



Modified Eccentric Connectivity Index and Polynomial of Antiviral Drugs used to Combat Viral Diseases of Graphs

Jyoti D K, Thukarama V

Abstract: The eccentric connectivity index of a graph is defined as the sum of the products of eccentricity with the degree of vertices over all vertices of the graph, and the modified eccentric connectivity index of a graph is defined as the sum of the products of eccentricity with the total degree of neighbouring vertices over all vertices of the graph. In this paper, we find the eccentric connectivity index and modified eccentric connectivity index, and their respective polynomial versions, for antiviral drugs.

Keywords: Eccentricity, Topological Index, Eccentric Connectivity Index, Modified Eccentric Connectivity Index, Zika Virus, Smallpox, Antiviral drugs.

AMS Subject Classification: 05C07, 05C09, 05C12, 05C90, 05C92.

Nomenclature:

HeV: Hendra Virus

NiV: Nipah Virus

I. INTRODUCTION

Topological indices are real numbers derived from the molecular graph structure to correlate chemical structure with various physical properties, chemical reactivity, and biological activity.

Graph theory was applied to chemistry, and the concept of chemical graph theory was developed to quantitatively describe molecular structures. The idea of topological descriptors was first introduced by H. Wiener in 1947. Eventually, many other topological descriptors were introduced following the pioneering works of Wiener and Randic. Suppose G be a simple connected graph and $V(G)$ and $E(G)$ respectively denote the vertex set and edge set of G . Let, for any vertex $v \in V(G)$, $\deg(v)$ denotes its degree, that is the number of neighbors of v and $N(v)$ denotes the set of vertices which are the neighbors of the vertex v , so that $|N(v)| = \deg(v)$. For vertices $v, u \in V$, the distance $d(v, u)$ is defined as the length of the shortest path between v and u in G . The eccentricity $e(v)$ of a vertex

v is the maximum distance from v to any other vertex [2]. Nilanjan De, Sk. Md. Abu Nayeem [4] introduced a distance-based molecular structure descriptor which they named eccentric connectivity index" and which is defined as:

$$\xi_c(G) = \sum_{v \in V(G)} \deg(v) \cdot e(v) \dots (1)$$

Which has numerous applications and is studied extensively in [1, 3, 5]. Medications used to combat those viruses are ribavirin and chloroquine. A class of drugs known as analgesics and antipyretics includes acetaminophen. Niclosamide is a member of the anthelmintic drug class, which is used to treat worm diseases. An experimental drug called PHA-690509 inhibits cyclin-dependent kinase. The most effective anti-death substance, a pan-caspase inhibitor called emricasan, was discovered. A high-throughput screen in 2002 led to the discovery of the antiviral medication tecovirimat. It is recommended for use in treating adults and pediatric patients with the condition and is effective against all Orthopox viruses, including Vaccinia, cowpox, ectromelia, rabbit pox and monkeypox. Patients with impaired immune systems may experience reduced tecovirimat effectiveness. It reduces viremia and helps stop viral spread. Brincidofovir is a lipid mimic of cidofovir, and cidofovir is an antiviral drug that is categorized as a nucleotide analogue. Ribavirin belongs to the group of antiviral drugs known as nucleoside analogues. The medication chloroquine belongs to the 4-aminoquinoline pharmacological class, and the eccentric connectivity polynomial and total eccentricity polynomial [3] of G are respectively defined as:

$$ECP(G, x) = \sum_{i=1}^n \deg(v_i) x^{e(v_i)} \dots (2)$$

and

$$\Theta(G, x) = \sum_{i=1}^n x^{e(v_i)} \dots (3)$$

The Zika virus is a flavivirus spread by mosquitoes. In India, reports of the Zika virus have been made in recent years. Acetaminophen, Niclosamide, PHA-690509 and Emricasan are the main repurposed medications used to treat the infection. The Variola virus, a member of the orthopoxvirus family, causes smallpox. Tecovirimat, Cidofovir and Brincidofovir are the main antiviral medications used to treat smallpox.

