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SOME NEW TOPOLOGICAL INDICES OF ASPIRIN

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Abstract. Acetylsalicylic acid (ASA), commonly known as Aspirin, is a medicinal drug prescribed to treat pain, fever, or inflammation. Topological indices are graph invariants computed by the distance or degree of vertices of the molecular graph. In chemical graph theory, topological indices have been successfully used to describe the structures and predict certain physicochemical properties of chemical compounds. In this paper, we compute new topological indices, including the first and second entire Zagreb indices, the first and second Zagreb eccentricity indices, the Zagreb degree eccentricity indices, first and second locating indices, and Sanskruti index of Aspirin. In addition, some other topological indices are calculated.

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1. Introduction

Aspirin, or acetylsalicylic acid (ASA), is an anti-inflammatory, pain relieving medicinal drug. Its molecular formula is $C_9H_8O_4$. See Fig. 1 below:

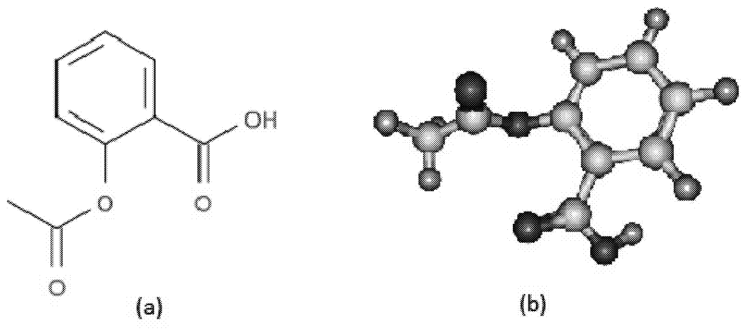

Figure 1. (a) Aspirin structure; (b) The chemical structure of aspirin as optimized at the DFT\B3LYB\$6-31+G\,(d,p)$ level of theory using Gaussian 09 package

Note that hydrogen atoms are often omitted. The molecular graph representing Aspirin is shown in Fig. 2:

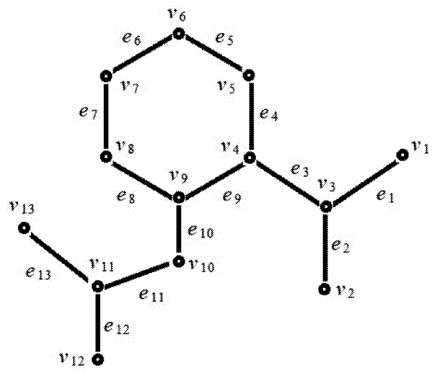

Figure 2. Molecular graph of Aspirin

The molecular structure of a drug determines its pharmacological characteristics. Topological indices can be considered as a transformation of a chemical structure into a positive real number and have been used as a predictor parameter. They are the molecular descriptors that describe the structure of chemical compounds and aid in the prediction of certain physicochemical properties, like boiling point, enthalpy of vaporizing, stability, etc. Molecules and molecular compounds are often modeled by molecular graphs, whose edges correspond to chemical bonds and vertices correspond to the atoms of the compound. For a detailed explanation, let $G = (V(G), E(G))$ be the molecular graph, then the topological index can be considered as a function of real values $f : G \to \mathbb{R}^+$. Let $G = (V, E)$ be a graph with vertex set V and edge set E. The degree of a vertex $v \in V(G)$ is denoted by d_v and is the number of vertices that are adjacent to v. $N(v)$ is the set of neighbors of v. Let uv represents the edge between the vertices v and u. Define $s_G(u)$ to be the sum of the degree of all neighbors of vertex u in G. i.e.

$$s_G(u) = \sum_{u \in N(u)} d_v. \tag{1}$$

Alwardi et al. in [1], introduced the first and second entire Zagreb indices of G as

$$M_1^{\varepsilon}(G) = \sum_{x \in V(G) \cup E(G)} (\deg(x))^2, \tag{2}$$

and

$$M_2^{\varepsilon}(G) = \sum_{\{x,y\} \in B(G)} \deg(x) \cdot \deg(y). \tag{3}$$

Where $deg(x)$ denotes the degree of a vertex or edge x in G and $B(G)$ to be the set of all $\{x, y\}$ such that $\{x, y\} \subseteq V(G) \cup E(G)$ and members of $\{x, y\}$ are adjacent or incident to each other.

