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SOME NEW VERSIONS OF MULTIPLICATIVE GEOMETRIC-ARITHMETIC INDEX OF CERTAIN CHEMICAL DRUGS

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ABSTRACT

A topological index is a numeric quantity from structural graph of a molecule. The methods of topological index computation can help to find out chemical information of drugs in Chemical Science. In this paper, we compute the first, second, third, fourth and fifth multiplicative geometric-arithmetic indices of some important chemical drugs such as chloroquine, hydroxychloroquine and remdesivir.

Keywords: *multiplicative geometric-arithmetic index, chemical drug.*

Mathematics Subject Classification: *05C05, 05C07, 05C35.*

1. INTRODUCTION

We consider only finite, simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d(u)$ of a vertex u is the number of vertices adjacent to u. For undefined term and notation, we refer the book [1].

A molecular graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. Chemical Graph Theory is a branch of Mathematical Chemistry, which has an important affect on the development of the Chemical Sciences. Topological indices are useful for establishing correlation between the structure of a molecular compound and its physicochemical properties. Several topological indices [2] have been considered in Theoretical Chemistry and have found some applications, especially in QSPR/QSAR study, see [3, 4].

In [5], Kulli introduced the first multiplicative geometric-arithmetic index of a graph G and it is defined as

$$GA_1II(G) = \prod_{uv\in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}.$$

Recently, many other multiplicative indices were studied, for example, in [6, 7, 8, 9, 10, 11, 12, 13, 14].

The second, third, fourth and fifth multiplicative geometric-arithmetic indices of a graph were introduced by Kulli in [15] as follows:

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

$$GA_2II(G) = \prod_{uv\in E(G)} \frac{2\sqrt{n(u)n(v)}}{n(u)+n(v)}$$

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 geometric-arithmetic index of a graph G is defined as

$$GA_3II(G) = \prod_{uv\in E(G)} \frac{2\sqrt{m(u)m(v)}}{m(u)+m(v)}$$

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.

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

$$GA_4II(G) = \prod_{uv \in E(G)} \frac{2\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)}$$

where the number $\varepsilon(u)$ is the eccentricity of all vertices adjacent to a vertex u.

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

$$GA_5II(G) = \prod_{uv \in E(G_1)} \frac{2\sqrt{s(u)s(v)}}{s(u)+s(v)}$$

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 [16, 17, 18, 19, 20].

In this paper; we determine the first, second, third, fourth and fifth multiplicative geometric-arithmetic indices of chloroquine, hydroxychloroquine, remdesivir. For chemical structures, see [21, 22].

2. RESULTS FOR 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.

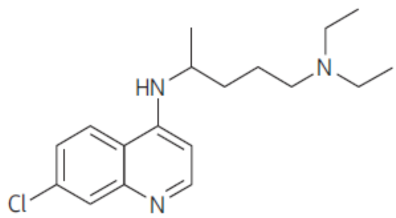

Figure-1: Chemical structure of chloroquine

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.

Table-1: Bond set partitions 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)
	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				
$s(u), s(v) \setminus uv \in E(G_1)$	(2,4)	(3,5)	(4,5)	(4,6)	(5,5)	
Number of bonds	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 geometric-arithmetic indices of chloroquine.

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

(i) $GA_1II(G_1)=\left(\frac{2\sqrt{2}}{3}\right)^2\times\left(\frac{\sqrt{3}}{2}\right)^2\times\left(\frac{2\sqrt{6}}{5}\right)^{12}.$

(ii) $GA_2II(G_1)=\left(\frac{\sqrt{19}}{10}\right)^2\times\left(\frac{4\sqrt{5}}{21}\right)^4\times\left(\frac{\sqrt{51}}{10}\right)^4\times\left(\frac{\sqrt{3}}{2}\right)^4\times\left(\frac{\sqrt{21}}{5}\right)^1\times\left(\frac{\sqrt{91}}{10}\right)^3\times\left(\frac{3\sqrt{11}}{10}\right)^1\times\left(\frac{36}{125}\right)^1.$

