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Article *in* Letters in Applied NanoBioScience · August 2024

DOI: 10.33263/LIANBS134.164

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Letters in Applied NanoBioScience
Open-Access Journal (ISSN: 2284-6808)

Article
Volume 13, Issue 4, 2024, 164
https://doi.org/10.33263/LIANBS134.164

Analysis of Topological Indices and Fractals in Amoxicillin

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Received: 1.10.2023; Accepted: 13.05.2024; Published: 25.08.2024

Abstract: Antibiotics are essential for curing diseases. Amoxicillin is indeed one of the antibiotics used to treat bacterial infections. Topological indices are mathematical values used to analyze and explore certain physicochemical properties of molecules. In this paper, various topological indices are computed based on the degree of the studied molecular graph. Topological indices values are utilized in drug design analysis to guide patient treatment strategies. The complexity derived from topological values can be further analyzed using mathematical concepts like Julia sets.

Keywords: Amoxicillin; chemical graph theory; fractals; Julia set; polynomial; topological indices; Zagreb index.

1. Introduction

In today's era, graph theory plays a crucial role in computer science, artificial intelligence engineering, machine learning, deep learning, data science, social networks, and drug design.

1.1. Graph.

A graph G=(V, E) is a mathematical and structural representation comprising nodes (also known as vertices) and edges that establish connections between these nodes. Graphs serve to illustrate relationships or associations among various elements [1].

In graph theory, the symbol "uv" is a standard notation for denoting an edge between two vertices, u and v, within a graph G. The notation "uv = E(G)" signifies that the edge represented by "uv" belongs to the set of edges in Graph G. Moreover, we describe the number of edges connected to a vertex as its "degree" [2]. This degree is also known as the "vertex valency." In this paper's context, we use the terms "du" and "dv" to represent the degrees of two particular vertices, u and v, respectively.

1.2. Chemical graph theory.

Chemical graph theory is a subfield within mathematical chemistry that utilizes graph theory to examine and assess chemical compounds. In this domain, molecules are depicted as graphs, with atoms serving as nodes and chemical bonds as the connecting edges [3].

1.3. Topological indices.

Topological indices(TIs) are numerical values or parameters derived from a molecule's structural graph in the chemical graph theory field [4]. These indices provide information about the structural and topological features of the molecule, such as its connectivity, shape, symmetry, branching, and cycles. Topological indices are used in quantitative structure-activity relationship (QSAR) studies [5], which help predict molecules' physical, chemical, and biological properties based on their structural characteristics. They are valuable tools in drug design, materials science, and various other fields of chemistry and biochemistry. Based on their degrees, topological indices are discovered in this study.

1.4. Julia set.

The Julia set is a mathematical concept in complex dynamics, which is a branch of mathematics studying the behavior of complex functions [6]. Specifically, in the context of the Julia set, it is associated with the iteration of complex numbers through a particular mathematical formula. The Julia set is a fractal, exhibiting intricate and complex geometric patterns at different scales. The behavior of the Julia set is Chaotic.

1.5. Amoxicillin.

Amoxicillin is a widely used antibiotic belonging to the penicillin class of drugs. It is effective against a wide range of bacterial infections. It is commonly prescribed to treat conditions like respiratory tract infections, urinary tract infections, skin infections, and certain types of bacterial sinus infections.

In this study, the structure of the drug is visualized as a graph. The molecular graph of Amoxicillin that has been considered here is A. The graph, denoted as A, consists of vertices and edges. In this context, each vertex in A corresponds to an individual atom, and each edge signifies a chemical bond between these atoms. The number of edges connected to a vertex determines its Valency [3]. Specifically, the graph under examination adheres to certain criteria: it is linked, simple, finite, has multiple edges, and contains no loops. Moreover, hydrogen atoms are omitted in the molecular graph being studied. The molecular formula of Amoxicillin is indeed $C_{16}H_{19}N_3O_5S$.

Figure 1 typically illustrates the chemical structure of Amoxicillin, including the arrangement of atoms and chemical bonds.