Wazzan and Saleh recently [15] introduced two new indices and named them first and second locating indices which are defined as

$$M_1^{\mathcal{L}}(G) = \sum_{v_i \in V(G)} (\overrightarrow{v}_i)^2, \tag{4}$$

and

$$M_2^{\mathcal{L}}(G) = \sum_{v_i v_j \in E(G)} \overrightarrow{v}_i \cdot \overrightarrow{v}_j. \tag{5}$$

Where $\overrightarrow{v}_i = (d(v_1, v_i), d(v_2, v_i), ..., d(v_n, v_i))$, such that $d(v_i, v_j)$ is the distance between the vertices v_i and v_j in G. The vector $\overrightarrow{v}_i$ is called the locating vector corresponding to the vertex v_i.Where $\overrightarrow{v}_i \cdot \overrightarrow{v}_j$ is the dot product of the vectors $\overrightarrow{v}_i$ and $\overrightarrow{v}_j$ in the integers space $\mathbb{Z}^+ \cup \{0\}$ such that v_i is adjacent to v_j.

Recently, Hosamani [11] proposed the Sanskruti index and defined it as

$$S(G) = \sum_{uv \in E(G)} \left(\frac{s_G(u)\, s_G(v)}{s_G(u) + s_G(v) - 2} \right)^3. \tag{6}$$

For vertices $v_i, v_j \in V(G)$, the distance $d_G(v_i, v_j)$ is defined as the length of the shortest path between v_i and v_j in G. The eccentricity $(ld)_i$ of v_i denote the largest distance between v_i and any other vertex of G, in other words

$$(ld)_i = \max_{v_j \in V(G)} d_G(v_i, v_j). \tag{7}$$

In analogy with the first and second Zagreb indices, Ghorbani et al. and Vukičecić et al. introduced the first and second Zagreb eccentricity indices, [8], by replacing the vertex degrees with the eccentricities. The first Zagreb eccentricity E_1 and the second Zagreb eccentricity E_2 indices of a graph G are defined as

$$E_1(G) = \sum_{v_i \in V(G)} (ld)_i^2, \tag{8}$$

and

$$E_2(G) = \sum_{v_i v_j \in E(G)} (ld)_i (ld)_j. \tag{9}$$

The Zagreb degree eccentricity indices are introduced in [12]. First Zagreb degree eccentricity DE_1 and second Zagreb degree eccentricity DE_2 indices of a graph G are defined as

$$DE_1(G) = \sum_{v_i \in V(G)} ((ld)_i + d_i)^2, \tag{10}$$

and

$$DE_2(G) = \sum_{v_i v_j \in E(G)} ((ld)_i + d_i)\left((ld)_j + d_j\right). \tag{11}$$

Other studies on Zagreb degree eccentricity indices can be found in [2] and [20].

2. Main results and proofs

Theorem 2.1. *The first and second entire Zagreb indices of Aspirin are* 156, *and* 358 *respectively.*

Proof. First, using equation 2, we compute the first entire Zagreb index as follows:

$$\begin{aligned} M_1^{\varepsilon}(C_9H_8O_4) &= \sum_{x\in V(G)\cup E(G)} (\deg(x))^2 \\ &= \sum_{i=1}^{13} (\deg(v_i))^2 + \sum_{i=1}^{13} (\deg(e_i))^2 \\ &= 4(1)^2 + 5(2)^2 + 4(3)^2 + 7(2)^2 + 4(3)^2 + 2(4)^2 \\ &= 156. \end{aligned}$$

