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Original Article

Comparative study of some Topological Indices of Zanamivir and Chloroquine

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Abstract - *Zanamivir is medication used to treat and prevent influenza caused by Influenza A and B viruses. Chloroquine is antiviral drug used for treating malaria and autoimmune disease. Gourava indices are degree-based indices. In this paper we study some topological indices of Zanamivir and Chloroquine by Graph theory polynomials.*

Keywords - *Chloroquine, Gourava exponential, Gourava index, M-polynomial, R-degree, R-index, topological index, Zanamivir.*

1. Introduction

Let G be a simple, finite, connected graph with vertex set V(G) and edge set E(G). The degree d_v of a vertex is the number of vertices adjacent to v. Antiviral drugs are a class of medication used for treating viral infections. The molecular formula of Zanamivir is $C_{12}H_{20}N_4O_7$.Recently many topological indices are used in the study of antiviral drugs applied in the treatment of COVID-19. Many research papers appear on topological indices of Chloroquine, Hydroxychloroquine and Remdesivir in the current study of Chemical graph theory [1-16]. Chloroquine is the most widely used medication to treat malaria [17]. For a simple connected graph G, the first and second Zagreb indices [18] are defined as

$$M_1(G) = \sum_{uv\in E(G)}(d_u + d_v) \quad \text{and} \quad M_2(G) = \sum_{uv\in E(G)} d_u\, d_v.$$

The hyper Zagreb index is defined as [19]

$$HZ(G) = \sum_{uv\in E(G)}(d_u + d_v)^2.$$

The hyper Zagreb is related to F(G) and $M_2(G)$ as [21],

$$HZ(G) = F(G) + 2M_2(G).$$

Many degree based topological indices are expressed in terms of function F(x,y) in [20].Different versions of harmonic indices of certain of carbon nanotubes were studied by S.Ediz et al. in [22].Sum connectivity Kulli-Basava index, product connectivity Kulli-Basava index was introduced and computed for a molecular graph by V.R.Kulli [23].M-polynomial for nanostructures are discussed in many papers on topological indices of a molecular graph for example [24-26].Topological indices of local anesthetic drugs was studied by N.K.Raut [27].

The first Gourava index and product connectivity Gourava index are defined as [28]

$$G_1O(G) = \sum_{uv\in E(G)}(d_u + d_v + d_u d_v) \text{ and } PGO(G) = \frac{1}{\sqrt{(d_u+d_v)\, d_u d_v}}.$$

The second Gourava index of molecular graph G is defined as

$$G_2O(G) = \sum_{uv\in E(G)}(d_u + d_v)\, d_u d_v .$$

The first and second hyper Gourava indices of a molecular graph are defined as

$$HG_1O(G) = \sum_{uv\in E(G)}(d_u + d_v + d_u d_v)^2 \text{ and } HG_2O(G) = \sum_{uv\in E(G)}[(d_u + d_v)d_u d_v]^2 .$$

We define reciprocal sum connectivity Gourava index and reciprocal product connectivity Gourava index as

$$RSGO(G) = \sum_{uv \in E(G)} \sqrt{d_u + d_v + d_u d_v} \text{ and } RPGO(G) = \sum_{uv \in E(G)} \sqrt{(d_u + d_v) d_u d_v}.$$

The R-degree and R-indices of a molecular graph G were defined and investigated by S. Ediz in [29]. We define reciprocal hyper second R-index and reciprocal hyper third R-index as

$$RHR^2(G) = \sum_{uv \in E(G)} \frac{1}{[r(u)r(v)]^2} \text{ and } RHR^3(G) = \sum_{uv \in E(G)} \frac{1}{[r(u)+r(v)]^2},$$

where $r(v) = S_v + M_v$, $S_v = \sum_{u \in N(v)} \deg(u)$ sum degree of v and $M_v = \prod_{u \in N(v)} \deg(u)$ the multiplication degree of v. The set of all vertices which are adjacent to v is called the open neighborhood of v and denoted by N(v). By using the first derivative of the Schultz, modified Schultz polynomials of Jahangir graph $J_{3,m}$ (evaluated at x = 1) one can compute the Schultz, modified Schultz indices [30] as