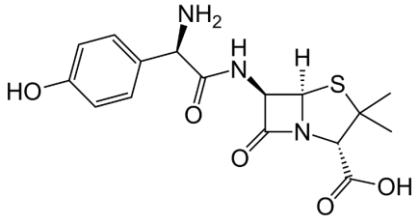

Figure 1. Amoxicillin's structure.

On the other hand, Figure 2 represents the graph of Amoxicillin, where vertices represent individual atoms (C for carbon, H for hydrogen, N for nitrogen, O for oxygen, and S for sulfur), and edges represent the chemical bonds connecting these atoms.

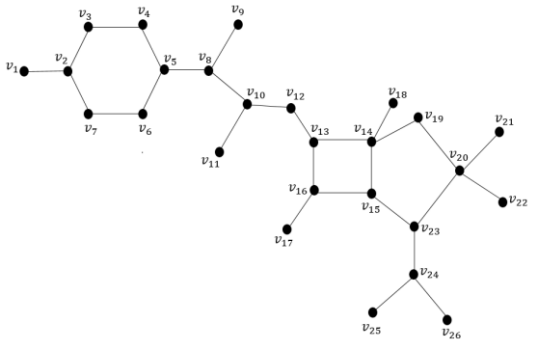

Figure 2. Graph of Amoxicillin A with vertices.

This graph representation simplifies the molecular structure into a visual framework commonly used in chemical graph theory and computational chemistry for various analyses. The figure makes it evident that Amoxicillin's graph comprises 26 vertices and 28 edges.

M.R. Rajesh Kanna and R. Jagadeesh [7] offered "Topological indices of Paracetamol". Several topological indices were calculated using vertex degree.

In this study, we introduced Theorem 2.1.1, in which we derived a set of topological indices using additive degrees. Specifically, we calculated a total of 18 topological indices for the drug amoxicillin.

Furthermore, Theorem 2.2.1 was formulated, focusing on the topological indices. We selectively utilized five of the 18 indices to create a polynomial. Subsequently, through our analysis of this polynomial, we established the existence of complex roots. Finally, we demonstrated that Amoxicillin's molecular structure conforms to a Julia set's characteristics, confirming its classification as a fractal set.

2. Materials and Methods

2.1. Topological indices of a graph of Amoxicillin.

The additive degree Topological indices(TI) have the general form of an edge between u and v, which is thought of as uv [8]

$$TI=TI\ (A)\ =\sum_{uv\in E(A)} \boldsymbol{F}(\boldsymbol{d_u}, \boldsymbol{d_v}) \quad (1)$$

Theorem 2.1.1.

If A represents the molecular structure of the antibiotic Amoxicillin $(C_{16}H_{19}N_3O_5S)$, the topological indices of graph A based on the additive degree are listed as follows.

ABC(A)=20.5047

M_1(A)=146

M_2 (A) =180.

Where each topological index is computed based on the additive degrees of the vertices in graph A.

Proof

Let A be a graph representing the molecular structure of Amoxicillin $(C_{16}H_{19}N_3O_5S)$.

Figure 3 displays the graph of Amoxicillin (denoted as A) the degrees of its vertices.

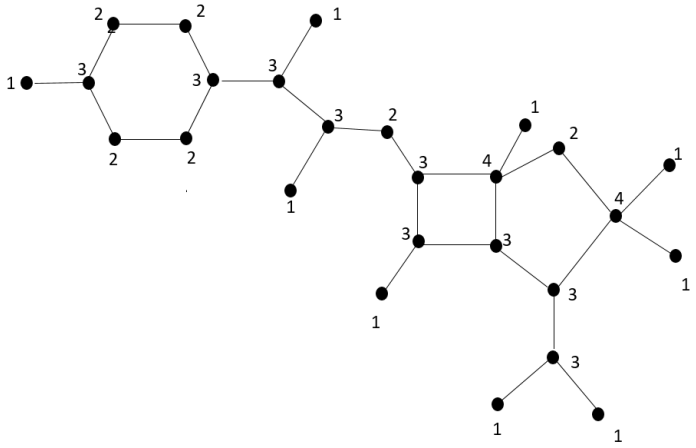

Figure 3. Graph of Amoxicillin A with degrees.