Second, through equation 3, we compute the second entire Zagreb index

$$\begin{aligned} M_2^{\varepsilon}(G) &= \sum_{\substack{x \text{ is either adjacent} \\ \text{or incident to } y}} \deg(x)\cdot\deg(y) \\ &= \deg(v_1)\deg(v_3) + \deg(v_2)\deg(v_3) + \deg(v_3)\deg(v_4) + \deg(v_4)\deg(v_5) + \\ &\quad \deg(v_5)\deg(v_6) + \deg(v_6)\deg(v_7) + \deg(v_7)\deg(v_8) + \deg(v_8)\deg(v_9) + \\ &\quad \deg(v_9)\deg(v_4) + \deg(v_9)\deg(v_{10}) + \deg(v_{10})\deg(v_{11}) + \deg(v_{11})\deg(v_{12}) + \\ &\quad \deg(v_{11})\deg(v_{13}) + \deg(e_1)\deg(e_2) + \deg(e_1)\deg(e_3) + \deg(e_2)\deg(e_3) + \\ &\quad \deg(e_3)\deg(e_4) + \deg(e_3)\deg(e_9) + \deg(e_4)\deg(e_5) + \deg(e_4)\deg(e_9) + \\ &\quad \deg(e_5)\deg(e_6) + \deg(e_6)\deg(e_7) + \deg(e_7)\deg(e_8) + \deg(e_8)\deg(e_9) + \\ &\quad \deg(e_8)\deg(e_{10}) + \deg(e_9)\deg(e_{10}) + \deg(e_{10})\deg(e_{11}) + \deg(e_{11})\deg(e_{12}) + \\ &\quad \deg(e_{11})\deg(e_{13}) + \deg(e_1)\deg(v_1) + \deg(e_1)\deg(v_3) + \deg(e_2)\deg(v_2) + \\ &\quad \deg(e_2)\deg(v_3) + \deg(e_3)\deg(v_3) + \deg(e_3)\deg(v_4) + \deg(e_4)\deg(v_4) + \\ &\quad \deg(e_4)\deg(v_5) + \deg(e_5)\deg(v_5) + \deg(e_5)\deg(v_6) + \deg(e_6)\deg(v_6) + \\ &\quad \deg(e_6)\deg(v_7) + \deg(e_7)\deg(v_7) + \deg(e_7)\deg(v_8) + \deg(e_8)\deg(v_8) + \\ &\quad \deg(e_8)\deg(v_9) + \deg(e_9)\deg(v_4) + \deg(e_9)\deg(v_9) + \deg(e_{10})\deg(v_9) + \\ &\quad \deg(e_{10})\deg(v_{10}) + \deg(e_{11})\deg(v_{10}) + \deg(e_{11})\deg(v_{11}) + \deg(e_{12})\deg(v_{11}) + \\ &\quad \deg(e_{12})\deg(v_{12}) + \deg(e_{13})\deg(v_{11}) + \deg(e_{13})\deg(v_{13}) \end{aligned}$$

Hence

$$\begin{aligned} M_2^{\varepsilon}(C_9H_8O_4) &= (1\times 3) + (3\times 1) + (3\times 3) + (3\times 2) + (2\times 2) + (2\times 2) + (2\times 2) + (3\times 2) + \\ &\quad (3\times 3) + (2\times 3) + (2\times 3) + (1\times 3) + (1\times 3) + (2\times 2) + (2\times 4) + (2\times 4) + \\ &\quad (4\times 3) + (4\times 4) + (3\times 2) + (3\times 4) + (2\times 2) + (2\times 2) + (2\times 3) + (3\times 4) + \\ &\quad (3\times 3) + (4\times 3) + (3\times 3) + (3\times 2) + (3\times 2) + (2\times 1) + (2\times 3) + (2\times 1) + \\ &\quad (2\times 3) + (4\times 3) + (4\times 3) + (3\times 3) + (3\times 2) + (2\times 2) + (2\times 2) + (2\times 2) + \\ &\quad (2\times 2) + (2\times 2) + (2\times 2) + (3\times 2) + (3\times 3) + (3\times 3) + (3\times 3) + (3\times 3) + \\ &\quad (3\times 2) + (3\times 2) + (3\times 3) + (2\times 3) + (2\times 1) + (2\times 3) + (2\times 1) \\ &= 358. \end{aligned}$$

The proof is complete. □

Theorem 2.2. *The first and second locating indices of Aspirin are* 1912, *and* 1600 *respectively.*

Proof. First, we compute $\overrightarrow{\vartheta}_i$ for each $v_i \in V\left(C_9H_8O_4\right)$:

$$\begin{aligned}
\overrightarrow{\vartheta}_1 &= (0,2,1,2,3,4,5,4,3,4,5,6,6)\,, \overrightarrow{\vartheta}_2 = (2,0,1,2,3,4,5,4,3,4,5,6,6)\,, \\
\overrightarrow{\vartheta}_3 &= (1,1,0,1,2,3,4,3,2,3,4,5,5)\,, \overrightarrow{\vartheta}_4 = (2,2,1,0,1,2,3,2,1,2,3,4,4)\,, \\
\overrightarrow{\vartheta}_5 &= (3,3,2,1,0,1,2,3,2,3,4,5,5)\,, \overrightarrow{\vartheta}_6 = (4,4,3,2,1,0,1,2,3,4,5,6,6)\,, \\
\overrightarrow{\vartheta}_7 &= (5,5,4,3,2,1,0,1,2,3,4,5,5)\,, \overrightarrow{\vartheta}_8 = (4,4,3,2,3,2,1,0,1,2,3,4,4)\,, \\
\overrightarrow{\vartheta}_9 &= (3,3,2,1,2,3,2,1,0,1,2,3,3)\,, \overrightarrow{\vartheta}_{10} = (4,4,3,2,3,4,3,2,1,0,1,2,2)\,, \\
\overrightarrow{\vartheta}_{11} &= (5,5,4,3,4,5,4,3,2,1,0,1,1)\,, \overrightarrow{\vartheta}_{12} = (6,6,5,4,5,6,5,4,3,2,1,0,2)\,, \\
\overrightarrow{\vartheta}_{13} &= (6,6,5,4,5,6,5,4,3,2,1,2,0)\,.
\end{aligned}$$

Then by use of equation 4, the first locating index of Aspirin is given by

$$\begin{aligned}
M_1^{\mathcal{L}}\left(C_9H_8O_4\right) &= \sum_{v_i \in V(G)} \left(\overrightarrow{\vartheta}_i\right)^2 \\
&= 197+197+120+73+116+173+160+105+ \\
&\quad 64+93+148+233+233 \\
&= 1912.
\end{aligned}$$

and by using equation 5, the second locating index of Aspirin is given by

$$\begin{aligned}
M_2^{\mathcal{L}}\left(C_9H_8O_4\right) &= \sum_{v_iv_j \in E(G)} \overrightarrow{\vartheta}_i \cdot \overrightarrow{\vartheta}_j \\
&= (\overrightarrow{\vartheta}_1 \cdot \overrightarrow{\vartheta}_3) + (\overrightarrow{\vartheta}_2 \cdot \overrightarrow{\vartheta}_3) + (\overrightarrow{\vartheta}_3 \cdot \overrightarrow{\vartheta}_4) + (\overrightarrow{\vartheta}_4 \cdot \overrightarrow{\vartheta}_5) + (\overrightarrow{\vartheta}_5 \cdot \overrightarrow{\vartheta}_6) + \\
&\quad (\overrightarrow{\vartheta}_6 \cdot \overrightarrow{\vartheta}_7) + (\overrightarrow{\vartheta}_7 \cdot \overrightarrow{\vartheta}_8) + (\overrightarrow{\vartheta}_8 \cdot \overrightarrow{\vartheta}_9) + (\overrightarrow{\vartheta}_9 \cdot \overrightarrow{\vartheta}_4) + (\overrightarrow{\vartheta}_9 \cdot \overrightarrow{\vartheta}_{10}) + \\
&\quad (\overrightarrow{\vartheta}_{10} \cdot \overrightarrow{\vartheta}_{11}) + (\overrightarrow{\vartheta}_{11} \cdot \overrightarrow{\vartheta}_{12}) + (\overrightarrow{\vartheta}_{11} \cdot \overrightarrow{\vartheta}_{13}) \\
&= 152+152+90+88+138+160+126+78+62+72+114 \\
&\quad +184+184 \\
&= 1600.
\end{aligned}$$

The proof is complete. □

Theorem 2.3. *The Sanskruti index of Aspirin is* 426.15.

Proof. Using equation 1

$$\begin{aligned}
s_{v_1} &= 3, s_{v_2} = 3, s_{v_3} = 5, s_{v_4} = 8, s_{v_5} = 5, s_{v_6} = 4, s_{v_7} = 4, s_{v_8} = 5, \\
s_{v_9} &= 7, s_{v_{10}} = 6, s_{v_{11}} = 4, s_{v_{12}} = 3, \text{ and } s_{v_{13}} = 3.
\end{aligned}$$