Smallpox immunisations, also known as Vaccinia virus vaccines, can prevent smallpox. The Asia-Pacific region is home to zoonotic diseases

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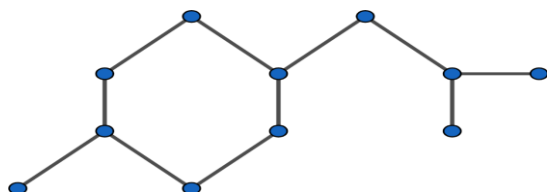
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like henipaviruses. Two henipaviruses that affect people are Hendra virus (HeV) and Nipah virus (NiV). Additionally, the World Health Organisation's Research and Development Blueprint has listed these illnesses as potential epidemic hazards. The repurposing is an antimalarial and amebicide. In regions where malaria is still susceptible to its effects, chloroquine is primarily used to prevent and cure malaria [1].

II. RESULTS AND DISCUSSION



[Fig.1: Chemical Graph of Acetaminophen]

Table-I: Degree and Eccentricity of Each Vertex

d(v). e(v)	No. of Vertices
1(7)	3
3(6)	2
2(5)	3
2(4)	2
3(4)	1

Theorem-1. Let G be a chemical graph of Acetaminophen, Then

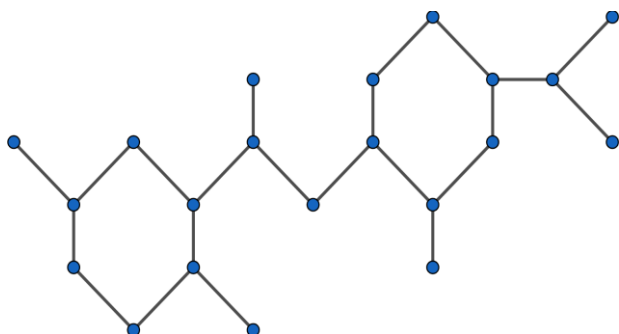
$$\begin{aligned}\zeta^c(G) &= 115, \\ ECP(G, x) &= 3x^7 + 6x^6 + 6x^5 + 7x^4, \\ \Theta(G, x) &= 3x^7 + 2x^6 + 3x^5 + 3x^4.\end{aligned}$$

Proof: Let G be a chemical graph for Acetaminophen. The graph consists of 11 vertices and 11 edges. By equations (1), (2) and (3), and Table-I, we have:

$$\zeta^c(G) = 3(1 \cdot 7) + 2(3 \cdot 6) + 3(2 \cdot 5) + 2(2 \cdot 4) + 3(4) = 21 + 36 + 30 + 16 + 12 = 115.$$

$$ECP(G, x) = 3x^7 + 2 \cdot 3x^6 + 3 \cdot 2x^5 + 2 \cdot 2x^4 + 3x^4 = 3x^7 + 6x^6 + 6x^5 + 7x^4.$$

$$\Theta(G, x) = 3x^7 + 2x^6 + 3x^5 + 2x^4 + x^4 = 3x^7 + 2x^6 + 3x^5 + 3x^4.$$



[Fig.2: Chemical Graph of Niclosamide]

Table-II: Degree and Eccentricity of Each Vertex

d(v). e(v)	No. of vertices	d(v). e(v)	No. of vertices
4(11)	3	3(5)	1
4(10)	2	3(4)	1
4(9)	1	4(2)	2
4(11)	1	2(5)	2
4(10)	1	3(6)	1
3(9)	1	2(3)	1
4(4)	1	2(5)	1
		3(12)	2

Theorem-2. Let G be a Niclosamide chemical graph. Then

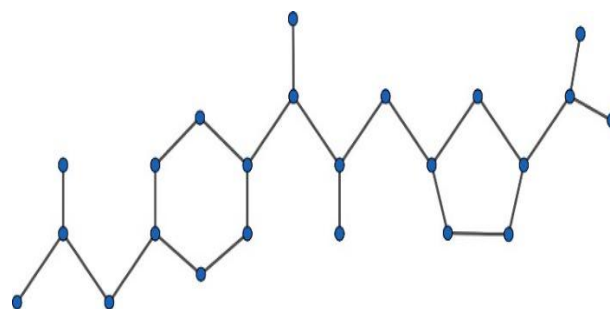
$$\begin{aligned}\zeta^c(G) &= 375 \\ ECP(G, x) &= 5x^{11} + 9x^{10} + 8x^9 + 9x^8 + 8x^7 + 5x^6 \\ \Theta(G, x) &= 4x^{11} + 4x^{10} + 3x^9 + 5x^8 + 3x^7 + 2x^6\end{aligned}$$