Amoxicillin's 2D structure, as illustrated in Figure 3, contains various types of edges denoted as $e_{1,3}$, $e_{1,4}$,$e_{2,2}$,$e_{2,3}$,$e_{2,4}$,$e_{3,3}$, and $e_{3,4}$.

Table 1 illustrates how the edges in Graph A are categorized and organized based on the connectivity of the vertices.

Table 1. Edge separation of Graph A dependent on Vertex connectivity.

Edge Set	Edge Partition	Degrees Type	Number of Edges
$E_1(A)$	$e_{1,3}$	$d_u=1$, $d_v=3$	$\lvert E_1(A)\rvert=6$
$E_2(A)$	$e_{1,4}$	$d_u=1$, $d_v=4$	$\lvert E_2(A)\rvert=3$
$E_3(A)$	$e_{2,2}$	$d_u=2$, $d_v=2$	$\lvert E_3(A)\rvert=2$
$E_4(A)$	$e_{2,3}$	$d_u=2$, $d_v=3$	$\lvert E_4(A)\rvert=6$
$E_5(A)$	$e_{2,4}$	$d_u=2$, $d_v=4$	$\lvert E_5(A)\rvert=2$
$E_6(A)$	$e_{3,3}$	$d_u=3$, $d_v=3$	$\lvert E6(A)\rvert=6$
$E_7(A)$	$e_{3,4}$	$d_u=3$, $d_v=4$	$\lvert E_7(A)\rvert=3$

Utilizing the information presented in Table 1, we derive the following results.

2.1.1.1 First part of the proof

For the graph A, the Atom Bond Connectivity Index (abbreviated ABC) [9] is

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

From equation (2)

$$=\{\sum_{uv\in E_1(A)}\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}+\sum_{uv\in E_2(A)}\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}+\sum_{uv\in E_3(A)}\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}$$
$$+\sum_{uv\in E_4(A)}\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}+\sum_{uv\in E_5(A)}\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}+\sum_{uv\in E_6(A)}\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}$$
$$+\sum_{uv\in E_7(A)}\sqrt{\frac{d_u+d_v-2}{d_u.d_v}} \quad (3)$$

$$=\{\left|E_{1(A)}\right|\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}+\left|E_{2(A)}\right|\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}+\left|E_{3(A)}\right|\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}+\left|E_{4(A)}\right|\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}$$
$$+\left|E_{5(A)}\right|\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}+\left|E_{6(A)}\right|\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}+\left|E_{7(A)}\right|\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}\} \quad (4)$$

$$=6\sqrt{\frac{1+3-2}{1.3}}+3\sqrt{\frac{1+4-2}{1.4}}+2\sqrt{\frac{2+2-2}{2.2}}+6\sqrt{\frac{2+3-2}{2.3}}+2\sqrt{\frac{2+4-2}{2.4}}+6\sqrt{\frac{3+3-2}{3.3}}+3\sqrt{\frac{3+4-2}{3.4}}$$

ABC(A)=20.5047.

2.1.1.2.Second part of the proof

For the graph A, the The first Zagrb Index (abbreviated M_1) [10] is

$$M_1(A)=\sum_{uv\epsilon E(A)}(d_u+d_v) \quad (5)$$

By Equation (5) and Table 1

$$\begin{aligned}&=\{|E_{1(A)}|(d_u+d_v)+|E_{2(A)}|(d_u+d_v)+|E_{3(A)}|(d_u+d_v)\\&+|E_{4(A)}|(d_u+d_v)+|E_{5(A)}|(d_u+d_v)+|E_{6(A)}|(d_u+d_v)\\&+|E_{7(A)}|(d_u+d_v)\} \quad (6)\\&=6(1+3)+3(1+4)+2(2+2)+6(2+3)+2(2+4)+6(3+3)+3(3+4)\end{aligned}$$

M_1(A)=146.

