International Journal of Engineering Sciences & Research Technology

(A Peer Reviewed Online Journal)
Impact Factor: 5.164

IJESRT

RESEARCHERID
THOMSON REUTERS

[Kulli *et al.*, 10(6): June, 2021]
IC™ Value: 3.00

ISSN: 2277-9655
Impact Factor: 5.164
CODEN: IJESS7

IJESRT

INTERNATIONAL JOURNAL OF ENGINEERING SCIENCES & RESEARCH TECHNOLOGY

DIFFERENT VERSIONS OF MULTIPLICATIVE ARITHMETIC-GEOMETRIC INDICES OF SOME CHEMICAL STRUCTURES

V. R. Kulli
Department of Mathematics, Gulbarga University, Kalaburgi(Gulbarga) 585 106, India

DOI: https://doi.org/10.29121/ijesrt.v10.i6.2021.5

ABSTRACT

In Chemical Graph Theory, several degree based topological indices were introduced and studied since 1972. In this paper, we compute the first, second, third, fourth and fifth multiplicative arithmetic-geometric indices of some important chemical drugs which appeared in medical science.

KEYWORDS: multiplicative arithmetic-geometric index, nanostructure.
Mathematics Subject Classification: 05C05, 05C07, 05C90.

1. INTRODUCTION

Let G be a finite, simple connected graph with a vertex set $V(G)$ and an edge set $E(G)$. The degree $d(v)$ of a vertex v is the number of vertices adjacent to v. We refer to [1] for undefined term and notation.

A molecular graph is a simple graph related to the structure of a chemical compound. Each vertex of this graph represents an atom of the molecule and its edges to the bonds between atoms. A topological index is a numeric quantity from structural graph of a molecule. These indices are useful for establishing correlation between the structures of a molecular compound and its physicochemical properties.

Very recently Kulli [2] introduced the first multiplicative arithmetic-geometric index of a graph G and it is defined as

$$AG_1II(G) = \prod_{uv \in E(G)} \frac{d(u)+d(v)}{2\sqrt{d(u)d(v)}}.$$

Many other multiplicative indices were studied, for example, in [3, 4, 5, 6, 7, 8, 9, 10].

Motivated by the definition of the first multiplicative arithmetic-geometric index and by previous research on topological indices, Kulli proposed the second, third, fourth and fifth multiplicative arithmetic-geometric indices [11] of a graph as follows:

The second multiplicative arithmetic-geometric index of a graph G is defined as

$$AG_2II(G) = \prod_{uv \in E(G)} \frac{n(u)+n(v)}{2\sqrt{n(u)n(v)}}$$

where the number $n(u)$ of vertices of G lying closer to the vertex u than to the vertex v for the edge uv of a graph G.

The third multiplicative arithmetic-geometric index of a graph G is defined as

$$AG_3II(G) = \prod_{uv \in E(G)} \frac{m(u)+m(v)}{2\sqrt{m(u)m(v)}}$$

ISSN: 2277-9655
Impact Factor: 5.164
CODEN: IJESS7

Where the number $m(u)$ of edges of G lying closer to the vertex u than to the vertex v for the edge uv of a graph G.

The fourth multiplicative arithmetic-geometric index of a graph G is defined as

$$AG_4II(G) = \prod_{uv \in E(G)} \frac{\varepsilon(u)+\varepsilon(v)}{2\sqrt{\varepsilon(u)\varepsilon(v)}}$$

where the number ε(u) is the eccentricity of vertex u.

The fifth multiplicative arithmetic-geometric index of a graph G is defined as

$$AG_5II(G) = \prod_{uv \in E(G)} \frac{s(u)+s(v)}{2\sqrt{s(u)s(v)}}$$

where $s(u)$ denote the sum of the degrees of all vertices adjacent to a vertex u.

Recently, some new versions of topological indices were studied [12, 13, 14, 15, 16].

In this paper, the first, second, third, fourth and fifth multiplicative arithmetic-geometric Zagreb indices of some important molecular structures such as chloroquine, hydrochloroquine, remdesivir are computed. For chemical drugs, see [17, 18].

2. RESULTS AND DISCUSSION: CHLOROQUINE

Chloroquine is an antiviral compound (drug) which was discovered in 1934 by H.Andersag. This drug is medication primarily used to prevent and treat malaria.

Let G_1 be the chemical structure of chloroquine. This structure has 21 atoms and 23 bonds, see Figure 1.

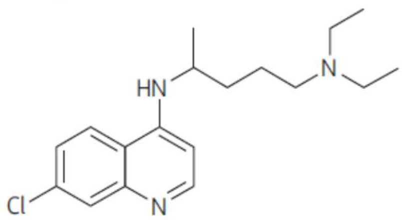

Figure 1. Chemical structure of chloroquine

From Figure 1, we obtain that
(i) $\{(d(u), d(v)) \setminus uv \in E(G_1)\}$ has 5 bond set partitions,
(ii) $\{(n(u), n(v)) \setminus uv \in E(G_1)\}$ has 10 bond set partitions,
(iii) $\{(m(u), m(v)) \setminus uv \in E(G_1)\}$ has 12 bond set partitions,
(iv) $\{(\varepsilon(u), \varepsilon(v)) \setminus uv \in E(G_1)\}$ has 7 bond set partitions,
(iv) $\{(s(u), s(v)) \setminus uv \in E(G_1)\}$ has 10 bond set partitions.