Proof: The Niclosamide chemical graph G has 21 vertices and 22 edges. By the equations (1), (2) and (3), we have

$$\begin{aligned}\zeta^c(G) &= 3(1(11)) + 2(30) + 18 + 22 + 20 + 2(27) + 10 \\ &\quad + 24 + 2(21) + 16 + 12 + 18 + 14 + 32 \\ &= 33 + 60 + 18 + 22 + 20 + 54 + 10 + 24 + 42 + 16 + \\ &\quad 12 + 18 + 14 + 32 = 375.\end{aligned}$$

$$\begin{aligned}ECP(G, x) &= 3x^{11} + 6x^{10} + 2x^9 + 2x^{11} + 2x^{10} + \\ &\quad 6x^{12} + 2x^{10} + 3x^8 + 6x^9 + 2x^7 + 2x^6 + 2x^7 + 4x^9 \\ &= 5x^{11} + 9x^{10} + 9x^9 + 9x^8 + 2x^7.\end{aligned}$$

$$\begin{aligned}\Theta(G, x) &= 3x^{11} + 2x^{10} + 2x^9 + x^{11} + x^{10} + 2x^9 + x^{10} \\ &\quad + x^8 + 2x^9 + 2x^8 + 2x^6 + x^7 + x^3 + 2x^8 \\ &= 4x^{11} + 4x^{10} + 3x^9 + 5x^8 + 3x^7 + 2x^6.\end{aligned}$$



[Fig.3: Chemical Graph of PHA-690509]

Theorem-3. Let G be a chemical graph of PHA-690509. Then,

$$\begin{aligned}\zeta^c(G) &= 466 \\ ECP(G, x) &= 4x^{14} + 6x^{13} + 7x^{12} + 7x^{11} + 7x^{10} + \\ &\quad 7x^9 + 7x^8 + 3x^7 \\ \Theta(G, x) &= 4x^{14} + 2x^{13} + 3x^{12} + \\ &\quad 3x^{11} + 3x^{10} + 4x^9 + 3x^8 + x^7.\end{aligned}$$

Proof: The chemical graph G of PHA-690509 has 21 vertices and 22 edges.

By using

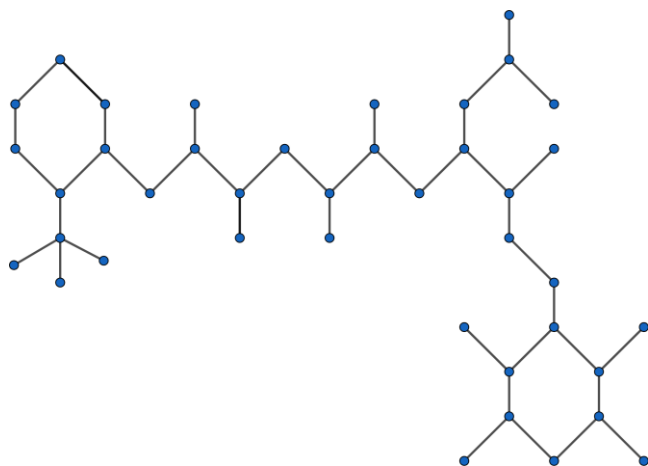


Table-III: Degree and Eccentricity of Each Vertex

d(v), e(v)	No. of vertices	d(v), e(v)	No. of vertices
1(14)	4	2(7)	1
3(13)	2	1(8)	1
2(12)	2	1(9)	1
3(11)	1	1(10)	1
2(10)	2	1(11)	2
2(9)	3	1(12)	1
3(8)	2		

