

Computation of Topological Indices for Aloe Emodin – A Potential Pharmacological Agent

K. B. Sudhakara¹  and P. S. Guruprasad² 

¹Department of Mathematics, Government Science College-Autonomous, Hassan-573201, India

²Department of Mathematics, Government First Grade College, K.G.F-563122, India

¹E-mail: sudhakarkb.maths@gmail.com

² Corresponding Author E-mail: guruprasad18881@gmail.com

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ABSTRACT

Aloe-emodin is an anthraquinone derivative that has been widely studied for its pharmacological potential. Graph theory provides a mathematical framework for modelling molecular structures and analysing their properties through numerical descriptors known as topological indices. In this study, the molecular graph of aloe-emodin is considered, and several degree-based topological indices are calculated. These include classical indices such as the Randić connectivity index, Zagreb indices, and other related descriptors. The computed values provide quantitative insights into the structural characteristics of aloe-emodin and may contribute to the understanding of its chemical and biological properties.

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1. Introduction

Aloe-emodin occurs naturally as an anthraquinone compound commonly found in plants such as *Aloe vera*. It has garnered significant interest in medicinal chemistry due to its diverse biological effects, including antimicrobial, anticancer, and anti-inflammatory properties[2,12]. Understanding its molecular structure through graph-theoretical descriptors offers valuable insights into its chemical behaviour.

In the field of chemical graph theory, a molecule can be represented as a graph where the vertices correspond to atoms and the edges represent chemical bonds. Characteristics obtained from these graphs, referred to as topological indices, are commonly utilized to estimate physical and chemical properties as well as to predict the biological activity of chemical substances.

The present work focuses on computing several topological indices that are determined by the degree of the vertices in the molecular graph of aloe-emodin. These include classical descriptors such as Randić connectivity index, Zagreb indices and other degree-based indices. The computed values provide quantitative measures for characterizing the molecular structure and potential reactivity of the compound.

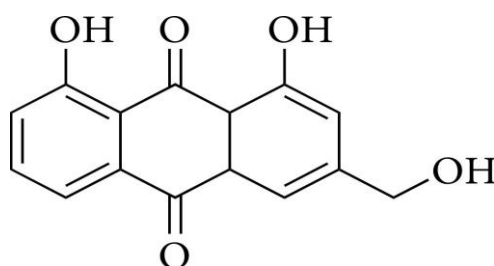


Figure 1: Chemical structure of aloe-emodin

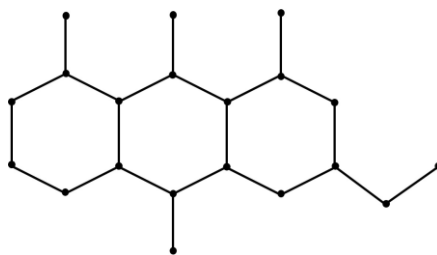


Figure 2 - Molecular graph of aloe-emodin

2. Preliminaries

Let $\mathcal{G} = (V, E)$ be a simple connected graph, where V represents vertices and E represents edges. The degree of a vertex v , written as $\mathbb{d}_v$, is defined as the total number of edges that are incident to it.

The following indices are used in this study:

Name	Mathematical Expression
Generalised Zagreb index [11]	$M_{\gamma, \delta} = M_{\gamma, \delta}(\mathcal{G}) = \sum_{mn \in E} \frac{(\mathbb{d}_m \cdot \mathbb{d}_n)^\gamma}{(\mathbb{d}_m + \mathbb{d}_n)^\delta}, \gamma, \delta \in \mathbb{R}$
First Zagreb index [10]	$M_1(\mathcal{G}) = \sum_{mn \in E} (\mathbb{d}_m + \mathbb{d}_n).$
Second Zagreb index [10]	$M_2(\mathcal{G}) = \sum_{mn \in E} (\mathbb{d}_m \cdot \mathbb{d}_n).$
Randić connectivity index [15]	$\chi(\mathcal{G}) = \sum_{mn \in E} \frac{1}{\sqrt{(\mathbb{d}_m \cdot \mathbb{d}_n)}}$
Sum connectivity index [22]	$SCI(\mathcal{G}) = \sum_{mn \in E} \frac{1}{\sqrt{(\mathbb{d}_m + \mathbb{d}_n)}}$
Hyper-Zagreb index [18]	$HM(\mathcal{G}) = \sum_{mn \in E} (\mathbb{d}_m + \mathbb{d}_n)^2.$
Second refined Zagreb index [16]	$ReZG_2(\mathcal{G}) = \sum_{mn \in E} \left(\frac{\mathbb{d}_m \cdot \mathbb{d}_n}{\mathbb{d}_m + \mathbb{d}_n} \right).$
Third refined Zagreb index or Inverse sum index [16]	$ReZG_3(\mathcal{G}) = \sum_{mn \in E} (\mathbb{d}_m \cdot \mathbb{d}_n)(\mathbb{d}_m + \mathbb{d}_n)$
Third Zagreb index [4]	$M_3(\mathcal{G}) = \sum_{mn \in E} \mathbb{d}_m - \mathbb{d}_n $
Fourth Zagreb index [17]	$M_4(\mathcal{G}) = \sum_{mn \in E} \mathbb{d}_m^2 - \mathbb{d}_n^2 $
First Zagreb polynomial [5]	$ZG_1(\mathcal{G}, x) = \sum_{mn \in E} x^{\mathbb{d}_m + \mathbb{d}_n},$
Second Zagreb polynomial [5]	$G_2(\mathcal{G}, x) = \sum_{mn \in E} x^{\mathbb{d}_m \cdot \mathbb{d}_n}$
Third Zagreb polynomial [1]	$ZG_3(\mathcal{G}, x) = \sum_{mn \in E} x^{ \mathbb{d}_m - \mathbb{d}_n }.$
Atom-Bond connectivity index [3]	$ABC(\mathcal{G}) = \sum_{mn \in E} \sqrt{\frac{\mathbb{d}_m + \mathbb{d}_n - 2}{\mathbb{d}_m \cdot \mathbb{d}_n}}.$
Fourth Atom-Bond connectivity index [8]	$ABC_4(\mathcal{G}) = \sum_{mn \in E} \sqrt{\frac{S_m + S_n - 2}{S_m \cdot S_n}},$ where, $S_m = \sum_{n \in N(m)} \mathbb{d}_n, N(m) = \{n \in V(\mathcal{G}) mn \in E(\mathcal{G})\}$
First multiplicative atom-bond connectivity index [13]	$ABCI(\mathcal{G}) = \prod_{mn \in E} \sqrt{\frac{\mathbb{d}_m + \mathbb{d}_n - 2}{\mathbb{d}_m \cdot \mathbb{d}_n}}$

Augmented Zagreb index [6]	$AZI(G) = \sum_{mn \in E} \left(\frac{d_m \cdot d_n}{d_m + d_n - 2} \right)^3$
Geometric-Arithmetic index [19]	$GA(G) = \sum_{mn \in E} \frac{2\sqrt{d_m \cdot d_n}}{d_m + d_n}$
Fifth Geometric-Arithmetic index [9]	$GA_5(G) = \sum_{mn \in E} \frac{2\sqrt{S_m \cdot S_n}}{S_m + S_n},$ where, $S_m = \sum_{n \in N(m)} d_n, N(m) = \{n \in V(G) mn \in E(G)\}$
First multiplicative Geometric-Arithmetic index [13]	$GA_1H(G) = \prod_{mn \in E} \frac{2\sqrt{d_m \cdot d_n}}{d_m + d_n}$
Symmetric division degree index [20]	$SDD(G) = \sum_{mn \in E} \left(\frac{d_m^2 + d_n^2}{d_m \cdot d_n} \right)$
Harmonic index [21]	$H(G) = \sum_{mn \in E} \left(\frac{2}{d_m + d_n} \right)$
Forgotten topological index [7]	$F(G) = \sum_{mn \in E} (d_m^2 + d_n^2)$
Forgotten polynomial [14]	$F(G, x) = \sum_{mn \in E} x^{(d_m^2 + d_n^2)}.$

Let the molecular graph of aloe-emodin be represented by $\mathcal{G}$. The edge set can be partitioned based on vertex degrees as $E(x, y)$, where edges connect vertices of degrees x and y .