(iii) $GA_3II(G_1)=\left(\frac{\sqrt{21}}{11}\right)^2\times\left(\frac{2\sqrt{22}}{23}\right)^4\times\left(\frac{2\sqrt{38}}{21}\right)^2\times\left(\frac{2\sqrt{6}}{7}\right)^4\times\left(\frac{4\sqrt{17}}{21}\right)^1\times\left(\frac{\sqrt{3}}{2}\right)^3$

$\times\left(\frac{8\sqrt{5}}{21}\right)^1\times\left(\frac{2\sqrt{10}}{7}\right)^1\times\left(\frac{2\sqrt{2}}{3}\right)^2\times\left(\frac{4\sqrt{26}}{21}\right)^1\times\left(\frac{3\sqrt{13}}{11}\right)^1\times\left(\frac{2\sqrt{30}}{11}\right)^1.$

$(iv) GA_4II(G_1)=\left(\frac{4\sqrt{14}}{15}\right)^3\times\left(\frac{12\sqrt{2}}{17}\right)^3\times\left(\frac{6\sqrt{10}}{19}\right)^4\times\left(\frac{2\sqrt{110}}{21}\right)^5\times\left(\frac{4\sqrt{33}}{23}\right)^4\times\left(\frac{4\sqrt{39}}{25}\right)^3.$

(v) $GA_5II(G_1)=\left(\frac{2\sqrt{2}}{3}\right)^2\times\left(\frac{\sqrt{15}}{4}\right)^2\times\left(\frac{4\sqrt{5}}{9}\right)^4\times\left(\frac{2\sqrt{6}}{5}\right)^2\times\left(\frac{2\sqrt{30}}{11}\right)^3$

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

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

(i) $GA_1II(G_1)=\prod_{uv\in E(G_1)}\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$

$=\left(\frac{2\sqrt{1\times2}}{1+2}\right)^2\times\left(\frac{2\sqrt{1\times3}}{1+3}\right)^2\times\left(\frac{2\sqrt{2\times2}}{2+2}\right)^5\times\left(\frac{2\sqrt{2\times3}}{2+3}\right)^{12}\times\left(\frac{2\sqrt{3\times3}}{3+3}\right)^2.$

After simplification, we obtain the desired result.

(ii) $GA_2II(G_1)=\prod_{uv\in E(G_1)}\frac{2\sqrt{n(u)n(v)}}{n(u)+n(v)}$

$=\left(\frac{2\sqrt{1\times19}}{1+19}\right)^2\times\left(\frac{2\sqrt{1\times20}}{1+20}\right)^4\times\left(\frac{2\sqrt{2\times18}}{2+18}\right)^2\times\left(\frac{2\sqrt{3\times17}}{3+17}\right)^4\times\left(\frac{2\sqrt{4\times16}}{4+16}\right)^1$

$\times\left(\frac{2\sqrt{5\times15}}{5+15}\right)^4\times\left(\frac{2\sqrt{6\times14}}{6+14}\right)^1\times\left(\frac{2\sqrt{7\times13}}{7+13}\right)^3\times\left(\frac{2\sqrt{9\times11}}{9+11}\right)^1\times\left(\frac{2\sqrt{10\times10}}{10+10}\right)^1.$

After simplification, we obtain the desired result.

(iii) $GA_3II(G_1)=\prod_{uv\in E(G_1)}\frac{2\sqrt{m(u)m(v)}}{m(u)+m(v)}$

$=\left(\frac{2\sqrt{1\times21}}{1+21}\right)^2\times\left(\frac{2\sqrt{1\times22}}{1+22}\right)^4\times\left(\frac{2\sqrt{2\times19}}{2+19}\right)^2\times\left(\frac{2\sqrt{3\times18}}{3+18}\right)^4\times\left(\frac{2\sqrt{4\times17}}{4+17}\right)^1\times\left(\frac{2\sqrt{5\times15}}{5+15}\right)^3$

$\times\left(\frac{2\sqrt{5\times16}}{5+16}\right)^1\times\left(\frac{2\sqrt{6\times15}}{6+15}\right)^1\times\left(\frac{2\sqrt{7\times14}}{7+14}\right)^2\times\left(\frac{2\sqrt{8\times13}}{8+13}\right)^1\times\left(\frac{2\sqrt{9\times13}}{9+13}\right)^1\times\left(\frac{2\sqrt{10\times12}}{10+12}\right)^1.$

After simplification, we obtain the desired result.