Figure 1. Chemical structure of chloroquine

$d(u), d(v) \setminus uv \in E(G_1)$	(1, 2)	(1,3)	(2, 2)	(2, 3)	(3, 3)	
Number of bonds	2	2	5	12	2	
$n(u), n(v) \setminus uv \in E(G_1)$	(1,19)	(1,20)	(2,18)	(3,17)	(4,16)	
Number of bonds	2	4	2	4	1	
	(5,15)	(6,14)	(7,13)	(9,11)	(10,10)	
	4	1	3	1	1	
$m(u), m(v) \setminus uv \in E(G_1)$	(1,21)	(1,22)	(2,19)	(3,18)	(4,17)	(5,15)
Number of bonds	2	4	2	4	1	3
	(5,16)	(6,15)	(7,14)	(8,13)	(9,13)	(10,12)

ISSN: 2277-9655
Impact Factor: 5.164
CODEN: IJESS7

	1	1	2	1	1	1
$\varepsilon(u), \varepsilon(v) \setminus uv \in E(G_1)$	(7,7)	(8,7)	(8,9)	(9,10)	(10,11)	
Number of bonds	1	3	3	4	5	
	(11,12)	(12,13)				
	4	3				
$s(u), s(v) \setminus uv \in E(G_1)$						
Number of bonds	(2,4)	(3,5)	(4,5)	(4,6)	(5,5)	
	2	2	4	2	3	
	(5,6)	(5,7)	(5,8)	(6,7)	(7,8)	
	3	2	1	2	2	

In the following theorem, we compute the different versions of multiplicative arithmetic-geometric indices of chloroquine.

Theorem 1. Let G_1 be the chemical structure of chloroquine. Then

(i) $$AG_1II(G_1) = \left(\frac{3}{2\sqrt{2}}\right)^2 \times \left(\frac{2}{\sqrt{3}}\right)^2 \times \left(\frac{5}{2\sqrt{6}}\right)^{12}.$$

(ii) $$AG_2II(G_1) = \left(\frac{10}{\sqrt{19}}\right)^2 \times \left(\frac{21}{4\sqrt{5}}\right)^4 \times \left(\frac{10}{\sqrt{51}}\right)^4 \times \left(\frac{2}{\sqrt{3}}\right)^4 \times \left(\frac{5}{\sqrt{21}}\right)^1$$
$$\times \left(\frac{10}{\sqrt{91}}\right)^3 \times \left(\frac{10}{3\sqrt{11}}\right)^1 \times \left(\frac{125}{36}\right)^1$$

(iii) $$AG_3II(G_1) = \left(\frac{11}{\sqrt{21}}\right)^2 \times \left(\frac{23}{2\sqrt{22}}\right)^4 \times \left(\frac{21}{2\sqrt{38}}\right)^2 \times \left(\frac{7}{2\sqrt{6}}\right)^4 \times \left(\frac{21}{4\sqrt{17}}\right)^1 \times \left(\frac{2}{\sqrt{3}}\right)^3$$
$$\times \left(\frac{21}{8\sqrt{5}}\right)^1 \times \left(\frac{7}{2\sqrt{10}}\right)^1 \times \left(\frac{3}{2\sqrt{2}}\right)^2 \times \left(\frac{21}{4\sqrt{26}}\right)^1 \times \left(\frac{11}{3\sqrt{13}}\right)^1 \times \left(\frac{11}{2\sqrt{30}}\right)^1$$

(iv) $$AG_4II(G_1) = \left(\frac{15}{4\sqrt{14}}\right)^3 \times \left(\frac{17}{12\sqrt{2}}\right)^3 \times \left(\frac{19}{6\sqrt{10}}\right)^4 \times \left(\frac{21}{2\sqrt{110}}\right)^5 \times \left(\frac{23}{4\sqrt{33}}\right)^4 \times \left(\frac{25}{4\sqrt{39}}\right)^3.$$

(v) $$AG_5II(G_1) = \left(\frac{3}{2\sqrt{2}}\right)^2 \times \left(\frac{4}{\sqrt{15}}\right)^2 \times \left(\frac{9}{4\sqrt{5}}\right)^4 \times \left(\frac{5}{2\sqrt{6}}\right)^2 \times \left(\frac{11}{2\sqrt{30}}\right)^3$$
$$\times \left(\frac{6}{\sqrt{35}}\right)^2 \times \left(\frac{13}{4\sqrt{10}}\right) \times \left(\frac{13}{2\sqrt{42}}\right)^2 \times \left(\frac{15}{4\sqrt{14}}\right)^2.$$

Proof: By using the definitions and cardinalities of the bond partitions of G_1, we deduce

(i) $$AG_1II(G_1) = \prod_{uv \in E(G_1)} \frac{d(u)+d(v)}{2\sqrt{d(u)d(v)}}$$
$$= \left(\frac{1+2}{2\sqrt{1\times 2}}\right)^2 \times \left(\frac{1+3}{2\sqrt{1\times 3}}\right)^2 \times \left(\frac{2+2}{2\sqrt{2\times 2}}\right)^5 \times \left(\frac{2+3}{2\sqrt{2\times 3}}\right)^{12} \times \left(\frac{3+3}{2\sqrt{3\times 3}}\right)^2$$

After simplification, we obtain the desired result.

(ii) $$AG_2II(G_1) = \prod_{uv \in E(G_1)} \frac{n(u)+n(v)}{2\sqrt{n(u)n(v)}}$$

$$=\left(\frac{1+19}{2\sqrt{1\times 19}}\right)^{2}\times\left(\frac{1+20}{2\sqrt{1\times 20}}\right)^{4}\times\left(\frac{2+18}{2\sqrt{2\times 18}}\right)^{2}\times\left(\frac{3+17}{2\sqrt{3\times 17}}\right)^{4}\times\left(\frac{4+16}{2\sqrt{4\times 16}}\right)^{1}$$
$$\times 4\left(\frac{5+15}{2\sqrt{5\times 15}}\right)^{4}\times\left(\frac{6+14}{2\sqrt{6\times 14}}\right)^{1}\times 3\left(\frac{7+13}{2\sqrt{7\times 13}}\right)^{3}\times\left(\frac{9+11}{2\sqrt{9\times 11}}\right)^{1}\times\left(\frac{10+10}{2\sqrt{10\times 10}}\right)^{1}.$$

After simplification, we obtain the desired result.