From the molecular graph (Figure 2), the edge distribution is:

$$\begin{aligned} |E(1,2)| &= 1 \\ |E(1,3)| &= 4 \\ |E(2,2)| &= 2 \\ |E(2,3)| &= 7 \\ |E(3,3)| &= 8 \end{aligned}$$

Similarly, based on the sums of the degrees of neighbouring vertices, the sets $S(x, y)$ are obtained, with the corresponding counts as follows:

$$\begin{aligned} |S(2,4)| &= 1 & |S(6,6)| &= 3 \\ |S(3,6)| &= 2 & |S(6,8)| &= 1 \\ |S(3,7)| &= 2 & |S(6,9)| &= 2 \\ |S(4,5)| &= 2 & |S(7,8)| &= 2 \\ |S(4,6)| &= 1 & |S(7,9)| &= 2 \\ |S(5,6)| &= 1 & |S(8,9)| &= 2 \\ |S(5,8)| &= 1 \end{aligned}$$

3. Results

Theorem 3.1 *The Generalized Zagreb index of aloe-emodin is*

$$\frac{2^\gamma}{3^\delta} + \frac{3^\gamma}{4^{\delta-1}} + 2 \cdot 4^{\gamma-\delta} + 7 \cdot \frac{6^\gamma}{5^\delta} + \frac{3^{2\gamma-\delta}}{2^{\delta-3}}, \text{ where } \gamma \text{ and } \delta \text{ are arbitrary real numbers.}$$

Proof. The $M_{\gamma, \delta}(\mathcal{G})$ of aloe-emodin is

$$\begin{aligned} M_{\gamma, \delta}(\mathcal{G}) &= \sum_{e=mn \in E(\mathcal{G})} \frac{(d_m \cdot d_n)^\gamma}{(d_m + d_n)^\delta} \\ &= \frac{(1 \cdot 2)^\gamma}{(1+2)^\delta} |E(1,2)| + \frac{(1 \cdot 3)^\gamma}{(1+3)^\delta} |E(1,3)| + \frac{(2 \cdot 2)^\gamma}{(2+2)^\delta} |E(2,2)| + \frac{(2 \cdot 3)^\gamma}{(2+3)^\delta} |E(2,3)| + \frac{(3 \cdot 3)^\gamma}{(3+3)^\delta} |E(3,3)| \\ &= \frac{2^\gamma}{3^\delta} + \frac{3^\gamma}{4^{\delta-1}} + 2 \cdot 4^{\gamma-\delta} + 7 \cdot \frac{6^\gamma}{5^\delta} + \frac{3^{2\gamma-\delta}}{2^{\delta-3}}. \end{aligned}$$

Note:

1. If $\gamma = 0$ and $\delta = -1$, then $M_1(G) = 110$.
2. If $\gamma = 1$ and $\delta = 0$, then $M_2(G) = 136$.
3. If $\gamma = -\frac{1}{2}$ and $\delta = 0$, then $\chi(G) = 9.540912$.
4. If $\gamma = 0$ and $\delta = \frac{1}{2}$, then $SCI(G) = 9.973831$.
5. If $\gamma = 0$ and $\delta = -2$, then $HM(G) = 568$.
6. If $\gamma = 1$ and $\delta = 1$, then $ReZG_2(G) = 26.066666$.
7. If $\gamma = 1$ and $\delta = -1$, then $ReZG_3(G) = 728$.

Theorem 3.2 The third Zagreb index of aloe-emodin is 16.

Proof. The $M_3(G)$ of aloe-emodin is

$$\begin{aligned} M_3(G) &= \sum_{e=mn \in E(G)} |\mathbb{d}_m - \mathbb{d}_n| \\ &= |1 - 2||E(1,2)| + |1 - 3||E(1,3)| + |2 - 2||E(2,2)| + |2 - 3||E(2,3)| + \\ &\quad |3 - 3||E(3,3)| = 16. \end{aligned}$$

Theorem 3.3 The fourth Zagreb index of aloe-emodin is 70.

Proof. The $M_4(G)$ of aloe-emodin is

$$\begin{aligned} M_4(G) &= \sum_{e=mn \in E(G)} |\mathbb{d}_m^2 - \mathbb{d}_n^2| \\ &= |1^2 - 2^2||E(1,2)| + |1^2 - 3^2||E(1,3)| + |2^2 - 2^2||E(2,2)| + \\ &\quad + |2^2 - 3^2||E(2,3)| + |3^2 - 3^2||E(3,3)| = 70. \end{aligned}$$

Theorem 3.4 The first Zagreb polynomial of aloe-emodin is $8x^6 + 7x^5 + 6x^4 + x^3$.