2.1.1.3.Third part of the proof

For the graph A, the The Second Zagrb Index (abbreviated M_2) [11] is

$$M_2(A)=\sum_{uv\epsilon E(A)}(d_u.d_v) \quad (7)$$

By Equation (7) and Table 1

$$\begin{aligned}&=\{\sum_{uv\epsilon E_1(A)}(d_u.d_v)+\sum_{uv\epsilon E_2(A)}(d_u.d_v)+\sum_{uv\epsilon E_3(A)}(d_u.d_v)\\&+\sum_{uv\epsilon E_4(A)}(d_u.d_v)+\sum_{uv\epsilon E_5(A)}(d_u.d_v)+\sum_{uv\epsilon E_6(A)}(d_u.d_v)\\&+\sum_{uv\epsilon E_7(A)}(d_u.d_v)\} \quad (8)\\&=\{|E_{1(A)}|(d_u.d_v)+|E_{2(A)}|(d_u.d_v)+|E_{3(A)}|(d_u.d_v)\\&+|E_{4(A)}|(d_u.d_v)+|E_{5(A)}|(d_u.d_v)+|E_{6(A)}|(d_u.d_v)\\&+|E_{7(A)}|(d_u.d_v)\}\\&=6(1\times3)+3(1\times4)+2(2\times2)+6(2\times3)+2(2\times4)+6(3\times3)+3(3\times4)\end{aligned}$$

M_2(A) =180.

This concludes the proof.

Remark 2.1.2.

Table 2 displays crucial topological indices for graph A (as shown in Figure 3), which include essential metrics like Zagreb indices, Harmonic indices, the Forgotten index, and the Randic[8,11-18]index.

Table 2. TIs of Graph A with additive degrees.

S.No	TI	Symbols	TI Formula	Values
1	Reduced second Zagreb index	$RM_2(A)$	$\sum_{uv\in(A)}(d_u-1)(d_v-1)$	32.9096
2	The first Hyper Zagreb index	$HM_1(A)$	$\sum_{uv\in E(A)}(d_u+d_v)^2$	788
3	The second Hyper Zagreb index	$HM_2(A)$	$\sum_{uv\in E(A)}(d_ud_v)^2$	1396
4	The Augmented Zagreb index	AZI(A)	$\sum_{uv\in E(A)}\left[\frac{d_ud_v}{d_u+d_v-2}\right]^3$	113.1487
5	Redefined First Zagreb index	$ReM_1(A)$	$\sum_{uv\in E(A)}\left(\frac{d_u+d_v}{d_ud_v}\right)$	25.9998

S.No	TI	Symbols	TI Formula	Values
6	Redefined second Zagreb index	$ReM_2(A)$	$\sum_{uv\in E(A)} \left(\frac{d_u.d_v}{d_u+d_v}\right)$	32.9096
7	Redefined third Zagreb index	$ReM_3(A)$	$\sum_{uv\in E(A)} d_u d_v(d_u+d_v)$	1016
8	Second Modified Zagreb index	$mM_2(A)$	$\sum_{uv\in E(A)} \frac{1}{d_u d_v}$	5.4167
9	Forgotten index[5]	F(A)	$\sum_{uv\in E(A)} ({d_u}^2+{d_v}^2)$	428
10	The Sum Connectivity index	χ (A)	$\sum_{uv\in E(A)} (d_u+d_v)^{-1/2}$	12.4248
11	Randic connectivity index	R(A)	$\sum_{uv\in E(A)} (d_u d_v)^{-1/2}$	11.9867
12	Reciprocal Randic index	ReR(A)	$\sum_{uv\in E(A)} (d_u d_v)^{1/2}$	69.1384
13	Harmonic index	H(A)	$\sum_{uv\in E(A)} \frac{2}{d_u+d_v}$	11.1238
14	SK index	SK (A)	$\sum_{uv\in E(A)} \frac{(d_u+d_v)}{2}$	73
15	Sk_1 index	$SK_1(A)$	$\sum_{uv\in E(A)} \frac{(d_u.d_v)}{2}$	81

2.2. Algebraic polynomials for topological indices of Amoxicillin graph a.

The field of mathematical chemistry explores a wide range of potential uses for algebraic polynomials. In this context, we have formulated Theorem 2.2.1, which specifically centers on topological indices. Out of the total of 18 available indices, we have intentionally chosen five to construct a polynomial.