(iii) $$AG_3II(G_1)=\prod_{uv\in E(G_1)}\frac{m(u)+m(v)}{2\sqrt{m(u)m(v)}}$$

$$=\left(\frac{1+21}{2\sqrt{1\times 21}}\right)^{2}\times\left(\frac{1+22}{2\sqrt{1\times 22}}\right)^{4}\times\left(\frac{2+19}{2\sqrt{2\times 19}}\right)^{2}\times\left(\frac{3+18}{2\sqrt{3\times 18}}\right)^{4}\times\left(\frac{4+17}{2\sqrt{4\times 17}}\right)^{1}\times\left(\frac{5+15}{2\sqrt{5\times 15}}\right)^{3}$$
$$\times\left(\frac{5+16}{2\sqrt{5\times 16}}\right)^{1}\times\left(\frac{6+15}{2\sqrt{6\times 15}}\right)^{1}\times\left(\frac{7+14}{2\sqrt{7\times 14}}\right)^{2}\times\left(\frac{8+13}{2\sqrt{8\times 13}}\right)^{1}\times\left(\frac{9+13}{2\sqrt{9\times 13}}\right)^{1}\times\left(\frac{10+12}{2\sqrt{10\times 12}}\right)^{1}.$$

After simplification, we obtain the desired result.

(iv) $$AG_4II(G_1)=\prod_{uv\in E(G_1)}\frac{\varepsilon(u)+\varepsilon(v)}{2\sqrt{\varepsilon(u)\varepsilon(v)}}$$

$$=\left(\frac{7+7}{2\sqrt{7\times 7}}\right)\times\left(\frac{8+7}{2\sqrt{8\times 7}}\right)^{3}\times\left(\frac{8+9}{2\sqrt{8\times 9}}\right)^{3}\times\left(\frac{9+10}{2\sqrt{9\times 10}}\right)^{4}\times\left(\frac{10+11}{2\sqrt{10\times 11}}\right)^{5}$$
$$\times\left(\frac{11+12}{2\sqrt{11\times 12}}\right)^{4}\times\left(\frac{12+13}{2\sqrt{12\times 13}}\right)^{3}.$$

After simplification, we obtain the desired result.

(v) $$AG_5II(G_1)=\prod_{uv\in E(G_1)}\frac{s(u)+s(v)}{2\sqrt{s(u)s(v)}}$$

$$=\left(\frac{2+4}{2\sqrt{2\times 4}}\right)^{2}\times\left(\frac{3+5}{2\sqrt{3\times 5}}\right)^{2}\times\left(\frac{4+5}{2\sqrt{4\times 5}}\right)^{4}\times\left(\frac{4+6}{2\sqrt{4\times 6}}\right)^{2}\times\left(\frac{5+5}{2\sqrt{5\times 5}}\right)^{3}$$
$$\times\left(\frac{5+6}{2\sqrt{5\times 6}}\right)^{3}\times\left(\frac{5+7}{2\sqrt{5\times 7}}\right)^{2}\times\left(\frac{5+8}{2\sqrt{5\times 8}}\right)^{1}\times\left(\frac{6+7}{2\sqrt{6\times 7}}\right)^{2}\times\left(\frac{7+8}{2\sqrt{7\times 8}}\right)^{2}$$

After simplification, we obtain the desired result.

3. RESULTS AND DISCUSSION: HYDROXYCHLOROQUINE

Hydroxychloroquine is another antiviral compound (drug) which has antiviral activity very similar to that of chloroquine. These compounds have been repurposed for the treatment of a number of other conditions including HIV, systemic lupus erythmatosus and rheumatoid arthritis .

Let G_2 be the chemical structure of hydroxychloroquine. This structure has 22 vertices and 24 edges, see Figure 2.

ISSN: 2277-9655
Impact Factor: 5.164
CODEN: IJESS7

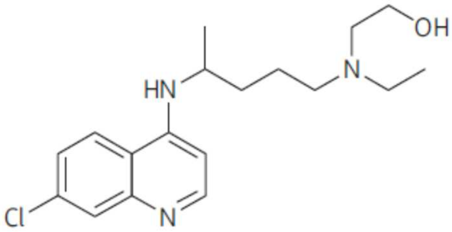

Figure 2. Chemical structure of hydroxychloroquine

From Figure 2, we obtain that

(i) $\{(d(u), d(v)) \setminus uv \in E(G_2)\}$ has 5 bond set partitions,

(ii) $\{(n(u), n(v)) \setminus uv \in E(G_2)\}$ has 9 bond set partitions,

(iii) $\{(m(u), m(v)) \setminus uv \in E(G_2)\}$ has 12 bond set partitions,

(iv) $\{(\varepsilon(u), \varepsilon(v)) \setminus uv \in E(G_2)\}$ has 7 bond set partitions,

(iv) $\{(s(u), s(v)) \setminus uv \in E(G_2)\}$ has 11 bond set partition

Table 2. Bond set partitions of hydroxychloroquine

$d(u), d(v) \setminus uv \in E(G_2)$	(1, 2)	(1,3)	(2, 2)	(2, 3)	(3, 3)	
Number of bonds	2	2	6	12	2	
$n(u), n(v) \setminus uv \in E(G_2)$	(1,20)	(1,21)	(2,19)	(3,18)	(5,16)	
Number of bonds	2	4	3	4	4	
	(6,15)	(7,14)	(10,11)	(8,13)		
	3	2	1	1		
$m(u), m(v) \setminus uv \in E(G_2)$	(1,22)	(1,23)	(2,20)	(2,21)	(3,19)	(5,16)
Number of bonds	2	4	2	1	4	3
	(5,17)	(6,16)	(7,15)	(8,14)	(10,13)	(11,12)
	1	1	1	3	1	1
$\varepsilon(u), \varepsilon(v) \setminus uv \in E(G_2)$	(7,8)	(8,9)	(9,10)	(10,11)	(11,12)	
Number of bonds	3	2	3	4	6	
	(12,13)	(13,14)				
	4	2				
$s(u), s(v) \setminus uv \in E(G_2)$						
Number of bonds	(2,3)	(2,4)	(3,5)	(4,5)	(4,6)	(5,5)
	1	1	3	4	1	3
	(5,6)	(5,7)	(5,8)	(6,7)	(7,8)	
	4	2	1	2	2	

In the following theorem, we compute the different versions of multiplicative arithmetic-geometric indices of hydroxychloroquine.