(iv) $$GA_4II(G_1) = \prod_{uv \in E(G_1)} \frac{2\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)}$$

$$= \left(\frac{2\sqrt{7\times 7}}{7+7}\right)^1 \times \left(\frac{2\sqrt{8\times 7}}{8+7}\right)^3 \times \left(\frac{2\sqrt{8\times 9}}{8+9}\right)^3 \times \left(\frac{2\sqrt{9\times 10}}{9+10}\right)^4 \times \left(\frac{2\sqrt{10\times 11}}{10+11}\right)^5$$

$$\times \left(\frac{2\sqrt{11\times 12}}{11+12}\right)^4 \times \left(\frac{2\sqrt{12\times 13}}{12+13}\right)^3.$$

After simplification, we obtain the desired result.

(v) $$GA_5II(G_1) = \prod_{uv \in E(G_1)} \frac{2\sqrt{s(u)s(v)}}{s(u)+s(v)}$$

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

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

After simplification, we obtain the desired result.

3. RESULTS FOR HYDROXYCHLOROQUINE

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

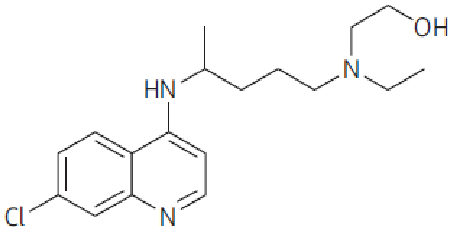

Figure-2: Chemical structure of hydroxychloroquine

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 partitions.

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 geometric-arithmetic indices of hydroxychloroquine.

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

(i) $GA_1II(G_2)=\left(\frac{2\sqrt{2}}{3}\right)^2\times\left(\frac{\sqrt{3}}{2}\right)^2\times\left(\frac{2\sqrt{6}}{5}\right)^{12}.$

(ii) $$GA_2II\left(G_2\right)=\left(\frac{4\sqrt{5}}{21}\right)^2\times\left(\frac{\sqrt{21}}{11}\right)^4\times\left(\frac{2\sqrt{38}}{21}\right)^3\times\left(\frac{2\sqrt{6}}{7}\right)^4\times\left(\frac{8\sqrt{5}}{21}\right)^4$$
$$\times\left(\frac{2\sqrt{10}}{7}\right)^3\times\left(\frac{2\sqrt{2}}{3}\right)^2\times\left(\frac{2\sqrt{110}}{21}\right)^1\times\left(\frac{4\sqrt{26}}{21}\right)^1.$$

(iii) $$GA_3II\left(G_2\right)=\left(\frac{2\sqrt{22}}{23}\right)^2\times\left(\frac{\sqrt{23}}{12}\right)^4\times\left(\frac{2\sqrt{10}}{11}\right)^2\times\left(\frac{2\sqrt{42}}{23}\right)^1\times\left(\frac{\sqrt{57}}{11}\right)^1\times\left(\frac{8\sqrt{5}}{21}\right)^3$$
$$+\left(\frac{\sqrt{85}}{11}\right)^1\times\left(\frac{4\sqrt{6}}{11}\right)^1\times\left(\frac{\sqrt{105}}{11}\right)^1\times\left(\frac{4\sqrt{7}}{11}\right)^3\times\left(\frac{2\sqrt{130}}{23}\right)^1\times\left(\frac{2\sqrt{132}}{23}\right)^1.$$

(iv) $$GA_4II\left(G_2\right)=\left(\frac{4\sqrt{14}}{15}\right)^3\times\left(\frac{12\sqrt{2}}{17}\right)^2\times\left(\frac{6\sqrt{10}}{19}\right)^3\times\left(\frac{2\sqrt{110}}{21}\right)^4\times\left(\frac{4\sqrt{33}}{23}\right)^6$$
$$\times\left(\frac{4\sqrt{39}}{25}\right)^4\times\left(\frac{4\sqrt{182}}{27}\right)^2.$$