Proof. The $ZG_1(G, x)$ of aloe-emodin is

$$\begin{aligned} ZG_1(G, x) &= \sum_{e=mn \in E(G)} x^{\mathbb{d}_m + \mathbb{d}_n} \\ &= |E(1,2)|x^{1+2} + |E(1,3)|x^{1+3} + |E(2,2)|x^{2+2} \\ &\quad + |E(2,3)|x^{2+3} + |E(3,3)|x^{3+3} = 8x^6 + 7x^5 + 6x^4 + x^3. \end{aligned}$$

Theorem 3.5 The second Zagreb polynomial of aloe-emodin is

$$8x^9 + 7x^6 + 2x^4 + 4x^3 + x^2.$$

Proof. The $ZG_2(G, x)$ of aloe-emodin is

$$\begin{aligned} ZG_2(G, x) &= \sum_{e=mn \in E(G)} x^{\mathbb{d}_m \cdot \mathbb{d}_n} \\ &= |E(1,2)|x^{1 \cdot 2} + |E(1,3)|x^{1 \cdot 3} + |E(2,2)|x^{2 \cdot 2} \\ &\quad + |E(2,3)|x^{2 \cdot 3} + |E(3,3)|x^{3 \cdot 3} = 8x^9 + 7x^6 + 2x^4 + 4x^3 + x^2. \end{aligned}$$

Theorem 3.6 The third Zagreb polynomial of aloe-emodin is $4x^2 + 8x + 10$.

Proof. The $ZG_3(G, x)$ of aloe-emodin is

$$\begin{aligned} ZG_3(G, x) &= \sum_{e=mn \in E(G)} x^{|\mathbb{d}_m - \mathbb{d}_n|} \\ &= |E(1,2)|x^{|1-2|} + |E(1,3)|x^{|1-3|} + |E(2,2)|x^{|2-2|} \\ &\quad + |E(2,3)|x^{|2-3|} + |E(3,3)|x^{|3-3|} = 4x^2 + 8x + 10. \end{aligned}$$

Theorem 3.7 The Atom-Bond connectivity index of aloe-emodin is 15.670387.

Proof. The $ABC(G)$ of aloe-emodin is

$$\begin{aligned} ABC(G) &= \sum_{e=mn \in E(G)} \sqrt{\frac{\mathbb{d}_m + \mathbb{d}_n - 2}{\mathbb{d}_m \cdot \mathbb{d}_n}} \\ &= \sqrt{\frac{1+2-2}{1 \cdot 2}}|E(1,2)| + \sqrt{\frac{1+3-2}{1 \cdot 3}}|E(1,3)| + \sqrt{\frac{2+2-2}{2 \cdot 2}}|E(2,2)| + \sqrt{\frac{2+3-2}{2 \cdot 3}}|E(2,3)| + \\ &\quad \sqrt{\frac{3+3-2}{3 \cdot 3}}|E(3,3)| = 15.670387. \end{aligned}$$

Theorem 3.8 The fourth Atom-Bond connectivity index of aloe-emodin is 11.903195.

Proof. The $ABC_4(G)$ of aloe-emodin is

$$\begin{aligned} ABC_4(G) &= \sum_{e=mn \in E(G)} \sqrt{\frac{S_m + S_n - 2}{S_m \cdot S_n}} \\ &= |S(2,4)| \sqrt{\frac{2+4-2}{2 \cdot 4}} + |S(3,6)| \sqrt{\frac{3+6-2}{3 \cdot 6}} + |S(3,7)| \sqrt{\frac{3+7-2}{3 \cdot 7}} + |S(4,5)| \sqrt{\frac{4+5-2}{4 \cdot 5}} + |S(4,6)| \sqrt{\frac{4+6-2}{4 \cdot 6}} + \\ &|S(5,6)| \sqrt{\frac{5+6-2}{5 \cdot 6}} + |S(5,8)| \sqrt{\frac{5+8-2}{5 \cdot 8}} + |S(6,6)| \sqrt{\frac{6+6-2}{6 \cdot 6}} + |S(6,8)| \sqrt{\frac{6+8-2}{6 \cdot 8}} + |S(6,9)| \sqrt{\frac{6+9-2}{6 \cdot 9}} + |S(7,8)| \sqrt{\frac{7+8-2}{7 \cdot 8}} + \\ &|S(7,9)| \sqrt{\frac{7+9-2}{7 \cdot 9}} + |S(8,9)| \sqrt{\frac{8+9-2}{8 \cdot 9}} = 11.903195. \end{aligned}$$

Theorem 3.9 The first multiplicative Atom-Bond connectivity index of aloe-emodin is 0.541922×10^{-3} .