Theorem 2. Let G_2 be the chemical structure of hydroxychloroquine. Then

(i) $$AG_1II(G_2) = \left(\frac{3}{2\sqrt{2}}\right)^2 \times \left(\frac{2}{\sqrt{3}}\right)^2 \times \left(\frac{5}{2\sqrt{6}}\right)^{12}.$$

(ii) $$AG_2II(G_2) = \left(\frac{21}{2\sqrt{20}}\right)^2 \times \left(\frac{11}{\sqrt{21}}\right)^4 \times \left(\frac{21}{2\sqrt{38}}\right)^4 \times \left(\frac{21}{2\sqrt{54}}\right)^4 \times \left(\frac{21}{8\sqrt{5}}\right)^1$$
$$\times \left(\frac{21}{6\sqrt{10}}\right)^3 \times \left(\frac{3}{2\sqrt{2}}\right)^2 \times \left(\frac{21}{2\sqrt{110}}\right)^1 \times \left(\frac{21}{2\sqrt{104}}\right)^1.$$

ISSN: 2277-9655
Impact Factor: 5.164
CODEN: IJESS7

(iii) $AG_3II(G_2)=\left(\frac{23}{2\sqrt{22}}\right)^2\times\left(\frac{12}{\sqrt{23}}\right)^4\times\left(\frac{11}{2\sqrt{10}}\right)^4\times\left(\frac{23}{2\sqrt{42}}\right)^4\times\left(\frac{11}{\sqrt{57}}\right)^1\times\left(\frac{21}{8\sqrt{5}}\right)^3$

$+\left(\frac{11}{\sqrt{85}}\right)^1\times\left(\frac{11}{4\sqrt{6}}\right)^1\times\left(\frac{11}{2\sqrt{105}}\right)^1\times\left(\frac{11}{4\sqrt{7}}\right)^3\times\left(\frac{23}{2\sqrt{130}}\right)^1\times\left(\frac{23}{2\sqrt{132}}\right)^1.$

(iv) $AG_4II(G_2)=\left(\frac{15}{4\sqrt{14}}\right)^3\times\left(\frac{17}{12\sqrt{2}}\right)^2\times\left(\frac{19}{6\sqrt{10}}\right)^3\times\left(\frac{21}{2\sqrt{110}}\right)^4\times\left(\frac{23}{4\sqrt{33}}\right)^6$

$\times\left(\frac{25}{4\sqrt{39}}\right)^4\times\left(\frac{27}{4\sqrt{182}}\right)^2.$

(v) $AG_5II(G_2)=\left(\frac{5}{2\sqrt{6}}\right)^1\times\left(\frac{3}{2\sqrt{2}}\right)^1\times\left(\frac{4}{\sqrt{15}}\right)^3\times\left(\frac{9}{4\sqrt{5}}\right)^4\times\left(\frac{5}{2\sqrt{6}}\right)^1\times\left(\frac{11}{2\sqrt{30}}\right)^4$

$\times\left(\frac{6}{\sqrt{35}}\right)^2\times\left(\frac{13}{4\sqrt{10}}\right)^1\times\left(\frac{13}{2\sqrt{42}}\right)^2\times\left(\frac{15}{4\sqrt{14}}\right)^2.$

Proof: By using the definitions and cardinalities of the bond partitions of G_2, we deduce

(i) $$AG_1II(G_2)=\prod_{uv\in E(G_2)}\frac{d(u)+d(v)}{2\sqrt{d(u)d(v)}}$$

$$=\left(\frac{1+2}{2\sqrt{1\times 2}}\right)^2\times\left(\frac{1+3}{2\sqrt{1\times 3}}\right)^2\times\left(\frac{2+2}{2\sqrt{2\times 2}}\right)^6\times\left(\frac{2+3}{2\sqrt{2\times 3}}\right)^{12}\times\left(\frac{3+3}{2\sqrt{3\times 3}}\right)^2.$$

After simplification, we obtain the desired result.

(ii) $$AG_2II(G_2)=\prod_{uv\in E(G_2)}\frac{n(u)+n(v)}{2\sqrt{n(u)n(v)}}$$

$$=2\left(\frac{1+20}{2\sqrt{1\times 20}}\right)^2\times 4\left(\frac{1+21}{2\sqrt{1\times 21}}\right)^4\times 3\left(\frac{2+19}{2\sqrt{2\times 19}}\right)^2\times 4\left(\frac{3+18}{2\sqrt{3\times 18}}\right)^4\times 4\left(\frac{5+16}{2\sqrt{5\times 16}}\right)^1$$

$$\times 3\left(\frac{6+15}{2\sqrt{6\times 15}}\right)^4\times 2\left(\frac{7+14}{2\sqrt{7\times 14}}\right)^1\times\left(\frac{10+11}{2\sqrt{10\times 11}}\right)^3\times\left(\frac{8+13}{2\sqrt{8\times 13}}\right)^1.$$

After simplification, we obtain the desired result.

(iii) $$AG_3II(G_2)=\prod_{uv\in E(G_2)}\frac{m(u)+m(v)}{2\sqrt{m(u)m(v)}}$$

$$=2\left(\frac{1+22}{2\sqrt{1\times 22}}\right)^2\times\left(\frac{1+23}{2\sqrt{1\times 23}}\right)^4\times\left(\frac{2+20}{2\sqrt{2\times 20}}\right)^2\times\left(\frac{2+21}{2\sqrt{2\times 21}}\right)^1\times\left(\frac{3+19}{2\sqrt{3\times 19}}\right)^4$$

$$\times\left(\frac{5+17}{2\sqrt{5\times 17}}\right)^1\times\left(\frac{6+16}{2\sqrt{6\times 16}}\right)^1\times\left(\frac{7+15}{2\sqrt{7\times 15}}\right)^3\times\left(\frac{8+14}{2\sqrt{8\times 14}}\right)^3\times\left(\frac{10+13}{2\sqrt{10\times 13}}\right)^1\times\left(\frac{11+12}{2\sqrt{11\times 12}}\right)^1.$$

After simplification, we obtain the desired result.