Hence by equation 6,

$$\begin{aligned}
S\left(C_9H_8O_4\right) &= \sum_{uv\in E(G)}\left(\frac{s_G(u)\,s_G(v)}{s_G(u)+s_G(v)-2}\right)^3 \\
&= \left(\frac{3\times 5}{3+5-2}\right)^3+\left(\frac{3\times 5}{3+5-2}\right)^3+\left(\frac{5\times 8}{5+8-2}\right)^3+\left(\frac{8\times 5}{8+5-2}\right)^3+ \\
&\quad \left(\frac{4\times 5}{4+5-2}\right)^3+\left(\frac{4\times 4}{4+4-2}\right)^3+\left(\frac{4\times 5}{4+5-2}\right)^3+\left(\frac{5\times 7}{5+7-2}\right)^3+ \\
&\quad \left(\frac{8\times 7}{8+7-2}\right)^3+\left(\frac{7\times 6}{7+6-2}\right)^3+\left(\frac{6\times 4}{6+4-2}\right)^3+\left(\frac{4\times 3}{4+3-2}\right)^3+ \\
&\quad \left(\frac{4\times 3}{4+3-2}\right)^3 \\
&= 426.15.
\end{aligned}$$

The proof is complete. $\square$

Theorem 2.4. *The first and second Zagreb eccentricity indices of Aspirin are* 337, *and* 296 *respectively.*

Proof. By equation 7, $(ld)_i = \max_{v_j\in V(G)} d_G(v_i,v_j)$. Hence

$$\begin{aligned}
(ld)_1 &= 6,(ld)_2=6,(ld)_3=5,(ld)_4=4,(ld)_5=5,(ld)_6=6,(ld)_7=5, \\
(ld)_8 &= 4,(ld)_9=3,(ld)_{10}=4,(ld)_{11}=5,(ld)_{12}=6,(ld)_{13}=6.
\end{aligned}$$

By equation 8

$$\begin{aligned}
E_1\left(C_9H_8O_4\right) &= \sum_{v_i\in V(G)} (ld)_i^2 \\
&= 5(6)^2+4(5)^2+3(4)^2+(3)^2 \\
&= 337.
\end{aligned}$$

and by equation 9

$$\begin{aligned}
E_2\left(C_9H_8O_4\right) &= \sum_{v_iv_j\in E(G)} (ld)_i\,(ld)_j \\
&= 6(5\times 6)+4(5\times 4)+3(4\times 3) \\
&= 296.
\end{aligned}$$

The proof is complete. $\square$

Theorem 2.5. *The Zagreb degree eccentricity indices of Aspirin are* 643, *and* 645 *respectively.*

Proof. By equation 10

$$\begin{aligned}
DE_1\left(C_9H_8O_4\right) &= \sum_{v_i\in V(G)} \left((ld)_i+d_i\right)^2 \\
&= 4(6+1)^2+2(5+3)^2+2(5+2)^2+2(4+2)^2+(6+2)^2+ \\
&\quad (4+3)^2+(3+3)^2 \\
&= 643.
\end{aligned}$$

and by equation 11

$$\begin{aligned} DE_2(G) &= \sum_{v_iv_j \in E(G)} ((ld)_i + d_i)\left((ld)_j + d_j\right) \\ &= (6+1)(5+3) + (6+1)(5+3) + (4+3)(5+3) + (4+3)(5+2) + \\ &\quad (5+2)(6+2) + (6+2)(5+2) + (5+2)(4+2) + (4+2)(3+3) + \\ &\quad (4+3)(3+3) + (3+3)(4+2) + (4+2)(5+3) + (6+1)(5+3) + \\ &\quad (6+1)(5+3) \\ &= 645. \end{aligned}$$

The proof is complete. □

Other topological indices calculated in this paper are all given in Table 1.

Table 1: The definition of topological indices.

Index Name	**Definition**	**Proposed**
Atom-bond connectivity	$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$	[3]
$ABC_4(G)$	$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{s_u + s_v - 2}{s_u s_v}}$	[7]
Randic connectivity	$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$	[14]
Sum connectivity	$S(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}$	[17]
Geometric-arithmetic	$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$	[16]
Fifth Geometric-arithmetic	$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{s_u s_v}}{s_u + s_v}$	[9]
First and second Zagreb	$M_1(G) = \sum_{uv \in E(G)} d_u + d_v,$	[10]
	$M_2(G) = \sum_{uv \in E(G)} d_u d_v$	
Multiple Zagreb	$PM_1(G) = \prod_{uv \in E(G)} (d_u + d_v),$	[6]
	$PM_2(G) = \prod_{uv \in E(G)} (d_u d_v)$	
Augmented Zagreb	$AZI(G) = \sum_{uv \in E(G)} \left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3$	[4]
Harmonic	$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$	[18]
Hyper-Zagreb	$HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2$	[13]
Symmetric division	$SDD(G) = \sum_{uv \in E(G)} \left[\frac{\min(d_u, d_v)}{\max(d_u, d_v)} + \frac{\max(d_u, d_v)}{\min(d_u, d_v)}\right]$	[19]
Forgotten topological	$F(G) = \sum_{uv \in E(G)} (d_u)^2 + (d_v)^2$	[5]