Proof. The $ABC_1H(G)$ of aloe-emodin is

$$\begin{aligned} ABC_1H(G) &= \prod_{e=mn \in E(G)} \sqrt{\frac{\mathbb{d}_m + \mathbb{d}_n - 2}{\mathbb{d}_m \cdot \mathbb{d}_n}} \\ &= \prod_{e=mn \in E(1,2)} \sqrt{\frac{\mathbb{d}_m + \mathbb{d}_n - 2}{\mathbb{d}_m \cdot \mathbb{d}_n}} \cdot \prod_{e=mn \in E(1,3)} \sqrt{\frac{\mathbb{d}_m + \mathbb{d}_n - 2}{\mathbb{d}_m \cdot \mathbb{d}_n}} \cdot \prod_{e=mn \in E(2,2)} \sqrt{\frac{\mathbb{d}_m + \mathbb{d}_n - 2}{\mathbb{d}_m \cdot \mathbb{d}_n}} \cdot \\ &\prod_{e=mn \in E(2,3)} \sqrt{\frac{\mathbb{d}_m + \mathbb{d}_n - 2}{\mathbb{d}_m \cdot \mathbb{d}_n}} \cdot \prod_{e=mn \in E(3,3)} \sqrt{\frac{\mathbb{d}_m + \mathbb{d}_n - 2}{\mathbb{d}_m \cdot \mathbb{d}_n}} = 0.541922 \times 10^{-3}. \end{aligned}$$

Theorem 3.10 The Augmented Zagreb index of aloe-emodin is 184.625.

Proof. The $AZI(G)$ of aloe-emodin is

$$\begin{aligned} AZI(G) &= \sum_{e=mn \in E(G)} \left(\frac{\mathbb{d}_m \cdot \mathbb{d}_n}{\mathbb{d}_m + \mathbb{d}_n - 2} \right)^3 \\ &= \left(\frac{1 \cdot 2}{1+2-2} \right)^3 |E(1,2)| + \left(\frac{1 \cdot 3}{1+3-2} \right)^3 |E(1,3)| + \left(\frac{2 \cdot 2}{2+2-2} \right)^3 |E(2,2)| \\ &\quad + \left(\frac{2 \cdot 3}{2+3-2} \right)^3 |E(2,3)| + \left(\frac{3 \cdot 3}{3+3-2} \right)^3 |E(3,3)| \\ &= 184.625. \end{aligned}$$

Theorem 3.11 The Geometric-Arithmetic index of aloe-emodin is 21.265481.

Proof. The $GA(G)$ of aloe-emodin is

$$\begin{aligned} GA(G) &= \sum_{e=mn \in E(G)} \frac{2\sqrt{\mathbb{d}_m \cdot \mathbb{d}_n}}{\mathbb{d}_m + \mathbb{d}_n} \\ &= \frac{2\sqrt{1 \cdot 2}}{1+2} |E(1,2)| + \frac{2\sqrt{1 \cdot 3}}{1+3} |E(1,3)| + \frac{2\sqrt{2 \cdot 2}}{2+2} |E(2,2)| \\ &\quad + \frac{2\sqrt{2 \cdot 3}}{2+3} |E(2,3)| + \frac{2\sqrt{3 \cdot 3}}{3+3} |E(3,3)| \\ &= 21.265481. \end{aligned}$$

Theorem 3.12 The fifth Geometric-Arithmetic index of aloe-emodin is 21.523472.

Proof. The $GA_5(G)$ of aloe-emodin is

$$\begin{aligned} GA_5(G) &= \sum_{e=mn \in E(G)} \frac{2\sqrt{S_m \cdot S_n}}{S_m + S_n} \\ &= |S(2,4)| \frac{2\sqrt{2 \cdot 4}}{2+4} + |S(3,6)| \frac{2\sqrt{3 \cdot 6}}{3+6} + |S(3,7)| \frac{2\sqrt{3 \cdot 7}}{3+7} + |S(4,5)| \frac{2\sqrt{4 \cdot 5}}{4+5} + |S(4,6)| \frac{2\sqrt{4 \cdot 6}}{4+6} + |S(5,6)| \frac{2\sqrt{5 \cdot 6}}{5+6} + \\ &|S(5,8)| \frac{2\sqrt{5 \cdot 8}}{5+8} + |S(6,6)| \frac{2\sqrt{6 \cdot 6}}{6+6} + |S(6,8)| \frac{2\sqrt{6 \cdot 8}}{6+8} + |S(6,9)| \frac{2\sqrt{6 \cdot 9}}{6+9} + |S(7,8)| \frac{2\sqrt{7 \cdot 8}}{7+8} + |S(7,9)| \frac{2\sqrt{7 \cdot 9}}{7+9} + |S(8,9)| \frac{2\sqrt{8 \cdot 9}}{8+9} = \\ &21.523472. \end{aligned}$$

Theorem 3.13 The first multiplicative Geometric-Arithmetic index of aloe-emodin is 0.459722.