(iv) $$AG_4II(G_2)=\prod_{uv\in E(G_2)}\frac{\varepsilon(u)+\varepsilon(v)}{2\sqrt{\varepsilon(u)\varepsilon(v)}}$$

ISSN: 2277-9655
Impact Factor: 5.164
CODEN: IJESS7

$$=\left(\frac{7+8}{2\sqrt{7\times 8}}\right)^{3}\times\left(\frac{8+9}{2\sqrt{8\times 9}}\right)^{2}\times\left(\frac{9+10}{2\sqrt{9\times 10}}\right)^{3}\times\left(\frac{10+11}{2\sqrt{10\times 11}}\right)^{4}\times\left(\frac{11+12}{2\sqrt{11\times 12}}\right)^{6}$$

$$\times\left(\frac{12+13}{2\sqrt{12\times 13}}\right)^{4}\times\left(\frac{13+14}{2\sqrt{13\times 14}}\right)^{2}.$$

After simplification, we obtain the desired result.

(v) $$AG_5II(G_2)=\prod_{uv\in E(G_2)}\frac{s(u)+s(v)}{2\sqrt{s(u)s(v)}}$$

$$=\left(\frac{2+3}{2\sqrt{2\times 3}}\right)^{1}\times\left(\frac{2+4}{2\sqrt{2\times 4}}\right)^{1}\times\left(\frac{3+5}{2\sqrt{3\times 5}}\right)^{3}\times\left(\frac{4+5}{2\sqrt{4\times 5}}\right)^{4}\times\left(\frac{4+6}{2\sqrt{4\times 6}}\right)^{1}\times\left(\frac{5+5}{2\sqrt{5\times 5}}\right)^{3}$$

$$\times\left(\frac{5+6}{2\sqrt{5\times 6}}\right)^{4}\times\left(\frac{5+7}{2\sqrt{5\times 7}}\right)^{2}\times\left(\frac{5+8}{2\sqrt{5\times 8}}\right)^{1}\times\left(\frac{6+7}{2\sqrt{6\times 7}}\right)^{2}\times\left(\frac{7+8}{2\sqrt{7\times 8}}\right)^{2}.$$

After simplification, we get the desired result.

4. RESULTS AND DISCUSSION : REMDESIVIR

Remdesivir is an antiviral drug which was developed by the biopharmaceutical company Gilead Sciences.Let G_3 be the molecular graph of remdesivir. This graph has 41 vertices and 44 edges.

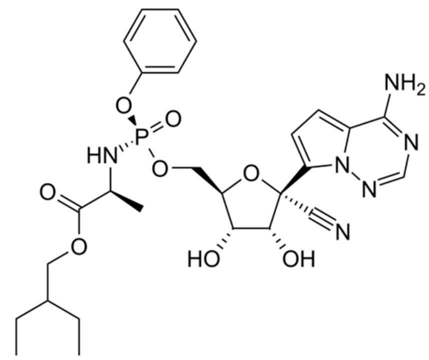

Figure 3. Chemical structure of remdesivir

From Figure 3, we obtain that

(i) $\{(d(u), d(v)) \setminus uv \in E(G_3)\}$ has 8 bond set partitions,
(ii) $\{(n(u), n(v)) \setminus uv \in E(G_3)\}$ has 25 bond set partitions,
(iii) $\{(m(u), m(v)) \setminus uv \in E(G_3)\}$ has 23 bond set partitions,
(iv) $\{(\varepsilon(u), \varepsilon(v)) \setminus uv \in E(G_3)\}$ has 11 bond set partitions,
(iv) $\{(s(u), s(v)) \setminus uv \in E(G_3)\}$ has 23 bond set partitions.

Table 3. Bond set partitions of remdesivir

$d(u), d(v)\setminus uv\in E(G_3)$	(1,2)	(1, 3)	(1, 4)	(2, 2)	(2, 3)	(2, 4)	(3, 3)	(3, 4)
Number of bonds	2	5	2	9	14	4	6	2
$n(u), n(v)\setminus uv\in E(G_3)$	(1,6)	(1,34)	(1,38)	(1,39)	(2,37)	(3,12)	(3,23)	(3,36)
Number of bonds	1	1	2	9	8	1	1	2
	(4,32)	(4,33)	(4,34)	(4,35)	(5,34)	(6,32)	(6,33)	(8,31)
	1	1	1	1	2	1	2	1
	(9,30)	(10,29)	(11,28)	(12,24)	(13,24)	(13,25)	(17,22)	(18,21)
	1	1	1	1	1	1	1	1
	(19,20)							

	1							
$m(u),m(v)\backslash uv\in E(G_3)$	(1,42)	(1,43)	(2,8)	(2,32)	(2,40)	(2,41)	(3,39)	(4,15)
Number of bonds	2	9	1	1	2	6	2	1
	(4,39)	(4,26)	(5,37)	(5,38)	(6,35)	(6,37)	(7,36)	(8,35)
	1	1	2	1	1	2	1	2
	(10,33)	(11,32)	(15,27)	(16,26)	(16,27)	(20,23)	(21,22)	
	1	2	1	1	1	1	2	
$\varepsilon(u),\varepsilon(v)\backslash uv\in E(G_3)$	(9,10)	(10,11)	(11,12)	(12,13)	(13,13)	(13,14)	(14,15)	(15,16)
Number of bonds	2	4	4	7	1	7	5	4
	(16,16)	(16,17)	(17,18)					
	1	4	5					
$s(u),s(v)\backslash uv\in E(G_3)$	(2,4)	(3,6)	(3,7)	(3,8)	(4,4)	(4,5)	(4,6)	(4,7)
Number of bonds	2	3	1	1	2	4	2	1
	(4,9)	(5,5)	(5,6)	(5,7)	(5,8)	(5,9)	(6,6)	(6,7)
	1	2	6	1	2	1	1	3
	(6,8)	(7,7)	(7,8)	(7,9)	(8,8)	(8,9)	(9,9)	
	1	4	1	1	1	2	1	

In the following theorem, we compute the different versions of multiplicative arithmetic-geometric indices of remdesivir.