From Table-III and equations (1), (2) and (3), we have,

$$\begin{aligned}\zeta^c(G) &= 4.14 + 3.13 + 4.12 + 3.11 + 4.10 + 5.9 + 6.8 \\ &\quad + 21 + 8 + 9 + 30 + 44 + 36 \\ &= 56 + 39 + 48 + 33 + 40 + 54 + 48 + 21 + 8 + 9 + 30 \\ &\quad + 44 + 36 = 466. \\ ECP(G, x) &= 4x^{14} + 6x^{13} + 4x^{12} + 3x^{11} + 4x^{10} + \\ &\quad 6x^9 + 6x^8 + 3x^7 + x^8 + x^9 + 3x^{10} + 4x^{11} + 3x^{12} \\ &= 4x^{14} + 6x^{13} + 7x^{12} + 7x^{11} + 7x^{10} + 7x^9 + 7x^8 + \\ &\quad 3x^7. \\ \theta(G, x) &= 4x^{14} + 2x^{13} + 2x^{12} + x^{11} + 2x^{10} + 3x^9 + \\ &\quad 2x^8 + x^7 + x^8 + x^9 + x^{10} + 2x^{11} + x^{12} \\ &= 4x^{14} + 2x^{13} + 3x^{12} + 3x^{11} + 3x^{10} + 4x^9 + 3x^8 + x^7.\end{aligned}$$



[Fig.4: Chemical Graph of Emricasan]

Table-IV: Degree and Eccentricity of Each Vertex

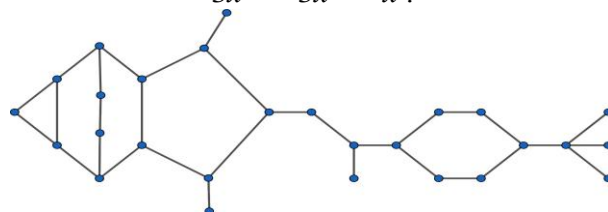
d(v), e(v)	No. of vertices	d(v), e(v)	No. of vertices
1(18)	5	3(10)	1
4(17)	1	1(11)	1
3(16)	3	3(9)	1
2(17)	2	1(10)	1
2(18)	2	2(10)	1
2(16)	1	3(11)	1
3(15)	2	2(12)	1
2(14)	2	1(14)	3
3(13)	2	1(13)	1
3(12)	2	2(13)	1
1(13)	2	1(17)	2
2(11)	1	3(17)	1

Theorem-4. Let G denote the chemical graph of Emricasan. Then,

$$\begin{aligned}\zeta^c(G) &= 1139. \\ ECP(G, x) &= 5x^{18} + 13x^{17} + 11x^{16} + 6x^{15} + 7x^{14} + \\ &\quad 11x^{13} + 8x^{12} + 6x^{11} + 6x^{10} + 3x^9. \quad \theta(G, x) = 5x^{18} + \\ &\quad 6x^{17} + 4x^{16} + 2x^{15} + 5x^{14} + 6x^{13} + 3x^{12} + 3x^{11} + \\ &\quad 3x^{10} + x^9 + 2x^8.\end{aligned}$$

Proof: Let G be a chemical graph of Emricasan with $|V(G)| = 40$ and $|E(G)| = 41$. By Table-IV and Equations (1), (2) and (3), we have,

$$\begin{aligned}\zeta^c(G) &= 5(18) + 4(12) + 9(16) + 4(17) + 4(18) + 32 \\ &\quad + 6(15) + 4(14) + 6(13) + 6(12) + 2(13) \\ &\quad + 22 + 30 + 11 + 27 + 10 + 20 + 33 + 24 + 3(14) + 13 \\ &\quad + 2(13) + 2(17) + 3(17) \\ &= 90 + 68 + 144 + 68 + 72 + 32 + 90 + 56 + 78 + 72 \\ &\quad + 26 + 22 + 30 + 11 + 27 \\ &\quad + 30 + 33 + 24 + 42 + 13 + 26 + 34 + 51 = 1,139 \\ ECP(G, x) &= 5x^{18} + 4x^{17} + 9x^{16} + 4x^{17} + 4x^{18} + \\ &\quad 2x^{16} + 6x^{15} + 4x^{14} + 6x^{13} + 6x^{12} + 2x^{13} + \\ &\quad x^{11} + 3x^{10} + x^{11} + 3x^9 + x^{10} + 2x^{10} + 3x^{11} + 2x^{12} + \\ &\quad 3x^{14} + x^{13} + 2x^{13} + 2x^{17} + 3x^{17}. \\ &= 9x^{18} + 13x^{17} + 11x^{16} + 6x^{15} + 7x^{14} + 11x^{13} + 8x^{12} \\ &\quad + 6x^{11} + 6x^{10} + 3x^9. \\ \theta(G, x) &= x^{18} + x^{17} + 3x^{16} + 2x^{17} + 2x^8 + x^{16} + 2x^{15} \\ &\quad + 2x^{14} + 2x^{13} + 2x^{12} + 2x^{13} + x^{11} + 2x^{10} + x^{11} \\ &\quad + x^9 + x^{10} + x^{10} + x^{11} + x^{12} + 3x^{14} + x^{13} + x^{13} + \\ &\quad 2x^{17} + x^{17} \\ &= 7x^{18} + 6x^{17} + 4x^{16} + 2x^{15} + 5x^{14} + 6x^{13} + 3x^{11} + \\ &\quad 3x^{12} + 3x^{10} + x^9.\end{aligned}$$