Theorem 2.2.1.

If A is a graph of the medication Amoxicillin ($C_{16}H_{19}N_3O_5S$). *The algebraic polynomials associated with the following topological indices are defined as follows:*

- *First index Polynomial* $M_1(A, x)= 3x^7+8x^6++9x^5+8x^4$
- *Second index Polynomial* $M_2(A, x)= 3x^{12}+6x^9+2x^8+6x^6+5x^4+6x^3$
- *Third index Polynomial* $M_3(A, x)=3x^3+8x^2+9x+8$
- *Harmonic index Polynomial* $H(A, x)= 3x^6+8x^5+9x^4+8x^3$
- *Forgotten index Polynomial* $F(A, x)=3x^{25}+2x^{20}+6x^{18}+3x^{17}+6x^{13}+6x^{10}+2x^8$

Proof

The chemical graph of Amoxicillin, represented as A in Figure 3, contains 26 vertices and 28 edges.

Clearly, Figure 3 and Table 1 provide information from which we have derived the edge partitions as follows:

$|E_1(A)|=6$, $|E_2(A)|=3$, $|E_3(A)|=2$, $|E_4(A)|=6$, $|E5(A)|=2$, $|E_6(A)|=6$

and $|E_7(A)|=3$.

Table 3 showcases graph invariants and specific polynomial expressions, offering valuable insights into their mathematical properties and chemical applications [8].

Table 3. Polynomial of a graph A with degree-based Tis.

S. No	Topological Index	Polynomial P(A ,x) formula	Differentiation from P(A,X)
1.	First Zagreb index	$M_1(A, x)=\sum_{uv\in E(G)} x^{d_u+d_v}$	$D_x(M_1(A, x)\|_{x=1}$
2.	Second Zagreb index	$M_2(A, x)=\sum_{uv\in E(G)} x^{d_u.d_v}$	$D_x(M_2(A, x)\|_{x=1}$
3.	Third Zagreb index	$M_3(A, x)=\sum_{uv\in E(G)} x^{\|d_u-d_v\|}$	$D_x(M_3(A, x)\|_{x=1}$
4.	Harmonic index	$H(A, x)=\sum_{uv\in E(G)} x^{d_u+d_v-1}$	$2I_x(H(A, x)\|_{x=1}$
5.	Forgotten index	$F(A, x)=\sum_{uv\in E(G)} x^{(d_u^2+d_v^2)}$	$D_x(F(A, x)\|_{x=1}$

Where $D_x = \frac{d(P(G,x)}{dx}$ (9)

And

$$I_x = \int_0^x P(A,t)dt \quad (10)$$

2.2.1.1. First Zagreb index polynomial $M_1(A, x)$

The first topological index polynomial for graph A, denoted as $M_1(A, x)$, is determined by

$$M_1(A, x)=\sum_{uv\epsilon E(A)} x^{d_u+d_v} \quad (11)$$

$$=\{|E_{1(A)}|(x^{d_u+d_v})+|E_{2(A)}|(x^{d_u+d_v})+ |E_{3(A)}|(x^{d_u+d_v})+ |E_{4(A)}|(x^{d_u+d_v}) + |E_{5(A)}|(x^{d_u+d_v})+ |E_{6(A)}|(x^{d_u+d_v})+ |E_{7(A)}|(x^{d_u+d_v}) \} \quad (12)$$

$$= 6x^{1+3} + 3x^{1+4} + 2x^{2+2} + 6x^{2+3} + 2x^{2+4} + 6x^{3+3} + 3x^{3+4}$$

$$\mathbf{M_1(A,x)=3x^7 + 8x^6 + 9x^5 + 8x^4} \quad (13)$$

2.2.1.2. Second Zagreb index polynomial $M_2(A, x)$

The second topological index polynomial for graph A, denoted as $M_2(A, x)$, is determined by