Proof. The $GA_1 II(G)$ of aloe-emodin is

$$\begin{aligned} GA_1 II(G) &= \prod_{e=mn \in E(G)} \frac{2\sqrt{d_m \cdot d_n}}{d_m + d_n} \\ &= \prod_{e=mn \in E(1,2)} \frac{2\sqrt{d_m \cdot d_n}}{d_m + d_n} \cdot \prod_{e=mn \in E(1,3)} \frac{2\sqrt{d_m \cdot d_n}}{d_m + d_n} \cdot \prod_{e=mn \in E(2,2)} \frac{2\sqrt{d_m \cdot d_n}}{d_m + d_n} \\ &\quad \cdot \prod_{e=mn \in E(2,3)} \frac{2\sqrt{d_m \cdot d_n}}{d_m + d_n} \cdot \prod_{e=mn \in E(3,3)} \frac{2\sqrt{d_m \cdot d_n}}{d_m + d_n} = 0.459722. \end{aligned}$$

Theorem 3.14 The symmetric division degree index of aloe-emodin is 51.

Proof. The $SDD(G)$ of aloe-emodin is

$$\begin{aligned} SDD(G) &= \sum_{e=mn \in E(G)} \left(\frac{d_m^2 + d_n^2}{d_m \cdot d_n} \right) \\ &= \left(\frac{1^2 + 2^2}{1 \cdot 2} \right) |E(1,2)| + \left(\frac{1^2 + 3^2}{1 \cdot 3} \right) |E(1,3)| + \left(\frac{2^2 + 2^2}{2 \cdot 2} \right) |E(2,2)| \\ &\quad + \left(\frac{2^2 + 3^2}{2 \cdot 3} \right) |E(2,3)| + \left(\frac{3^2 + 3^2}{3 \cdot 3} \right) |E(3,3)| = 51. \end{aligned}$$

Theorem 3.15 The Harmonic index of aloe-emodin is 9.133333.

Proof. The Harmonic index of aloe-emodin is

$$\begin{aligned} H(G) &= \sum_{e=mn \in E(G)} \left(\frac{2}{d_m + d_n} \right) \\ &= \left(\frac{2}{1+2} \right) |E(1,2)| + \left(\frac{2}{1+3} \right) |E(1,3)| + \left(\frac{2}{2+2} \right) |E(2,2)| \\ &\quad + \left(\frac{2}{2+3} \right) |E(2,3)| + \left(\frac{2}{3+3} \right) |E(3,3)| = 9.133333. \end{aligned}$$

Theorem 3.16 The Forgotten index of aloe-emodin is 296.

Proof. The $F(G)$ of aloe-emodin is

$$\begin{aligned} F(G) &= \sum_{e=mn \in E(G)} (d_m^2 + d_n^2) \\ &= |E(1,2)|(1^2 + 2^2) + |E(1,3)|(1^2 + 3^2) + |E(2,2)|(2^2 + 2^2) \\ &\quad + |E(2,3)|(2^2 + 3^2) + |E(3,3)|(3^2 + 3^2) = 296. \end{aligned}$$

Theorem 3.17 The Forgotten polynomial of aloe-emodin is

$$8x^{18} + 7x^{13} + 4x^{10} + 2x^8 + x^5.$$

Proof. The $F(G, x)$ of aloe-emodin is

$$\begin{aligned} F(G, x) &= \sum_{e=mn \in E(G)} x^{(d_m^2 + d_n^2)} \\ &= |E(1,2)|x^{(1^2 + 2^2)} + |E(1,3)|x^{(1^2 + 3^2)} + |E(2,2)|x^{(2^2 + 2^2)} \\ &\quad + |E(2,3)|x^{(2^2 + 3^2)} + |E(3,3)|x^{(3^2 + 3^2)} = 8x^{18} + 7x^{13} + 4x^{10} + 2x^8 + x^5. \end{aligned}$$

4. Conclusion

This study presents a graph-theoretical evaluation of aloe-emodin using degree-based topological indices. By representing the molecule as a graph and computing various indices, including the Zagreb, Randić, atom-bond connectivity (ABC), and geometric-arithmetic (GA) indices, its structural characteristics are quantitatively characterized. These findings may be useful in further studies of its chemical and pharmacological behavior.

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