(v) $$GA_5II\left(G_2\right)=\left(\frac{2\sqrt{6}}{5}\right)^1\times\left(\frac{2\sqrt{2}}{3}\right)^1\times\left(\frac{\sqrt{15}}{4}\right)^3\times\left(\frac{4\sqrt{5}}{9}\right)^4\times\left(\frac{2\sqrt{6}}{5}\right)^1\times\left(\frac{2\sqrt{30}}{11}\right)^4$$
$$\times\left(\frac{\sqrt{35}}{6}\right)^2\times\left(\frac{4\sqrt{10}}{13}\right)^1\times\left(\frac{2\sqrt{42}}{13}\right)^2\times\left(\frac{4\sqrt{14}}{15}\right)^2.$$

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

(i) $$GA_1II\left(G_2\right)=\prod_{uv\in E\left(G_2\right)}\frac{2\sqrt{d\left(u\right)d\left(v\right)}}{d\left(u\right)+d\left(v\right)}$$
$$=\left(\frac{2\sqrt{1\times 2}}{1+2}\right)^2\times\left(\frac{2\sqrt{1\times 3}}{1+3}\right)^2\times\left(\frac{2\sqrt{2\times 2}}{2+2}\right)^6\times\left(\frac{2\sqrt{2\times 3}}{2+3}\right)^{12}\times\left(\frac{2\sqrt{3\times 3}}{3+3}\right)^2.$$

After simplification, we obtain the desired result.

(ii) $$GA_2II\left(G_2\right)=\prod_{uv\in E\left(G_2\right)}\frac{2\sqrt{n(u)n(v)}}{n(u)+n(v)}$$
$$=\left(\frac{2\sqrt{1\times 20}}{1+20}\right)^2\times\left(\frac{2\sqrt{1\times 21}}{1+21}\right)^4\times\left(\frac{2\sqrt{2\times 19}}{2+19}\right)^3\times\left(\frac{2\sqrt{3\times 18}}{3+18}\right)^4\times\left(\frac{2\sqrt{5\times 16}}{5+16}\right)^1$$
$$\times\left(\frac{2\sqrt{6\times 15}}{6+15}\right)^3\times\left(\frac{2\sqrt{7\times 14}}{7+14}\right)^2\times\left(\frac{2\sqrt{10\times 11}}{10+11}\right)^1\times\left(\frac{2\sqrt{8\times 13}}{8+13}\right)^1.$$

After simplification, we obtain the desired result.

(iii) $$GA_3II(G_2)=\prod_{uv\in E(G_2)}\frac{2\sqrt{m(u)m(v)}}{m(u)+m(v)}$$

$$=\left(\frac{2\sqrt{1\times 22}}{1+22}\right)^2\times\left(\frac{2\sqrt{1\times 23}}{1+23}\right)^4\times\left(\frac{2\sqrt{2\times 20}}{2+20}\right)^2\times\left(\frac{2\sqrt{2\times 21}}{2+21}\right)^1\times\left(\frac{2\sqrt{3\times 19}}{3+19}\right)^4$$
$$\times\left(\frac{2\sqrt{5\times 17}}{5+17}\right)^1\times\left(\frac{2\sqrt{6\times 16}}{6+16}\right)^1\times\left(\frac{2\sqrt{7\times 15}}{7+15}\right)^1\times\left(\frac{2\sqrt{8\times 14}}{8+14}\right)^3\times\left(\frac{2\sqrt{10\times 13}}{10+13}\right)^1$$
$$\times\left(\frac{2\sqrt{11\times 12}}{11+12}\right)^1.$$

After simplification, we obtain the desired result.

(iv) $$GA_4II(G_2)=\prod_{uv\in E(G_2)}\frac{2\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)}$$

$$=\left(\frac{2\sqrt{7\times 8}}{7+8}\right)^3\times\left(\frac{2\sqrt{8\times 9}}{8+9}\right)^2\times\left(\frac{2\sqrt{9\times 10}}{9+10}\right)^3\times\left(\frac{2\sqrt{10\times 11}}{10+11}\right)^4\times\left(\frac{2\sqrt{11\times 12}}{11+12}\right)^6$$
$$\times\left(\frac{2\sqrt{12\times 13}}{12+13}\right)^4\times\left(\frac{2\sqrt{13\times 14}}{13+14}\right)^2.$$

After simplification, we obtain the desired result.