$$M_2(A, x)=\sum_{uv\epsilon E(A)} x^{d_u.d_v} \quad (14)$$

$$=\{|E_{1(A)}|(x^{d_u d_v}) + |E_{2(A)}|(x^{d_u d_v}) + |E_{3(A)}|(x^{d_u d_v}) + |E_{4(A)}|(x^{d_u d_v}) + |E_{5(A)}|(x^{d_u d_v}) + |E_{6(A)}|(x^{d_u d_v}) + |E_{7(A)}|(x^{d_u d_v})\} \quad (15)$$

$$\mathbf{M_2(A,x)= 3x^{12} + 6x^9 + 2x^8 + 6x^6 + 5x^4 + 6x^3} \quad (16)$$

2.2.1.3. Third Zagreb index polynomial $M_3(A, x)$

The third topological index polynomial for graph A, denoted as $M_3(A, x)$, is determined by

$$M_3(A,x)=\sum_{uv\epsilon E(A)} x^{|d_u-d_v|} \quad (17)$$

$$=6x^{|1-3|} + 3x^{|1-4|} + 2x^{|2-2|} + 6x^{|2-3|} + 2x^{|2-4|} + 6x^{|3-3|} + 3x^{|3-4|}$$

$$\mathbf{M_3(A,x) = 3x^3 + 8x^2 + 9x+8} \quad (18)$$

2.2.1.4. Harmonic index polynomial H(A, x)

The Harmonic topological index polynomial for graph A, denoted as H(A, x), is determined by

$$\mathbf{H(A,x)}=\sum_{uv\in E(A)} x^{d_u+d_v-1} \quad (19)$$

$$=6x^{1+3-1} + 3x^{1+4-1} + 2x^{2+2-1} + 6x^{2+3-1} + 2x^{2+4-1} + 6x^{3+3-1} + 3x^{3+4-1}$$

$$\mathbf{H(A,x)=3x^6 + 8x^5 + 9x^4 + 8x^3} \quad (20)$$

2.2.1.5. Forgotten index polynomial F(A, x)

The Forgotten topological index polynomial for graph A, denoted as F(A, x), is determined by

$$\mathbf{F(A,x)}=\sum_{uv\in E(A)} x^{(d_u^2+d_v^2)} \quad (21)$$

$$=6x^{(1^2+3^2)}+2x^{(2^2+2^2)}+6x^{(2^2+3^2)}+2x^{(2^2+4^2)}+6x^{(3^2+3^2)}+3x^{(3^2+4^2)}+3x^{(1^2+4^2)}$$

$$\mathbf{F(A,x)}=\mathbf{3x^{25}+2x^{20}+6x^{18}+3x^{17}+6x^{13}+6x^{10}+2x^{8}} \quad (22)$$

Hence, the theorem.

Corollary 2.2.2.

If A is a Chemical graph of Amoxicillin ($C_{16}H_{19}N_3O_5S$) drug. Then, the topological indices are given by using the polynomials, which are

- *First Zagreb index M1(A)=146*
- *Second Zagreb Index M2(A)=180*
- *Third Zagreb index M3(A)=34*
- *Harmonic index H(A)=11.1238*
- *Forgotten index F(A)=428*

Proof

By using theorem 2.2.1 and Table 3, we obtain

- $First\ Zagreb\ index M_1(A)=\frac{d}{dx}(3x^7+8x^6+9x^5+8x^4)|_{x=1}=\mathbf{146}$
- $Second\ Zagreb\ index\ M_2(A)=\frac{d}{dx}(3x^{12}+6x^9+2x^8+6x^6+5x^4+6x^3)|_{x=1}=\mathbf{180}$
- $Third\ Zagreb\ index M_3(A)=\frac{d}{dx}(3x^3+8x^2+9x+8)|_{x=1}=\mathbf{34}$
- $Harmonic\ index H(A)=2\int_0^x(3t^6+8t^5+9t^4+8t^3)dt|_{x=1}=\mathbf{11.123}$
- $Forgotten\ index\ F(A)=\frac{d}{dx}(3x^{25}+2x^{10}+6x^{18}+3x^{17}+6x^{13}+6x^{10}+2x^8)|_{x=1}$ =**428**

Hence, the Proof.