$$Sc(J_{3,m}) = \frac{\partial Sc(J_{3,m},x,y)}{\partial x}\Big|_{x=1}.$$

The M-polynomial of graph G is defined as

$$M(G;x,y) = \sum_{\delta \le i \le j \le \Delta} m_{ij}(G)\, x^i y^j,$$

where $\delta = \min\{d_v | v \in V(G)\}$, $\Delta = \max\{d_v | v \in V(G)\}$, and $m_{ij}(G)$ is the edge vu ∈ E(G) such that

$i \le j$, with $D_x = x\frac{\partial f(x,y)}{\partial x}$, $D_y = y\frac{\partial f(x,y)}{\partial y}$, $S_x = \int_0^x \frac{f(t,y)}{t}dt$, $S_y = \int_0^y \frac{f(x,t)}{t}dt$, $J(f(x,y)) = f(x,x)$,

$Q_\alpha(f(x,y)) = x^\alpha f(x,y)$.

The notations used in this paper are standard and mainly taken from books of chemical graph theory [31-33]. In this paper first and second Gourava indices, first and second hyper Gourava indices and reciprocal hyper second R-index and reciprocal hyper third R-index are studied by M-polynomials and the reciprocal sum connectivity Gourava index and reciprocal product connectivity Gourava index for Zanamivir and Chloroquine is computed by Gourava exponential.

2. Materials and Methods

A molecular graph is a simple and connected graph. The molecular formula of Zanamivir is $C_{12}H_{20}N_4O_7$.The number of vertices is 12+4+7 = 23 that is vertex set |V(G)| = 23 and edge set |E(G)| = 23. The molecular graph of Zanamivir is shown in figure 1. The molecular graph of Chloroquine is considered in the determination of M-polynomials and exponential is also shown in figure 1. Degree-based topological indices are computed by using vertex degree of Zanamivir and Chloroquine. To study reciprocal hyper second R-index and reciprocal hyper third R-index, the sum degree and multiplication degree of the end vertices are used. The topological indices of Zanamivir and Chloroquine are compared graphically. The bond set partition of Zanamivir and Chloroquine are determined from molecular graph of respective structures. The M-polynomial of molecular graph of Zanamivir and Chloroquine is written from edge set of molecular graphs. The reciprocal sum connectivity Gourava index and reciprocal product connectivity Gourava index for Zanamivir and Chloroquine are computed by Gourava exponential.

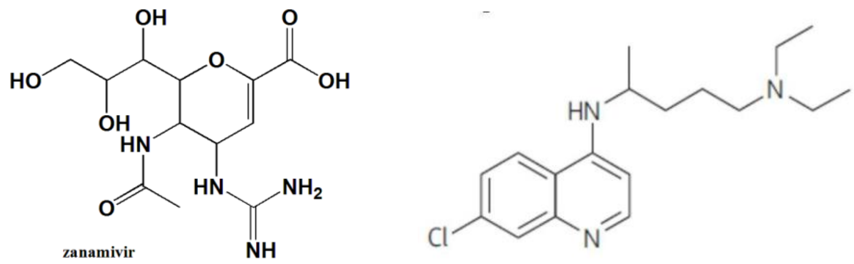
3. Results and Discussion

3.1. Topological indices of Zanamivir

In this section we compute some topological indices of Zanamivir by M-polynomial and Gourava exponential. Antiviral drugs are class of medication used specifically for treating viral infections. Zanamivir is medication used to treat and prevent influenza caused by influenza A and B viruses. The molecular graph of Zanamivir is shown figure 1. From 2-dimensional graph of Zanamivir we see that (d_u,d_v) = (1,2) = 1,(1,3) = 8,(2,3) = 9 and (3,3) = 5.The M-polynomial is written as

$$M(G;x,y) = xy^2+8xy^3+9x^2y^3+5x^3y^3.$$

Let G be the molecular graph of Zanamivir. The degree-based edge partition is used for computing the topological indices such as first Gourava index, second Gourava index, first and second hyper Gourava indices, reciprocal sum connectivity Gourava index and product connectivity Gourava index. The edge partitions are given in table I-IV and M-polynomial based formulas for topological indices are represented in table-V.The bond edge partitions of Zanamivir are used to investigate reciprocal hyper second R-index and reciprocal hyper third R-index.