Theorem 3. Let G_3 be the chemical structure of remdesivir. Then

(i) $$AG_1II(G_3)=\left(\frac{3}{2\sqrt{2}}\right)^2\times\left(\frac{2}{\sqrt{3}}\right)^5\times\left(\frac{5}{4}\right)^2\cdot\times\left(\frac{5}{2\sqrt{6}}\right)^{14}\times\left(\frac{3}{2\sqrt{2}}\right)^4\times\left(\frac{7}{4\sqrt{3}}\right)^2.$$

(ii) $$AG_2II(G_3)=\left(\frac{7}{2\sqrt{6}}\right)^1\times\left(\frac{35}{2\sqrt{34}}\right)^1\times\left(\frac{39}{2\sqrt{38}}\right)^2\times\left(\frac{20}{\sqrt{39}}\right)^9\times\left(\frac{39}{2\sqrt{74}}\right)^8\times\left(\frac{5}{4}\right)^1\times\left(\frac{13}{\sqrt{69}}\right)^1$$
$$\times\left(\frac{13}{4\sqrt{3}}\right)^2\times\left(\frac{9}{4\sqrt{2}}\right)^1\times\left(\frac{37}{4\sqrt{33}}\right)^1\times\left(\frac{19}{2\sqrt{34}}\right)^1\times\left(\frac{39}{4\sqrt{35}}\right)^1\times\left(\frac{39}{2\sqrt{170}}\right)^2$$
$$\times\left(\frac{19}{8\sqrt{3}}\right)^1\times\left(\frac{13}{2\sqrt{22}}\right)^2\times\left(\frac{39}{4\sqrt{62}}\right)^1\times\left(\frac{13}{2\sqrt{30}}\right)^1\times\left(\frac{39}{2\sqrt{290}}\right)^1\times\left(\frac{39}{4\sqrt{77}}\right)^1.$$
$$\times\left(\frac{3}{2\sqrt{2}}\right)^1\times\left(\frac{37}{4\sqrt{78}}\right)^1\times\left(\frac{19}{5\sqrt{13}}\right)^1\times\left(\frac{39}{2\sqrt{374}}\right)^1\times\left(\frac{13}{2\sqrt{42}}\right)^1\times\left(\frac{39}{4\sqrt{95}}\right)^1.$$

(iii) $$AG_3II(G_3)=\left(\frac{43}{2\sqrt{42}}\right)^2\times\left(\frac{22}{\sqrt{43}}\right)^9\times\left(\frac{5}{4}\right)^1\times\left(\frac{17}{8}\right)^1\times\left(\frac{21}{4\sqrt{5}}\right)^2\times\left(\frac{43}{2\sqrt{82}}\right)^6$$
$$+\left(\frac{7}{\sqrt{13}}\right)^2\times\left(\frac{19}{4\sqrt{15}}\right)^1\times\left(\frac{43}{4\sqrt{39}}\right)^1\times\left(\frac{15}{2\sqrt{26}}\right)^1\times\left(\frac{21}{\sqrt{185}}\right)^2\times\left(\frac{43}{2\sqrt{190}}\right)^1$$
$$+\left(\frac{41}{2\sqrt{210}}\right)^1\times\left(\frac{43}{2\sqrt{222}}\right)^2\times\left(\frac{43}{12\sqrt{7}}\right)^1\times\left(\frac{43}{4\sqrt{70}}\right)^2\times\left(\frac{43}{2\sqrt{330}}\right)^1\times\left(\frac{43}{8\sqrt{22}}\right)^2$$
$$+\left(\frac{7}{\sqrt{45}}\right)^1\times\left(\frac{21}{4\sqrt{26}}\right)^1\times\left(\frac{43}{24\sqrt{3}}\right)^1\times\left(\frac{43}{4\sqrt{115}}\right)^1\times\left(\frac{43}{2\sqrt{483}}\right)^2.$$

(iv) $$AG_4II(G_3)=\left(\frac{19}{6\sqrt{10}}\right)^2\times\left(\frac{21}{2\sqrt{110}}\right)^4\times\left(\frac{23}{4\sqrt{33}}\right)^4\times\left(\frac{25}{4\sqrt{39}}\right)^7\times\left(\frac{27}{2\sqrt{182}}\right)^7$$

$$\times\left(\frac{29}{2\sqrt{210}}\right)^5\times\left(\frac{31}{8\sqrt{15}}\right)^4\times\left(\frac{33}{8\sqrt{17}}\right)^4\times\left(\frac{35}{6\sqrt{34}}\right)^5.$$

(v) $$AG_5II(G_3)=\left(\frac{3}{2\sqrt{2}}\right)^2\times\left(\frac{3}{2\sqrt{2}}\right)^3\times\left(\frac{5}{\sqrt{21}}\right)^1\times\left(\frac{11}{4\sqrt{6}}\right)^1\times\left(\frac{9}{4\sqrt{5}}\right)^4\times\left(\frac{5}{2\sqrt{6}}\right)^2$$

$$\times\left(\frac{11}{4\sqrt{7}}\right)^1\times\left(\frac{13}{12}\right)^1\times\left(\frac{11}{2\sqrt{30}}\right)^6\times\left(\frac{12}{2\sqrt{35}}\right)^1\times\left(\frac{13}{4\sqrt{10}}\right)^2\times\left(\frac{7}{3\sqrt{5}}\right)^1$$

$$\times\left(\frac{13}{2\sqrt{42}}\right)^3\times\left(\frac{7}{4\sqrt{3}}\right)^1\times\left(\frac{15}{4\sqrt{14}}\right)^1\times\left(\frac{8}{3\sqrt{7}}\right)^1\times\left(\frac{17}{12\sqrt{2}}\right)^2.$$

Proof: By using the definitions and cardinalities of the bond partitions of G_3, we deduce

(i) $$AG_1II(G_3)=\prod_{uv\in E(G_3)}\frac{d(u)+d(v)}{2\sqrt{d(u)d(v)}}$$

$$=\left(\frac{1+2}{2\sqrt{1\times 2}}\right)^2\times\left(\frac{1+3}{2\sqrt{1\times 3}}\right)^5\times\left(\frac{1+4}{2\sqrt{1\times 4}}\right)^2\times\left(\frac{2+2}{2\sqrt{2\times 2}}\right)^9\times\left(\frac{2+3}{2\sqrt{2\times 3}}\right)^{14}$$

$$\times\left(\frac{2+4}{2\sqrt{2\times 4}}\right)^4\times\left(\frac{3+3}{2\sqrt{3\times 3}}\right)^6\times\left(\frac{3+4}{2\sqrt{3\times 4}}\right)^2.$$

After simplification, we get the desired result.