(iv) $$GA_5II(G_2)=\prod_{uv\in E(G_2)}\frac{2\sqrt{s(u)s(v)}}{s(u)+s(v)}$$

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

After simplification, we get the desired result.

3. RESULTS FOR REMDESIVIR

Let G_3 be the molecular graph of remdesivir. This graph has 41 vertices and 44 edges.

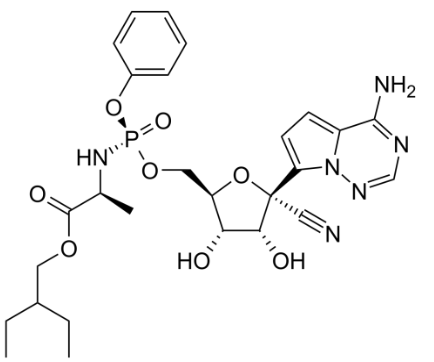

Figure-3: Chemical structure of remdesivir

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

$d(u), d(v)\backslash uv\in E(G_3)$	(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
$n(u), n(v)\backslash uv\in E(G_3)$	(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 geometric-arithmetic indices of remdesivir.

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

(i) $$GA_1II(G_3)=\left(\frac{2\sqrt{2}}{3}\right)^{2}\times\left(\frac{\sqrt{3}}{2}\right)^{5}\times\left(\frac{4}{5}\right)^{2}.\times\left(\frac{2\sqrt{6}}{5}\right)^{14}\times\left(\frac{2\sqrt{2}}{3}\right)^{4}\times\left(\frac{4\sqrt{3}}{7}\right)^{2}.$$

(ii) $$\begin{aligned}GA_2II(G_3)=&\left(\frac{2\sqrt{6}}{7}\right)^{1}\times\left(\frac{2\sqrt{34}}{35}\right)^{1}\times\left(\frac{2\sqrt{38}}{39}\right)^{2}\times\left(\frac{\sqrt{39}}{20}\right)^{9}\times\left(\frac{2\sqrt{74}}{39}\right)^{8}\times\left(\frac{4}{5}\right)^{1}\times\left(\frac{\sqrt{69}}{13}\right)^{1}\\&\times\left(\frac{4\sqrt{3}}{13}\right)^{2}\times\left(\frac{4\sqrt{2}}{9}\right)^{1}\times\left(\frac{4\sqrt{33}}{37}\right)^{1}\times\left(\frac{2\sqrt{34}}{19}\right)^{1}\times\left(\frac{4\sqrt{35}}{39}\right)^{1}\times\left(\frac{2\sqrt{170}}{39}\right)^{2}\\&\times\left(\frac{8\sqrt{3}}{19}\right)^{1}\times\left(\frac{2\sqrt{22}}{13}\right)^{2}\times\left(\frac{4\sqrt{62}}{39}\right)^{1}\times\left(\frac{2\sqrt{30}}{13}\right)^{1}\times\left(\frac{2\sqrt{290}}{39}\right)^{1}\times\left(\frac{4\sqrt{77}}{39}\right)^{1}\\&\times\left(\frac{2\sqrt{2}}{3}\right)^{1}\times\left(\frac{4\sqrt{78}}{37}\right)^{1}\times\left(\frac{5\sqrt{13}}{19}\right)^{1}\times\left(\frac{2\sqrt{374}}{39}\right)^{1}\times\left(\frac{2\sqrt{42}}{13}\right)^{1}\times\left(\frac{4\sqrt{95}}{39}\right)^{1}.\end{aligned}$$