Zanamivir Chloroquine

Fig. 1.2-D graphs of Zanamivir and Chloroquine.

Table 1. Edge partitions of Zanamivir

(d_u,d_v)\uv∈E(G)	(1,2)	(1,3)	(2,3)	(3,3)
Number of edges	1	8	9	5

Table 2. Bond set partitions of Zanamivir

(d_u,d_v)	Frequency	(S_u,S_v)	(M_u,Mv)
(1,2)	1	(2,4)	(2,3)
(1,3)	1 2 4	(3,7),(3,6) (3,5) (3,4)	(3,9),(3,6) (3,3) (3,2)
(2,3)	1 4 2 2	(4,6) (6,7) (6,8) (6,4)	(3,6) (9,12) (9,12) (9,2)
(3,3)	5	(6,7),(7,8),(7,5),(7,8),(8,8)	(6,9),(9,18),(12,3),(12,!8),(18,18)

Some topological indices of Zanamivir and Chloroquine are computed by M-polynomial and reciprocal sum connectivity Gourava index, reciprocal product connectivity Gourava index by Gourava exponential.

Theorem 1. First Gourava index of Zanamivir is 235.

Proof. Consider a molecular graph of Zanamivir as shown in figure 1. Using table I and formula of first Gourava index $G_1O(G) = \sum_{uv\in E(G)}(d_u+d_v + d_u d_v)$, we get first Gourava index.

M-polynomial expression for molecular graph G is

$M(G;x,y) = xy^2+8xy^3+9x^2y^3+5x^3y^3$.

$D_xM(G;x,y) = xy^2+8xy^3+18x^2y^3+15x^3y^3$.

$D_yM(G;x,y) = 2xy^2+24\, xy^3+27x^2y^3+15x^3y^3$.

$D_xD_yM(G;x,y) = 2xy^2+24\, xy^3+54x^2y^3+45x^3y^3$.

$G_1O(G) = (D_x+D_y+D_xD_y)(M(G;x,y))|_{x=y=1} = 235$.

Theorem 2. Second Gourava index of Zanamivir is 642.

Proof. Using table I and the formula of second Gourava index

$G_2O(G) = \sum_{uv\in E(G)}(d_u+d_v)d_ud_v$,we get second Gourava index.

The M-polynomial of graph G of Zanamivir is

$M(G;x,y) = xy^2+8xy^3+9x^2y^3+5x^3y^3$.

$D_yM(G;x,y) = 2xy^2+24\, xy^3+27x^2y^3+15x^3y^3$.

$(D_xD_y)M(G;x,y) = 2xy^2+24\, xy^3+54x^2y^3+45x^3y^3$.

$D_xM(G;x,y) = xy^2+8\, xy^3+18x^2y^3+15x^3y^3$.

$D_y(D_xD_y)M(G;x,y) = 4xy^2+72\, xy^3+162x^2y^3+135x^3y^3$.

$D_x(D_xD_y)M(G;x,y) = 2xy^2+24xy^3+108x^2y^3+135x^3y^3$.

$G_2O(G) = (D_x+D_y)D_xD_y\,(M(G;x,y))|_{x=y=1} = 642$.

Theorem 3. First hyper Gourava index of Zanamivir is 2631.

Proof. Using table I and the formula of first hyper Gourava index

$HG_1O(G) = \sum_{uv\in E(G)}[d_u+d_v + d_ud_v]^2$,we get first hyper Gourava index.

The M-polynomial of graph G of Zanamivir is

$M(G;x,y) = xy^2+8xy^3+9x^2y^3+5x^3y^3$.

$D_x^2M(G;x,y) = xy^2+8\, xy^3+36x^2y^3+45x^3y^3$.