Theorem 2.6. *The atom bond connectivity index of Aspirin is* 10.902.

Proof. Let $n_{i,j}$ denote the edges connecting the vertices of degrees d_i and d_j. The molecular graph of Aspirin contains edges of types $n_{1,3}, n_{3,3}, n_{3,2}$, and $n_{2,2}$. The number of edges of these types are

$$|n_{1,3}| = 4, |n_{3,3}| = 2, |n_{3,2}| = 4, \text{ and } |n_{2,2}| = 3.$$

Hence the atom bond connectivity index of Aspirin is

$$\begin{aligned}
ABC\,(C_9H_8O_4) &= \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\
&= |n_{1,3}| \sqrt{\frac{1+3-2}{3}} + |n_{3,3}| \sqrt{\frac{3+3-2}{9}} + |n_{3,2}| \sqrt{\frac{3+2-2}{6}} \\
&\quad + |n_{2,2}| \sqrt{\frac{2+2-2}{4}} \\
&= 4\sqrt{\frac{4}{3}} + 2\sqrt{\frac{4}{9}} + 4\sqrt{\frac{3}{6}} + +3\sqrt{\frac{2}{4}} \\
&= 10.902.
\end{aligned}$$

This completes the proof. □

Theorem 2.7. *The forth atom bond connectivity index of Aspirin is* 7.5057.

Proof. The forth atom bond index of Aspirin is given by

$$\begin{aligned}
ABC_4(C_9H_8O_4) &= \sum_{uv\in E(G)} \sqrt{\frac{s_u + s_v - 2}{s_u s_v}} \\
&= \sqrt{\frac{3+5-2}{15}} + \sqrt{\frac{5+3-2}{15}} + \sqrt{\frac{5+8-2}{40}} + \sqrt{\frac{5+8-2}{40}} \\
&\quad + \sqrt{\frac{4+5-2}{20}} + \sqrt{\frac{4+4-2}{16}} + \sqrt{\frac{4+5-2}{20}} + \sqrt{\frac{5+7-2}{35}} \\
&\quad + \sqrt{\frac{8+7-2}{56}} + \sqrt{\frac{7+6-2}{42}} + \sqrt{\frac{6+4-2}{24}} + \sqrt{\frac{4+3-2}{12}} \\
&\quad + \sqrt{\frac{4+3-2}{12}} \\
&= 7.5057.
\end{aligned}$$

This completes the proof. □

Theorem 2.8. *The Randic connectivity index of Aspirin is* 6.1091.

Proof. The Randic connectivity index of Aspirin is given by

$$\begin{aligned}
\chi(C_9H_8O_4) &= \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}} \\
&= |n_{1,3}| \frac{1}{\sqrt{1\times 3}} + |n_{3,3}| \frac{1}{\sqrt{3\times 3}} + |n_{3,2}| \frac{1}{\sqrt{3\times 2}} + |n_{2,2}| \frac{1}{\sqrt{2\times 2}} \\
&= 4\frac{1}{\sqrt{3}} + 2\frac{1}{\sqrt{9}} + 4\frac{1}{\sqrt{6}} + 3\frac{1}{\sqrt{4}} \\
&= 6.1091.
\end{aligned}$$

The proof is complete. □

Theorem 2.9. *The Sum connectivity index $S(G)$ of Aspirin is* 6.1054.

Proof. The sum connectivity index of Aspirin is given by

$$\begin{aligned}
S(C_9H_8O_4) &= \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u+d_v}} \\
&= |n_{1,3}|\frac{1}{\sqrt{1+3}} + |n_{3,3}|\frac{1}{\sqrt{3+3}} + |n_{3,2}|\frac{1}{\sqrt{3+2}} + |n_{2,2}|\frac{1}{\sqrt{2+2}} \\
&= 4\frac{1}{\sqrt{4}} + 2\frac{1}{\sqrt{6}} + 4\frac{1}{\sqrt{5}} + 3\frac{1}{\sqrt{4}} \\
&= 6.1054.
\end{aligned}$$

The proof is complete. □

Theorem 2.10. *The Geometric-arithmetic index $GA(G)$ of Aspirin is* 12. 383.