(ii) $$AG_2II(G_3)=\prod_{uv\in E(G_3)}\frac{n(u)+n(v)}{2\sqrt{n(u)n(v)}}$$

$$=\left(\frac{1+6}{2\sqrt{1\times 6}}\right)^1\times\left(\frac{1+34}{2\sqrt{1\times 34}}\right)^1\times\left(\frac{1+38}{2\sqrt{1\times 38}}\right)^2\times\left(\frac{1+39}{2\sqrt{1\times 39}}\right)^9\times\left(\frac{2+37}{2\sqrt{2\times 37}}\right)^8$$

$$\times\left(\frac{3+12}{2\sqrt{3\times 12}}\right)^1\times\left(\frac{3+23}{2\sqrt{3\times 23}}\right)^1\times\left(\frac{3+36}{2\sqrt{3\times 36}}\right)^2\times\left(\frac{4+32}{2\sqrt{4\times 32}}\right)^1\times\left(\frac{4+33}{2\sqrt{4\times 33}}\right)^1$$

$$\times\left(\frac{4+34}{2\sqrt{4\times 34}}\right)^1\times\left(\frac{4+35}{2\sqrt{4\times 35}}\right)^1\times\left(\frac{5+34}{2\sqrt{5\times 34}}\right)^2\times\left(\frac{6+32}{2\sqrt{6\times 32}}\right)^1\times\left(\frac{6+33}{2\sqrt{6\times 33}}\right)^2$$

$$\times\left(\frac{8+31}{2\sqrt{8\times 31}}\right)^1\times\left(\frac{9+30}{2\sqrt{9\times 30}}\right)^1\times\left(\frac{10+29}{2\sqrt{10\times 29}}\right)^1\times\left(\frac{11+28}{2\sqrt{11\times 28}}\right)^1\times\left(\frac{12+24}{2\sqrt{12\times 24}}\right)^1$$

$$\times\left(\frac{13+24}{2\sqrt{13\times 24}}\right)^1\times\left(\frac{13+25}{2\sqrt{13\times 25}}\right)^1\times\left(\frac{17+22}{2\sqrt{17\times 22}}\right)^1\times\left(\frac{18+21}{2\sqrt{18\times 21}}\right)^1\times\left(\frac{19+20}{2\sqrt{19\times 20}}\right)^1.$$

After simplification, we get the desired result.

(iii) $$AG_3II(G_3)=\prod_{uv\in E(G_3)}\frac{m(u)+m(v)}{2\sqrt{m(u)m(v)}}$$

$$=\left(\frac{1+42}{2\sqrt{1\times 42}}\right)^2\times\left(\frac{1+43}{2\sqrt{1\times 43}}\right)^9\times\left(\frac{2+8}{2\sqrt{2\times 8}}\right)^1\times\left(\frac{2+32}{2\sqrt{2\times 32}}\right)^1\times\left(\frac{2+40}{2\sqrt{2\times 40}}\right)^2$$

$$\times\left(\frac{2+41}{2\sqrt{2\times 41}}\right)^6\times\left(\frac{3+39}{2\sqrt{3\times 39}}\right)^2\times\left(\frac{4+15}{2\sqrt{4\times 15}}\right)^1\times\left(\frac{4+39}{2\sqrt{4\times 39}}\right)^1\times\left(\frac{4+26}{2\sqrt{4\times 26}}\right)^1$$

$$\times\left(\frac{5+37}{2\sqrt{5\times 37}}\right)^{2}\times\left(\frac{5+38}{2\sqrt{5\times 38}}\right)^{1}\times\left(\frac{6+35}{2\sqrt{6\times 35}}\right)^{1}\times\left(\frac{6+37}{2\sqrt{6\times 37}}\right)^{2}\times\left(\frac{7+36}{2\sqrt{7\times 36}}\right)^{1}$$
$$\times\left(\frac{8+35}{2\sqrt{8\times 35}}\right)^{2}\times\left(\frac{10+33}{2\sqrt{10\times 33}}\right)^{1}\times\left(\frac{11+32}{2\sqrt{11\times 32}}\right)^{2}\times\left(\frac{15+27}{2\sqrt{15\times 27}}\right)^{1}\times\left(\frac{16+26}{2\sqrt{16\times 26}}\right)^{1}$$
$$\times\left(\frac{16+27}{2\sqrt{16\times 27}}\right)^{1}\times\left(\frac{20+23}{2\sqrt{20\times 23}}\right)^{1}\times\left(\frac{21+22}{2\sqrt{21\times 22}}\right)^{2}.$$

After simplification, we get the desired result.

(iv) $$AG_4II(G_3)=\prod_{uv\in E(G_3)}\frac{\varepsilon(u)+\varepsilon(v)}{2\sqrt{\varepsilon(u)\varepsilon(v)}}$$
$$=\left(\frac{9+10}{2\sqrt{9\times 10}}\right)^{2}+\left(\frac{10+11}{2\sqrt{10\times 11}}\right)^{4}+\left(\frac{11+12}{2\sqrt{11\times 12}}\right)^{4}+\left(\frac{12+13}{2\sqrt{12\times 13}}\right)^{7}+\left(\frac{13+13}{2\sqrt{13\times 13}}\right)^{1}$$
$$+\left(\frac{13+14}{2\sqrt{13\times 14}}\right)^{7}+\left(\frac{14+15}{2\sqrt{14\times 15}}\right)^{5}+\left(\frac{15+16}{2\sqrt{15\times 16}}\right)^{4}+\left(\frac{16+16}{2\sqrt{16\times 16}}\right)^{1}+\left(\frac{16+17}{2\sqrt{16\times 17}}\right)^{4}$$
$$+\left(\frac{17+18}{2\sqrt{17\times 18}}\right)^{5}.$$

After simplification, we get the desired result.