[Fig.5: Chemical Graph of Tecovirimat]

Table-V: Degree and Eccentricity of Each Vertex

d(v), e(v)	No. of vertices	d(v), e(v)	No. of vertices
2(13)	1	2(7)	1
3(12)	2	3(7)	1
3(11)	3	1(8)	1
2(12)	2	2(9)	2
3(10)	2	2(10)	2
3(9)	2	4(12)	1
1(10)	2	1(13)	3
3(8)	2		

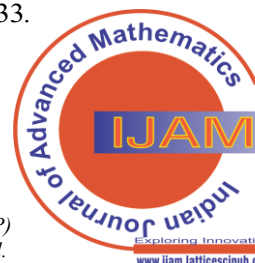
Theorem-5. Let G be a chemical graph of Tecovirimat. Then

$$\begin{aligned}\zeta^c(G) &= 633. \\ ECP(G, x) &= 5x^{13} + 14x^{12} + 9x^{11} + 12x^{10} + 10x^9 + \\ &\quad 7x^8 + 5x^7. \\ \theta(G, x) &= 4x^{13} + 5x^{12} + 3x^{11} + 6x^{10} + 4x^9 + 3x^8 + \\ &\quad 2x^7.\end{aligned}$$

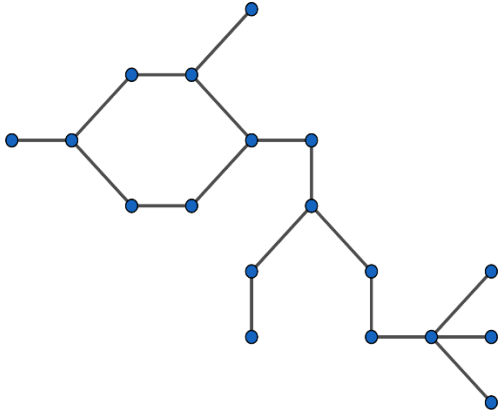
Proof: Let G be a chemical graph of Tecovirimat. Then G has $V(G) = 27$ and $E(G) = 31$.

Then, by tables and equations (1), (2) and (3), we have

$$\begin{aligned}\zeta^c(G) &= 2(13) + 6(12) + 9(11) + 4(12) + 6(10) + 6(9) \\ &\quad + 2(10) + 6(8) + 2(7) + 3(7) \\ &\quad + 4(9) + 4(10) + 4(12) + 3(13). \\ &= 26 + 72 + 99 + 48 + 60 + 54 + 20 + 48 + 14 + 21 + \\ &\quad 8 + 36 + 40 + 48 + 39 = 633. \\ ECP(G, x) &= 2x^{13} + 6x^{12} \\ &\quad + 9x^{11} + 4x^{12} + 6x^{10} + \\ &\quad 6x^9 + 2x^{10} + 6x^8 + 2x^7 + \\ &\quad 3x^7.\end{aligned}$$



$$\begin{aligned}
 &+ x^8 + 4x^9 + 4x^{10} + 4x^{12} + \\
 &\quad 3x^{13} \\
 &= 5x^{13} + 14x^{12} + 9x^{11} + 12x^{10} + 10x^9 + 7x^8 + 5x^7. \\
 \theta(G, x) &= x^{13} + 2x^{12} + 3x^{11} + 2x^{12} + 2x^{10} + 2x^9 + \\
 &\quad 2x^{10} + 2x^8 + x^7 + x^7 + x^8 \\
 &\quad + 2x^9 + 2x^{10} + x^{12} + 2x^{13} \\
 &= 4x^{13} + 5x^{12} + 3x^{11} + 6x^{10} + 4x^9 + 3x^8 + 2x^7.
 \end{aligned}$$