(iii) $$\begin{aligned}GA_3II(G_3)=&\left(\frac{2\sqrt{42}}{43}\right)^{2}\times\left(\frac{\sqrt{43}}{22}\right)^{9}\times\left(\frac{4}{5}\right)^{1}\times\left(\frac{8}{17}\right)^{1}\times\left(\frac{4\sqrt{5}}{21}\right)^{2}\times\left(\frac{2\sqrt{82}}{43}\right)^{6}\\&+\left(\frac{\sqrt{13}}{7}\right)^{2}\times\left(\frac{4\sqrt{15}}{19}\right)^{1}\times\left(\frac{4\sqrt{39}}{43}\right)^{1}\times\left(\frac{2\sqrt{26}}{15}\right)^{1}\times\left(\frac{\sqrt{185}}{21}\right)^{2}\times\left(\frac{2\sqrt{190}}{43}\right)^{1}\\&+\left(\frac{2\sqrt{210}}{41}\right)^{1}\times\left(\frac{2\sqrt{222}}{43}\right)^{2}\times\left(\frac{12\sqrt{7}}{43}\right)^{1}\times\left(\frac{4\sqrt{70}}{43}\right)^{2}\times\left(\frac{2\sqrt{330}}{43}\right)^{1}\times\left(\frac{8\sqrt{22}}{43}\right)^{2}\\&+\left(\frac{3\sqrt{5}}{7}\right)^{1}\times\left(\frac{4\sqrt{26}}{21}\right)^{1}\times\left(\frac{24\sqrt{3}}{43}\right)^{1}\times\left(\frac{4\sqrt{115}}{43}\right)^{1}\times\left(\frac{2\sqrt{483}}{43}\right)^{2}.\end{aligned}$$

(iv) $$GA_4II(G_3)=\left(\frac{6\sqrt{10}}{19}\right)^2\times\left(\frac{2\sqrt{110}}{21}\right)^4\times\left(\frac{4\sqrt{33}}{23}\right)^4\times\left(\frac{4\sqrt{39}}{25}\right)^7\times\left(\frac{2\sqrt{182}}{27}\right)^7$$
$$\times\left(\frac{2\sqrt{210}}{29}\right)^5\times\left(\frac{8\sqrt{15}}{31}\right)^4\times\left(\frac{8\sqrt{17}}{33}\right)^4\times\left(\frac{6\sqrt{34}}{35}\right)^5.$$

(v) $$GA_5II(G_3)=\left(\frac{2\sqrt{2}}{3}\right)^2\times\left(\frac{2\sqrt{2}}{3}\right)^3\times\left(\frac{\sqrt{21}}{\sqrt{21}}\right)^1\times\left(\frac{4\sqrt{6}}{11}\right)^1\times\left(\frac{4\sqrt{5}}{9}\right)^4\times\left(\frac{2\sqrt{6}}{5}\right)^2$$
$$\times\left(\frac{4\sqrt{7}}{11}\right)^1\times\left(\frac{12}{13}\right)^1\times\left(\frac{2\sqrt{30}}{11}\right)^6\times\left(\frac{2\sqrt{35}}{12}\right)^1\times\left(\frac{4\sqrt{10}}{13}\right)^2\times\left(\frac{3\sqrt{5}}{7}\right)^1$$
$$\times\left(\frac{2\sqrt{42}}{13}\right)^3\times\left(\frac{4\sqrt{3}}{7}\right)^1\times\left(\frac{4\sqrt{14}}{15}\right)^1\times\left(\frac{3\sqrt{7}}{8}\right)^1\times\left(\frac{12\sqrt{2}}{17}\right)^2.$$

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

(i) $$GA_1II(G_3)=\prod_{uv\in E(G_3)}\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$$
$$=\left(\frac{2\sqrt{1\times2}}{1+2}\right)^2\times\left(\frac{2\sqrt{1\times3}}{1+3}\right)^5\times\left(\frac{2\sqrt{1\times4}}{1+4}\right)^2\times\left(\frac{2\sqrt{2\times2}}{2+2}\right)^9\times\left(\frac{2\sqrt{2\times3}}{2+3}\right)^{14}$$
$$\times\left(\frac{2\sqrt{2\times4}}{2+4}\right)^4\times\left(\frac{2\sqrt{3\times3}}{3+3}\right)^6\times\left(\frac{2\sqrt{3\times4}}{3+4}\right)^2.$$

After simplification, we get the desired result.