2.3. Complexity of polynomial.

According to Theorem 2.2.1, it is evident that the first index polynomial, third index polynomial, and harmonic polynomial (refer to equation (13),(18),(20)) all possess a common characteristic—they can be expressed as the function f(x) = 0. Specifically,

$M_1(A,x)=x^4(3x^3+8x^2+9x+8)$

$M_3(A,x)=3x^3+8x^2+9x+8$

$H(A,x)=x^3(3x^3+8x^2+9x+8)$

This observation underscores the finding established in Theorem 2.2.1 regarding the mathematical representations of these polynomials. Based on this observation, we can establish the following result "If A is a non-constant polynomial with real coefficients, then there exists at least one complex root ".

The complex roots for the polynomial $M_3(x) = 3x^3 + 8x^2 + 9x + 8$ is obtained from Python programming is:

(-1.8234+0j)

(-0.4216+1.1334j)

(-0.4216-1.1334j).

Figure 4 depicts the graphical representation of the polynomial M3(A,x). Python programming was utilized to generate a surface plot of the polynomial.

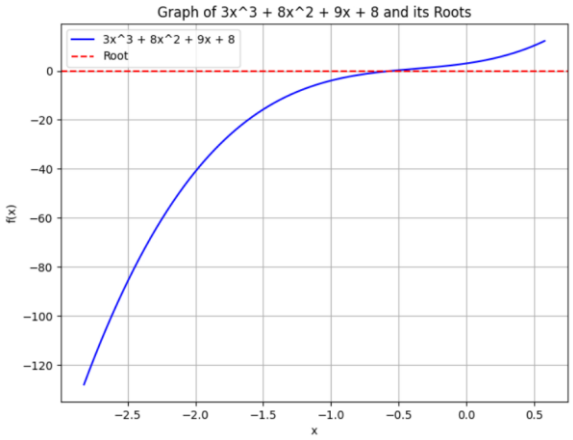

Figure 4. Plotting M_3(A,x) Polynomial of Amoxicillin ($C_{16}H_{19}N_3O_5S$).

3. Results and Discussion

This paper comprehensively analyzes various topological indices for the antibiotic drug Amoxicillin. These indices include the ABC index, Reduced second Zagreb index, Redefined first, second, and third Zagreb indices, forgotten index, Harmonic index, The Hyper Zagreb index, The augmented Zagreb index, Second modified Zagreb index, The Amoxicillin antibiotic's sum connection index, Randic connectivity index, reciprocal Randic index, and Sk index. The purpose of computing these topological indices was to gain insights into the physiochemical properties of the drug.

Through the analysis of these topological indices, several algebraic polynomials are derived. These polynomials played a significant role in constructing the graph of a function, specifically f(x) = 0, which led to the generation of various complex roots. This process helped us better understand Amoxicillin's mathematical properties and structural characteristics at a molecular level.

The Julia set is formed using a complex number denoted as $z = x + iy$ where $i^2 = -1$ and x and y represent the pixel coordinates in an image, typically falling between -2 and 2. The topological indices values give more complexity. Julia analyzes this complexity set. The Julia set exhibits chaotic behavior. As the structure of Amoxicillin demonstrates characteristics similar to those found in the Julia set, this can infer that it shares properties with a Julia set.

4. Conclusions

In this paper, a comprehensive analysis of several additive degree-based topological indices is computed for the antibiotic Amoxicillin. These indices serve as valuable tools for elucidating the physiochemical traits of drugs, offering a quantitative depiction of molecular structure. They are commonly employed in Quantitative Structure-Activity Relationship

(QSAR) investigations and the design and prediction of drug properties. Additionally, we established that the polynomial associated with Amoxicillin possesses at least one complex root, and intriguingly, it exhibits characteristics resembling those of a Julia set. These findings contribute significantly to our understanding of the mathematical aspects and structural properties of Amoxicillin at the molecular level**.**

Funding

This research received no external funding.

Acknowledgments

This research does not include any acknowledgments.

Conflicts of Interest

The authors declare no conflict of interest.

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