[Fig.6: Chemical Graph of Cidofovir]

Table-VI: Degree and Eccentricity of Each Vertex

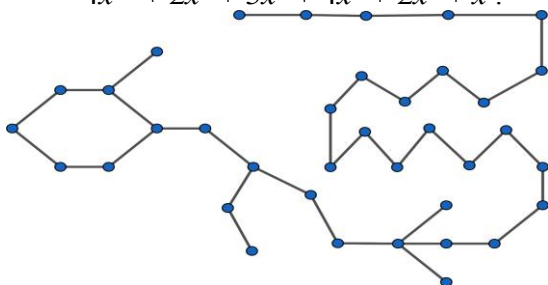
deg(v). e(v)	No. of vertices
1(10)	4
3(9)	1
2(8)	3
3(7)	1
1(8)	2
3(6)	2
2(7)	3
4(9)	1
2(5)	1

Theorem-6. Let G denote the chemical graph of Cidofovir. Then,

$$\begin{aligned}
 \zeta^c(G) &= 276. \\
 ECP(G, x) &= 4x^{10} + 7x^9 + 8x^8 + 9x^7 + 6x^6 + 2x^5. \\
 \theta(G, x) &= 4x^{10} + 2x^9 + 5x^8 + 4x^7 + 2x^6 + x^5.
 \end{aligned}$$

Proof: Let G be a chemical graph of Cidofovir, which has 18 vertices and 18 edges. By Table-VI and equations (1), (2) and (3), we have

$$\begin{aligned}
 \zeta^c(G) &= 4(10) + 3(9) + 6(8) + 3(7) + 2(8) + 6(6) + \\
 &\quad 6(7) + 4(9) + 2(5). \\
 &= 40 + 27 + 48 + 21 + 16 + 36 + 42 + 36 + 10 = 276. \\
 ECP(G, x) &= 4x^{10} + 3x^9 + 6x^8 + 3x^7 + 2x^8 + 6x^6 + \\
 &\quad 6x^7 + 4x^9 + 2x^5 \\
 &= 4x^{10} + 7x^9 + 8x^8 + 9x^7 + 6x^6 + 2x^5. \\
 \theta(G, x) &= 4x^{10} + x^9 + 3x^8 + x^7 + 2x^8 + 2x^6 + 3x^7 + \\
 &\quad x^6 + x^5 \\
 &= 4x^{10} + 2x^9 + 5x^8 + 4x^7 + 2x^6 + x^5.
 \end{aligned}$$



[Fig.7: Chemical Graph of Brincidofovir]

Table-VII: Degree and Eccentricity of Each Vertex

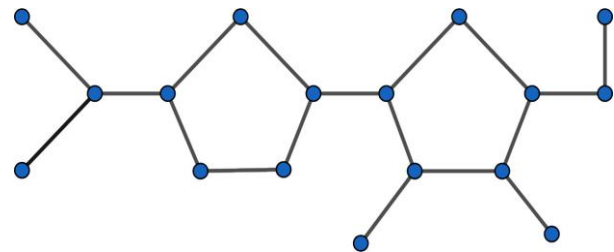
d(v). e(v)	No. of Vertices	d(v). e(v)	No. of Vertices
1(30)	2	2(22)	2
3(29)	1	3(21)	1
2(28)	3	1(22)	2
3(27)	1	2(20)	3
2(27)	2	2(19)	2
1(28)	1	2(21)	2
3(26)	1	2(16)	2
2(25)	3	2(15)	1
3(24)	1	2(17)	2
2(23)	2	2(18)	2
1(26)	1	2(24)	1

Theorem-7. Let G denote the chemical graph of Brincidofovir. Then

$$\begin{aligned}
 \zeta^c(G) &= 1657 \\
 ECP(G, x) &= 2x^{30} + 3x^{29} + 7x^{28} + 7x^{27} + 4x^{26} + \\
 &\quad 6x^{25} + 5x^{24} + 4x^{23} + 6x^{22} + 4x^{21} + 6x^{20} \\
 &\quad + 4x^{19} + 4x^{18} + 4x^{17} + 4x^{16} + 2x^{15}. \\
 \theta(G, x) &= 2x^{30} + x^{29} + 2x^{28} + 3x^{27} + 2x^{26} + 3x^{25} + \\
 &\quad 2x^{24} + 2x^{23} + 4x^{22} + 3x^{21} + 3x^{20} + 2x^{19} + 2x^{18} + \\
 &\quad 2x^{17} + 2x^{16} + x^{15}.
 \end{aligned}$$