$D_y^2M(G;x,y) = 4xy^2+72xy^3+81x^2y^3+45x^3y^3$.

$(D_x^2D_y^2)M(G;x,y) = 4xy^2+72\, xy^3+324x^2y^3+405x^3y^3$.

$(2D_xD_y)M(G;x,y) = 4xy^2+48\, xy^3+108x^2y^3+90x^3y^3$.

$(2D_xD_y^2)M(G;x,y) = 8xy^2+144\, xy^3+304x^2y^3+270x^3y^3$.

$(2D_x^{\,2}D_y)M(G;x,y) = 4xy^2+48\, xy^3+216x^2y^3+270x^3y^3$.

$HG_1O(G) = (D_x^2+D_y^2+D_x^2D_y^2+2D_yD_x+2D_x^2D_y+2D_xD_y^2)(M(G;x,y))|_{x=y=1} = 2631$.

Theorem 4. Second hyper Gourava index of Zanamivir is 23868.

Proof. Using table I and the formula of second hyper Gourava index

$HG_2O(G) = \sum_{uv\in E(G)}[(d_u+d_v)d_ud_v]^2$, we get second hyper Gourava index.

The M-polynomial of graph G of Zanamivir is

$M(G;x,y) = xy^2+8xy^3+9x^2y^3+5x^3y^3$.

$D_xM(G;x,y) = xy^2+8\, xy^3+18x^2y^3+15x^3y^3$.

$D_yM(G;x,y) = 2xy^2+24xy^3+27x^2y^3+15x^3y^3$.

$D_y^2M(G;x,y) = 4xy^2+72xy^3+81x^2y^3+45x^3y^3$.

$(D_x^4D_y^2)M(G;x,y) = 4xy^2+72xy^3+1296x^2y^3+3645x^3y^3$.

$D_y^3M(G;x,y) = 8xy^2+216xy^3+243x^2y^3+135x^3y^3$.

$(2D_x^3D_y^2)M(G;x,y) = 8xy^2+144xy^3+1296x^2y^3+2430x^3y^3$.

$D_y^4M(G;x,y) = 16xy^2+648xy^3+729x^2y^3+405x^3y^3$.

$D_x^2D_y^4M(G;x,y) = 16xy^2+648xy^3+2916x^2y^3+405x^3y^3$.

$HG_2O(G) = (D_x^4D_y^2+2D_x^3D_y^2+D_x^2D_y^4)(M(G;x,y))|_{x=y=1} = 23868$.

Theorem 5. Reciprocal sum connectivity Gourava index of Zanamivir is 72.6.

Proof. Using table I and the formula of reciprocal sum connectivity Gourava exponential we get RSGO(G).

$RSGO(G,x) = \sum_{uv\in E(G)} x^{\sqrt{d_u+d_v+d_ud_v}}$

$= \sum_{12\in E(G)} x^{\sqrt{1+2+1*2}} + \sum_{13\in E(G)} x^{\sqrt{1+3+1*3}} + \sum_{23\in E(G)} x^{\sqrt{2+3+2*3}} + \sum_{33\in E(G)} x^{\sqrt{3+3+3*3}}$.

$= x^{\sqrt{5}}+8x^{\sqrt{7}}+9x^{\sqrt{11}}+5x^{\sqrt{15}}$.

$RSGO(G) = \frac{\partial(RSG(G,x))}{\partial x}|_{x=1} = [\sqrt{5}+8\sqrt{7}+9\sqrt{11}+5\sqrt{15}] = 72.6$.

Theorem 6. Reciprocal product connectivity Gourava index of Zanamivir is 116.1.

Proof. Using table I and the formula of reciprocal product connectivity Gourava exponential we get reciprocal product connectivity Gourava index.

$RPGO(G,x) = \sum_{uv\in E(G)} x^{\sqrt{(d_u+d_v)d_ud_v}}$,

$= \sum_{12\in E(G)} x^{\sqrt{(1+2)1*2}} + \sum_{13\in E(G)} x^{\sqrt{(1+3)1*3}} + \sum_{23\in E(G)} x^{\sqrt{(2+3)2*3}} + \sum_{33\in E(G)} x^{\sqrt{(3+3)3*3}}$.