Proof. The Geometric-arithmetic index of Aspirin is given by

$$\begin{aligned}
GA(C_9H_8O_4) &= \sum_{uv\in E(G)} \frac{2\sqrt{d_ud_v}}{d_u+d_v} \\
&= |n_{1,3}|\frac{2\sqrt{1\times 3}}{1+3} + |n_{3,3}|\frac{2\sqrt{3\times 3}}{3+3} + |n_{3,2}|\frac{2\sqrt{3\times 2}}{3+2} + |n_{2,2}|\frac{2\sqrt{2\times 2}}{2+2} \\
& \quad 4\frac{2\sqrt{1\times 3}}{1+3} + 2\frac{2\sqrt{3\times 3}}{3+3} + 4\frac{2\sqrt{3\times 2}}{3+2} + 3\frac{2\sqrt{2\times 2}}{2+2} \\
&= 12.383.
\end{aligned}$$

The proof is complete. □

Theorem 2.11. *The fifth Geometric-arithmetic index $GA_4(G)$ of Aspirin is* 12.81.

Proof. The fifth Geometric-arithmetic index of Aspirin is given by

$$\begin{aligned}
GA_5(C_9H_8O_4) &= \sum_{uv\in E(G)} \frac{2\sqrt{s_us_v}}{s_u+s_v} \\
&= \frac{2\sqrt{3\times 5}}{3+5} + \frac{2\sqrt{3\times 5}}{3+5} + \frac{2\sqrt{5\times 8}}{5+8} + \frac{2\sqrt{8\times 5}}{8+5} + \frac{2\sqrt{5\times 4}}{5+4} + \\
&= \frac{2\sqrt{4\times 4}}{4+4} + \frac{2\sqrt{4\times 5}}{4+5} + \frac{2\sqrt{5\times 7}}{5+7} + \frac{2\sqrt{8\times 7}}{8+7} + \frac{2\sqrt{7\times 6}}{7+6} + \\
&= \frac{2\sqrt{6\times 4}}{6+4} + \frac{2\sqrt{4\times 3}}{4+3} + \frac{2\sqrt{4\times 3}}{4+3} \\
&= 12.81.
\end{aligned}$$

The proof is complete. □

Theorem 2.12. *The First and second Zagreb indices of Aspirin are* 60, *and* 66 *respectively.*

Proof. The First Zagreb index of Aspirin is given by

$$\begin{aligned} M_1\left(C_9H_8O_4\right) &= \sum_{uv\in E(G)} d_u + d_v \\ &= \left|n_{1,3}\right|(1+3) + \left|n_{3,3}\right|(3+3) + \left|n_{3,2}\right|(3+2) + \left|n_{2,2}\right|(2+2) \\ &= (4\times 4) + (2\times 6) + (4\times 5) + (3\times 4) \\ &= 60. \end{aligned}$$

and the second Zagreb index is given by

$$\begin{aligned} M_2\left(C_9H_8O_4\right) &= \sum_{uv\in E(G)} d_u d_v \\ &= 4(1\times 3) + 2(3\times 3) + 4(3\times 2) + 3(2\times 2) \\ &= 66. \end{aligned}$$

The proof is complete. □

Theorem 2.13. *The first and second multiple Zagreb indices of Aspirin are* 3.6864×10^8, *and* 5.4420×10^8 *respectively.*

Proof. The first multiple Zagreb index is

$$\begin{aligned} PM_1\left(C_9H_8O_4\right) &= \prod_{uv\in E(G)} (d_u + d_v) \\ &= \prod_{uv\in 1,3} (d_u + d_v) \prod_{uv\in 3,3} (d_u + d_v) \prod_{uv\in 3,2} (d_u + d_v) \prod_{uv\in 2,2} (d_u + d_v) \\ &= 4^4 \times 6^2 \times 5^4 \times 4^3 = 3.6864\times 10^8. \end{aligned}$$

and

$$\begin{aligned} PM_2\left(C_9H_8O_4\right) &= \prod_{uv\in E(G)} (d_u d_v) \\ &= \prod_{uv\in 1,3} (d_u \cdot d_v) \prod_{uv\in 3,3} (d_u \cdot d_v) \prod_{uv\in 3,2} (d_u \cdot d_v) \prod_{uv\in 2,2} (d_u \cdot d_v) \\ &= 3^4 \times 9^2 \times 6^4 \times 4^3 = 5.4420\times 10^8. \end{aligned}$$

The proof is complete. □

Theorem 2.14. *The augmented Zagreb index* $AZI(G)$ *of Aspirin is* 92. 281.