Proof: The chemical graph of Brincidofovir, G , has 38 vertices and 38 edges. By the Table-VII. and equations (1), (2) and (3), we have

$$\begin{aligned}
 \zeta^c(G) &= 2(30) + 3(29) + 6(28) + 3(27) + 4(27) + \\
 &\quad 2(28) + 3(26) + 4(25) + 3(24) \\
 &\quad + 4(23) + 2(20) + \\
 &\quad 4(22) + 3(21) + 2(22) + 6(20) + 4(19) + 4(21) + 4(16) \\
 &\quad + 2(15) + 4(17) + 4(18) + 2(24) \\
 &= 1657. \\
 ECP(G, x) &= 2x^{30} + 3x^{29} + 6x^{28} + 3x^{27} + 4x^{27} + \\
 &\quad 2x^{28} + 3x^{26} + 6x^{25} + 3x^{24} + 4x^{23} + 2x^{20} \\
 &\quad + 4x^{22} + 3x^{21} + 2x^{22} + 6x^{20} + 4x^{19} + 4x^{21} + 4x^{16} + \\
 &\quad 2x^{15} + 4x^{17} + 4x^{18} + 2x^{24} \\
 &= 2x^{30} + 3x^{29} + 7x^{28} + 7x^{27} + 4x^{26} + 6x^{25} + 5x^{24} + \\
 &\quad 4x^{23} + 6x^{22} + 4x^{21} + 6x^{20} + 4x^{19} \\
 &\quad + 4x^{18} + 4x^{17} + 4x^{16} + 2x^{15} \\
 \theta(G, x) &= 2x^{30} + x^{29} + x^{28} + x^{27} + 2x^{27} + x^{28} + x^{26} \\
 &\quad + 3x^{25} + x^{24} + 2x^{23} + x^{20} + 2x^{22} + x^{21} \\
 &\quad + x^{22} + 3x^{20} + 2x^{19} + 2x^{21} + 2x^{16} + x^{15} + 2x^{17} + \\
 &\quad 2x^{18} + x^{24} \\
 &= 2x^{30} + x^{29} + 2x^{28} + 3x^{27} + 2x^{26} + 3x^{25} + 2x^{24} + \\
 &\quad 2x^{23} + 4x^{22} + 3x^{21} + 3x^{20} \\
 &\quad + 2x^{19} + 2x^{18} + 2x^{17} + 2x^{16} + x^{15}.
 \end{aligned}$$



[Fig.8: Chemical Graph of Ribavirin]



Table-VIII: Degree and Eccentricity of Each Vertex

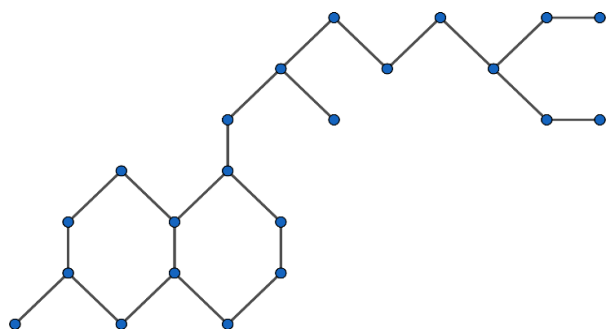
deg(v). e(v)	No. of Vertices
1(0)	3
3(8)	1
3(7)	3
2(7)	1
2(6)	3
3(5)	2
3(6)	1
1(7)	1
1(8)	1
2(8)	1

Theorem-8. Let G denote the chemical graph of Ribavirin. Then

$$\begin{aligned}\zeta(G) &= 243 \\ ECP(G, x) &= 3x^9 + 6x^8 + 12x^3 + 9x^6 + 6x^5 \\ \theta(G, x) &= 3x^9 + 3x^8 + 5x^7 + 4x^6 + 2x^5\end{aligned}$$

Proof: Let G be the chemical graph of Ribavirin. Then G has $V(G) = 17$ and $E(G) = 18$.