$= x^{\sqrt{6}}+8x^{\sqrt{12}}+9x^{\sqrt{30}}+5x^{\sqrt{54}}$.

$RPGO(G) = \frac{\partial(RPGO(G,x))}{\partial x}|_{x=1} = [\sqrt{6}+8\sqrt{12}+9\sqrt{30}+5\sqrt{54}] = 116.1$.

Theorem 7. Reciprocal hyper second R-index of Zanamivir is $4.6*10^{-3}$.

Proof. Using table II and the formula of reciprocal hyper second R-index

$RHR^2(G) = \sum_{uv\in E(G)} x^{\left(\frac{1}{(r(u)\,r(v))^2}\right)}$, we get reciprocal hyper second R-index.

The M-polynomial of graph G of Zanamivir is

$M(G;x,y)=x^4y^7+x^6y^{16}+2x^6y^8+4x^6y^6+x^6y^{12}+x^7y^{12}+2x^{15}y^{26}+4x^{15}y^{19}+2x^{15}y^6+x^{12}y^{16}+x^{16}y^{26}+x^{19}y^{18}+x^{19}y^{26}+x^{26}y^{26}$.

$S_y{}^2M(G;x,y)=\frac{1}{16}x^4y^7+\frac{1}{36}x^6y^{16}+\frac{2}{36}x^6y^8+4\frac{1}{36}x^6y^6+\frac{1}{36}x^6y^{12}+\frac{1}{49}x^7y^{12}+\frac{2}{225}x^{15}y^{26}+\frac{4}{225}x^{15}y^{19}+\frac{2}{225}x^{15}y^6+\frac{1}{144}x^{12}y^{16}+\frac{1}{256}x^{16}y^{26}+\frac{1}{361}x^{19}y^{18}+\frac{1}{361}x^{19}y^{26}+\frac{1}{676}x^{26}y^{26}$.

$S_x{}^2S_y{}^2M(G;x,y)=\frac{1}{16*49}x^4y^7+\frac{1}{36*256}x^6y^{16}+\frac{2}{36*64}x^6y^8+4\frac{1}{36*36}x^6y^6+\frac{1}{36*144}x^6y^{12}+\frac{1}{49*144}x^7y^{12}+\frac{2}{225*676}x^{15}y^{26}+\frac{4}{225*361}x^{15}y^{19}+\frac{2}{225*36}x^{15}y^6+\frac{1}{144*256}x^{12}y^{16}+\frac{1}{256*676}x^{16}y^{26}+\frac{1}{361*324}x^{19}y^{18}+\frac{1}{361*676}x^{19}y^{26}+\frac{1}{676*676}x^{26}y^{26}$.

$RHR^2(G) = S_x{}^2S_y{}^2(M(G;x,y))|_{x=y=1} = 4.6*10^{-3}$.

Theorem 8. Reciprocal hyper third R-index of Zanamivir is 0.066.

Proof. Using table II and the formula of reciprocal hyper third R-index $RHR^3(G) = \sum_{uv\in E(G)} x^{\left(\frac{1}{(r(u)+r(v))^2}\right)}$, we get reciprocal hyper third R-index.

The M-polynomial of graph G of Zanamivir is

$M(G;x,y)=x^4y^7+x^6y^{16}+2x^6y^8+4x^6y^6+x^6y^{12}+x^7y^{12}+2x^{15}y^{26}+4x^{15}y^{19}+2x^{15}y^6+x^{12}y^{16}+x^{16}y^{26}+$

$x^{19}y^{18}+x^{19}y^{26}+x^{26}y^{26}$.

$JM(G;x,y)=x^{11}+x^{22}+2x^{14}+4x^{12}+x^{18}+x^{19}+2x^{41}+4x^{34}+2x^{21}+x^{28}+x^{42}+x^{37}+x^{45}+x^{52}$.

