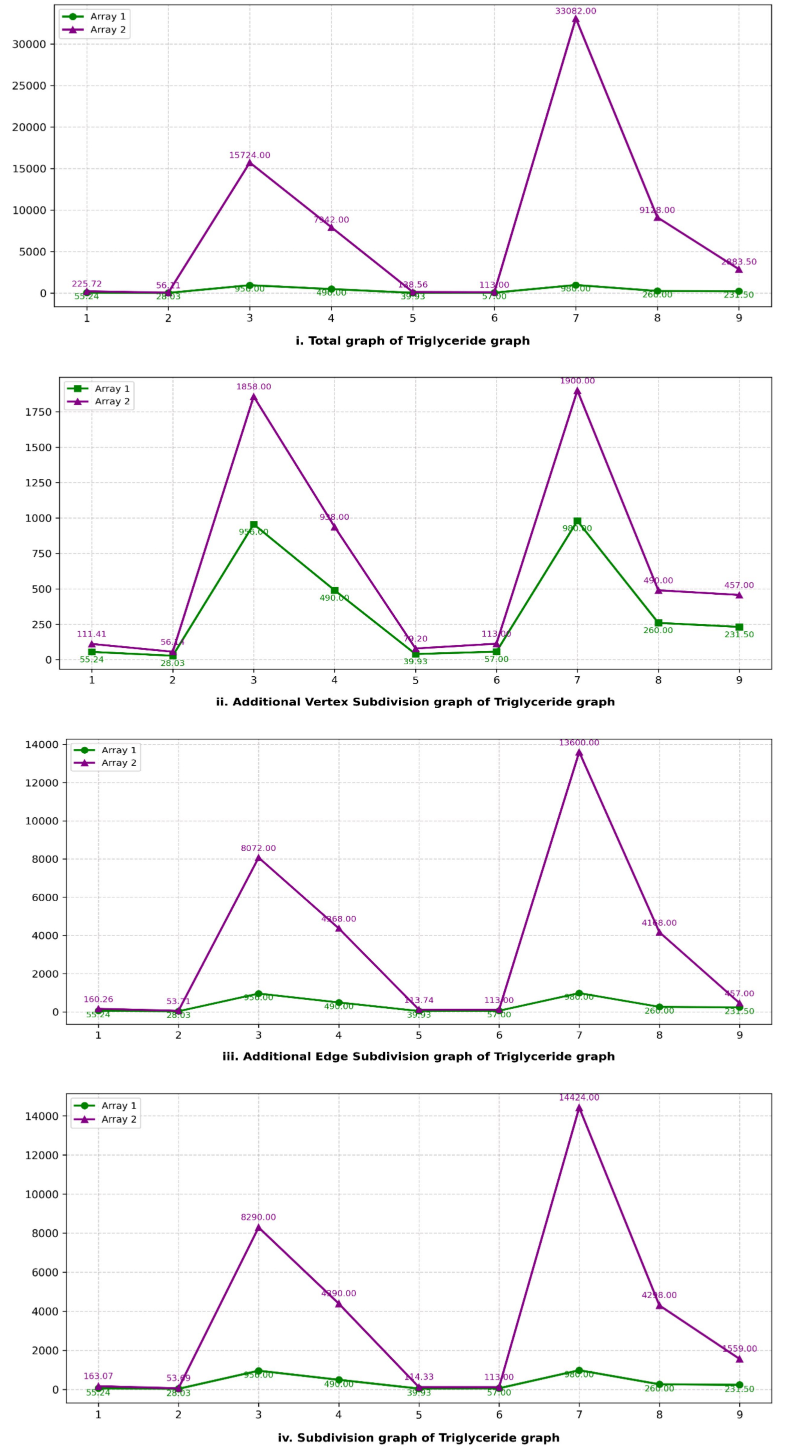

Figure 2: Evaluation of the graph indices of the derived graphs of triglyceride.

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