By Table-VIII and equations (1), (2) and (3), we have

$$\begin{aligned}\zeta(G) &= 3(9) + 3(8) + 9(7) + 2(7) + 6(6) + 6(5) + 3(5) + 7 + 8 + 2(8). \\ &= 27 + 24 + 63 + 14 + 36 + 30 + 15 + 15 + 16 = 243. \\ ECP(G, x) &= 3x^9 + 3x^8 + 9x^7 + 2x^7 + 6x^6 + 6x^5 + 3x^6 + x^7 + x^8 + 2x^8. \\ &= 3x^9 + 6x^8 + 12x^7 + 9x^6 + 6x^5 \\ \theta(G, x) &= 3x^9 + x^8 + 3x^7 + x^7 + 3x^6 + 2x^5 + x^6 + x^7 + x^8 + x^8. \\ &= 3x^9 + 3x^8 + 5x^7 + 4x^6 + 2x^5.\end{aligned}$$


[Fig.9: Chemical Graph of Chloroquine]

Table-IX: Degree and Eccentricity of Each Vertex

d(v). e(v)	No. of Vertices	d(v). e(v)	No. of Vertices
1 (13)	3	3 (8)	1
3 (12)	1	2 (7)	1
2 (11)	3	3 (7)	1
2 (10)	3	1 (8)	1
3 (9)	1	2 (8)	1
3 (10)	1	3 (11)	1
2 (9)	2	2 (12)	2

III. CONCLUSION

Theorem-1. Let G be the chemical graph of Chloroquine. Then,

$$\begin{aligned}\zeta(G) &= 458 \\ ECP(G, x) &= 3x^{13} + 7x^{12} + 9x^{11} + 9x^{10} + 7x^9 + 6x^8 + 5x^7, \\ \theta(G, x) &= 3x^{13} + 3x^{12} + 4x^{11} + 4x^{10} + 3x^9 + 3x^8 + 2x^7.\end{aligned}$$

Proof: Chemical graph of Chloroquine G has $V(G)$

$= 22$ and $E(G) = 23$. By Table-IX and equations (1), (2) and (3), we have

$$\begin{aligned}\zeta(G) &= 3(13) + 3(12) + 6(11) + 6(10) + 3(9) + 3(10) + 4(9) + 3(8) + 2(7) + 3(7) + 8 + 16 + 33 + 4(12) = 458. \\ ECP(G, x) &= 3x^{13} + 3x^{12} + 6x^{11} + 6x^{10} + 3x^9 + 3x^{10} + 4x^9 + 3x^8 + 2x^7 + 3x^7 + x^8 + 2x^8 + 3x^{11} + 4x^{12} \\ &= 3x^{13} + 7x^{12} + 9x^{11} + 9x^{10} + 7x^9 + 6x^8 + 5x^7. \\ \theta(G, x) &= 3x^{13} + x^{12} + 3x^{11} + 3x^{10} + x^9 + x^{10} + 2x^9 + x^8 + x^7 + x^7 + x^8 + x^8 + x^{11} + 2x^{12} \\ &= 3x^{13} + 3x^{12} + 4x^{11} + 4x^{10} + 3x^9 + 3x^8 + 2x^7.\end{aligned}$$

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DECLARATION STATEMENT

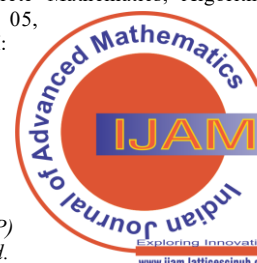
Some of the cited references are older and are noted explicitly as [4]. However, these works remain significant for the current study, as they are pioneering in their fields.

After aggregating input from all authors, I must verify the accuracy of the following information as the article's author.

- **Conflicts of Interest:** Based on my understanding, this article has no conflicts of interest.
- **Funding Support:** This article has not been sponsored or funded by any organization or agency.
- **Ethical Approval and Consent to Participate:** The data provided in this article are exempt from ethical approval or participant consent requirements.
- **Data Access Statement and Material Availability:** The adequate resources of this article are publicly accessible.
- **Author's Contributions:** The authorship of this article is contributed equally by all participating individuals.

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