Proof. The augmented Zagreb index of Aspirin is given by

$$\begin{aligned} AZI(C_9H_8O_4) &= \sum_{uv\in E(G)} \left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3 \\ &= 4\left(\frac{3}{4-2}\right)^3 + 2\left(\frac{9}{6-2}\right)^3 + 4\left(\frac{6}{5-2}\right)^3 + 3\left(\frac{4}{4-2}\right)^3 \\ &= 92.281. \end{aligned}$$

The proof is complete. □

Theorem 2.15. *The Harmonic index of Aspirin is* 5.7667.

Proof. The Harmonic index of Aspirin is given by

$$\begin{aligned} H(C_9H_8O_4) &= \sum_{uv\in E(G)} \frac{2}{d_u+d_v} \\ &= \left(4\times\frac{2}{4}\right)+\left(2\times\frac{2}{6}\right)+\left(4\times\frac{2}{5}\right)+\left(3\times\frac{2}{4}\right) \\ &= 5.7667. \end{aligned}$$

The proof is complete. □

Theorem 2.16. *The Hyper Zagreb index of Aspirin is* 284.

Proof. The Hyper Zagreb index of Aspirin is given by

$$\begin{aligned} HM(C_9H_8O_4) &= \sum_{uv\in E(G)} (d_u+d_v)^2 \\ &= 4(1+3)^2+2(3+3)^2+4(3+2)^2+3(2+2)^2 \\ &= 284. \end{aligned}$$

The proof is complete. □

Theorem 2.17. *The Symmetric division index of Aspirin is* 32.

Proof. The Symmetric division index of Aspirin is given by

$$\begin{aligned} SDD(C_9H_8O_4) &= \sum_{uv\in E(G)} \left[\frac{\min(d_u,d_v)}{\max(d_u,d_v)}+\frac{\max(d_u,d_v)}{\min(d_u,d_v)}\right] \\ &= 4\left[\frac{\min(1,3)}{\max(1,3)}+\frac{\max(1,3)}{\min(1,3)}\right]+2\left[\frac{\min(3,3)}{\max(3,3)}+\frac{\max(3,3)}{\min(3,3)}\right]+ \\ &\quad 4\left[\frac{\min(2,3)}{\max(2,3)}+\frac{\max(2,3)}{\min(2,3)}\right]+3\left[\frac{\min(2,2)}{\max(2,2)}+\frac{\max(2,2)}{\min(2,2)}\right] \\ &= 4\left[\frac{1}{3}+\frac{3}{1}\right]+2\left[\frac{3}{3}+\frac{3}{3}\right]+4\left[\frac{2}{3}+\frac{3}{2}\right]+3\left[\frac{2}{2}+\frac{2}{2}\right] \\ &= 4\left(\frac{10}{3}\right)+2(2)+4\left(\frac{13}{6}\right)+3(2)=32. \end{aligned}$$

The proof is complete. □

Theorem 2.18. *The forgotten topological index of Aspirin is* 152.

Proof. The forgotten topological index of Aspirin is given by

$$\begin{aligned} F(C_9H_8O_4) &= \sum_{uv\in E(G)} (d_u)^2+(d_v)^2 \\ &= 4(1+9)+2(9+9)+4(4+9)+3(4+4) \\ &= 152. \end{aligned}$$

The proof is complete. □

Conclusion 2.19. *Topological indices help to test the chemical properties of drugs. In this paper, we calculate different new and old topological indices of Aspirin such as the first and second entire Zagreb indices, the first and second Zagreb eccentricity indices, the Zagreb degree eccentricity indices, first* *and second locating indices, etc. The results of this paper offer promising pharmaceutical application. Future work on in this area may be done to investigate the topological indices for other drugs.*

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