$S_x{}^2JM(G;x,y)=\frac{1}{121}x^{11}+\frac{1}{484}x^{22}+\frac{2}{196}x^{14}+\frac{4}{144}x^{12}+\frac{1}{324}x^{18}+\frac{1}{361}x^{19}+\frac{2}{1681}x^{41}+\frac{4}{1156}x^{34}+\frac{2}{441}x^{21}+$

$\frac{1}{784}x^{28}+\frac{1}{1764}x^{42}+\frac{1}{1369}x^{37}+\frac{1}{2025}x^{45}+\frac{1}{2704}x^{52}$.

$RHR^3(G) = S_x{}^2J(M(G;x,y))|_{x=y=1} = 0.066$.

3.2. Topological indices of Chloroquine

The 2-D molecular graph of Chloroquine with vertices 22 and edges 23 is shown in figure 1. Edge partitions of Chloroquine is given in table III. The molecular formula of Chloroquine is $C_{18}H_{26}ClN_3$. First and second Gourava indices, first and second hyper Gourava indices, reciprocal hyper second R-index and reciprocal hyper third R-index are computed by using M-polynomial and reciprocal sum connectivity Gourava index, reciprocal product connectivity Gourava index by Gourava exponential.

R-degree of a vertex v is defined as $r(v) = S_v+ M_v$, where S_v is sum degree of v and M_v is the multiplication degree of v. Reciprocal hyper second and third R-indices are computed by using bond set partitions of chloroquine. The bond set partitions are in given table IV. The derivational formulas of topological indices by M-polynomial are given in table 5. The topological indices computed for Chloroquine are given below. The values of some topological indices for Chloroquine are First Gourava index = 226, second Gourava index = 584, first hyper Gourava index = 2370, second hyper Gourava index = 18272, reciprocal sum connectivity index = 71, reciprocal product connectivity index = 109.8, reciprocal hyper second R-index = 0.0044 and reciprocal hyper third R-index = 0.00058.

Table 3. Edge partitions of Chloroquine

$(d_u,d_v)\backslash uv\in E(G)$	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
Number of edges	2	2	5	12	2

Table 4. Bond set partitions of Chloroquine

(d_u,d_v)	Frequency	(S_u,S_v)	(M_u,Mv)
(1,2)	2	(2,4)	(2,3)
(1,3)	2	(3,5)	(3,4)
(2,3)	2 1	(5,5),(6,5),(6,7),(5,7),(4,6) (5,8),(5,6)	(6,4), (9,4),(9,12),(6,12),(3,8) (9,18),(6,8)
(2,2)	1	(5,5),(5,5),(5,7),(5,4),(5,5)	(6,6),(4,6),(4,8),(6,4),(4,6)
(3,3)	1	(7,8),(8,7)	(12,8),(18,12)

Table 5. Derivational formulas for topological indices by M-polynomial

Topological index	Derivation from M(G;x,y)
First Gourava index	$(D_x+D_y+D_x D_y)(M(G;x,y))\|_{x=y=1}$
Second Gourava index	$(D_x+D_y) D_xD_y(M(G;x,y))\|_{x=y=1}$
First hyper Gourava index	$(D_x+D_y+D_x D_y)^2(M(G;x,y))\|_{x=y=1}$
Second hyper Gourava index	$[(D_x+D_y) D_x D_y]^2(M(G;x,y))\|_{x=y=1}$
Reciprocal hyper second R-index	$S_x^2 S_y^2(M(G;x,y))\|_{x=y=1}$
Reciprocal hyper third R-index	$S_x^2 J(M(G;x,y))\|_{x=1}$

6. Conclusion

Some topological indices of Zanamivir and Chloroquine are computed by M-polynomial. Reciprocal sum connectivity Gourava index and reciprocal product connectivity Gourava index are investigated by Gourava exponential. The values of reciprocal hyper second R-index and reciprocal hyper second R-index of Zanamivir and Chloroquine are nearly equal. Reciprocal hyper second and reciprocal hyper third R-index has low values as compared to other considered topological indices.

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