(v) $$AG_5II(G_3)=\prod_{uv\in E(G_3)}\frac{s(u)+s(v)}{2\sqrt{s(u)s(v)}}$$
$$=\left(\frac{2+4}{2\sqrt{2\times 4}}\right)^{2}+\left(\frac{3+6}{2\sqrt{3\times 6}}\right)^{3}+\left(\frac{3+7}{2\sqrt{3\times 7}}\right)^{1}+\left(\frac{3+8}{2\sqrt{3\times 8}}\right)^{1}+\left(\frac{4+4}{2\sqrt{4\times 4}}\right)^{2}$$
$$+\left(\frac{4+5}{2\sqrt{4\times 5}}\right)^{4}+\left(\frac{4+6}{2\sqrt{4\times 6}}\right)^{2}+\left(\frac{4+7}{2\sqrt{4\times 7}}\right)^{1}+\left(\frac{4+9}{2\sqrt{4\times 9}}\right)^{1}+\left(\frac{5+5}{2\sqrt{5\times 5}}\right)^{2}$$
$$+\left(\frac{5+6}{2\sqrt{5\times 6}}\right)^{6}+\left(\frac{5+7}{2\sqrt{5\times 7}}\right)^{1}+\left(\frac{5+8}{2\sqrt{5\times 8}}\right)^{2}+\left(\frac{5+9}{2\sqrt{5\times 9}}\right)^{1}+\left(\frac{6+6}{2\sqrt{6\times 6}}\right)^{1}$$
$$+\left(\frac{6+7}{2\sqrt{6\times 7}}\right)^{3}+\left(\frac{6+8}{2\sqrt{6\times 8}}\right)^{1}+\left(\frac{7+7}{2\sqrt{7\times 7}}\right)^{4}+\left(\frac{7+8}{2\sqrt{7\times 8}}\right)^{1}+\left(\frac{7+9}{2\sqrt{7\times 9}}\right)^{1}$$
$$+\left(\frac{8+8}{2\sqrt{8\times 8}}\right)^{1}+\left(\frac{8+9}{2\sqrt{8\times 9}}\right)^{2}+\left(\frac{9+9}{2\sqrt{9\times 9}}\right)^{1}.$$

After simplification, we get the desired result.

5. CONCLUSION

In this paper, we have computed the first, second, third, fourth and fifth multiplicative arithmetic-geometric indices of some important chemical drugs which appeared in medical science.

REFERENCES

[1] V.R.Kulli, *College Graph Theory*, Vishwa International Publications, Gulbarga, India (2012).
[2] V.R.Kulli, A new multiplicative arithmetic-geometric index, *Journal of Fuzzy Mathematical Archive,* 12(2) (2017) 49-53.

[3] W.Gao, Y. Wang and W. Wang, and Li Shi, The first multiplication atom bond connectivity index of molecular structures in drugs, *Saudi Pharmaceutical Journal*, (2017), http://dx.doi.org/10.1016/j.jsps.2017.04.021.
[4] V.R.Kulli, Multiplicative connectivity KV indices of dendrimers, *Journal of Mathematics and Informatics*, 15(2019) 1-7.
[5] V.R.Kulli, Multiplicative Gourava indices of armchair and zigzag polyhax nanotube, *Journal of Mathematics and Informatics*, 17(2019) 107-112
[6] V.R.Kulli, Computation of Multiplicative (a, b)-status index of certain graphs, *Journal of Mathematics and Informatics*, 18(2020) 50-55.
[7] V.R.Kulli, Computation of multiplicative Banhatti-Sombor indices of certain benzenoid systems, *International Journal of Mathematical Archive,* 12(4) (2021) 24-30.
[8] V.R.Kulli, On multiplicative inverse Nirmala indices, *Annals of Pure and Applied Mathematics*, 23(2) (2021) 57-61.
[9] V.R.Kulli, Computation of Multiplicative minus F-indices of titania nanotubes, *Journal of Mathematics and Informatics*, 18(2020) 135-140.
[10] V.R.Kulli, Multiplicative Sombor indices of certain nanotubes, *International Journal of Mathematical Archive,* 12(3) (2021) 1-5.
[11] V.R.Kulli, New multiplicative arithmetic-geometric indices, *Journal of Ultra Scientist of Physical Sciences*, A, 29(6) (2017) 205-211.
[12] M.Ghorbaniand M.A.Hosseinzadeh, A new version of Zagreb indices, *Filomat* 26(1) (2012) 93-100.
[13] A.Graovac and M.Ghorbani, A new version of atom bond connectivity index, *Acta Cimica Slovenica,* 57(2) (2010) 609-612.
[14] V.R.Kulli, Two new multiplicative atom bond connectivity indices, *Annals of Pure and Applied Mathematics*, 13(1) (2017) 1-7.
[15] V.R.Kulli, Some new multiplicative geometric-arithmetic indices, *Journal of Ultra Scientist of Physical Sciences*, A, 29(2) (2017) 52-57.
[16] V.R.Kulli, New arithmetic-geometric indices, *Annals of Pure and Applied Mathematics*, 13(2) (2017) 165-172.
[17] B.Chaluvaraju and A.B.Shaikh, Different versions of atom bond connectivity indices of some molecular structures: Applied for the treatment and prevention of COVID-19, *Polycyclic Aromatic Compounds,* DOI: 10.1080/10406638.2021.1872655.
[18] V.R.Kulli, Revan indices of chloroquine, hydroxychloroquine, remdesivir: Research Advances for the treatment of COVOD-19, *International Journal of Engineering Sciences and research technology,* 9(5) (2020) 73-84.