(ii) $$GA_2II(G_3)=\prod_{uv\in E(G_3)}\frac{2\sqrt{n(u)n(v)}}{n(u)+n(v)}$$
$$=\left(\frac{2\sqrt{1\times6}}{1+6}\right)^1\times\left(\frac{2\sqrt{1\times34}}{1+34}\right)^1\times\left(\frac{2\sqrt{1\times38}}{1+38}\right)^2\times\left(\frac{2\sqrt{1\times39}}{1+39}\right)^9\times\left(\frac{2\sqrt{2\times37}}{2+37}\right)^8$$
$$\times\left(\frac{2\sqrt{3\times12}}{3+12}\right)^1\times\left(\frac{2\sqrt{3\times23}}{3+23}\right)^1\times\left(\frac{2\sqrt{3\times36}}{3+36}\right)^2\times\left(\frac{2\sqrt{4\times32}}{4+32}\right)^1\times\left(\frac{2\sqrt{4\times33}}{4+33}\right)^1$$
$$\times\left(\frac{2\sqrt{4\times34}}{4+34}\right)^1\times\left(\frac{2\sqrt{4\times35}}{4+35}\right)^1\times\left(\frac{2\sqrt{5\times34}}{5+34}\right)^2\times\left(\frac{2\sqrt{6\times32}}{6+32}\right)^1\times\left(\frac{2\sqrt{6\times33}}{6+33}\right)^2$$
$$\times\left(\frac{2\sqrt{8\times31}}{8+31}\right)^1\times\left(\frac{2\sqrt{9\times30}}{9+30}\right)^1\times\left(\frac{2\sqrt{10\times29}}{10+29}\right)^1\times\left(\frac{2\sqrt{11\times28}}{11+28}\right)^1\times\left(\frac{2\sqrt{12\times24}}{12+24}\right)^1$$
$$\times\left(\frac{2\sqrt{13\times24}}{13+24}\right)^1\times\left(\frac{2\sqrt{13\times25}}{13+25}\right)^1\times\left(\frac{2\sqrt{17\times22}}{17+22}\right)^1\times\left(\frac{2\sqrt{18\times21}}{18+21}\right)^1\times\left(\frac{2\sqrt{19\times20}}{19+20}\right)^1.$$

After simplification, we get the desired result.

(iii) $$GA_3II(G_3)=\prod_{uv\in E(G_3)}\frac{2\sqrt{m(u)m(v)}}{m(u)+m(v)}$$
$$=\left(\frac{2\sqrt{1\times42}}{1+42}\right)^2\times\left(\frac{2\sqrt{1\times43}}{1+43}\right)^9\times\left(\frac{2\sqrt{2\times8}}{2+8}\right)^1\times\left(\frac{2\sqrt{2\times32}}{2+32}\right)^1\times\left(\frac{2\sqrt{2\times40}}{2+40}\right)^2$$
$$\times\left(\frac{2\sqrt{2\times41}}{2+41}\right)^6\times\left(\frac{2\sqrt{3\times39}}{3+39}\right)^2\times\left(\frac{2\sqrt{4\times15}}{4+15}\right)^1\times\left(\frac{2\sqrt{4\times39}}{4+39}\right)^1\times\left(\frac{2\sqrt{4\times26}}{4+26}\right)^1$$

$$\times\left(\frac{2\sqrt{5\times37}}{5+37}\right)^{2}\times\left(\frac{2\sqrt{5\times38}}{5+38}\right)^{1}\times\left(\frac{2\sqrt{6\times35}}{6+35}\right)^{1}\times\left(\frac{2\sqrt{6\times37}}{6+37}\right)^{2}\times\left(\frac{2\sqrt{7\times36}}{7+36}\right)^{1}$$

$$\times\left(\frac{2\sqrt{8\times35}}{8+35}\right)^{2}\times\left(\frac{12\sqrt{10\times33}}{10+33}\right)^{1}\times\left(\frac{2\sqrt{11\times32}}{11+32}\right)^{2}\times\left(\frac{2\sqrt{15\times27}}{15+27}\right)^{1}\times\left(\frac{2\sqrt{16\times26}}{16+26}\right)^{1}$$

$$\times\left(\frac{2\sqrt{16\times27}}{16+27}\right)^{1}\times\left(\frac{2\sqrt{20\times23}}{20+23}\right)^{1}\times\left(\frac{2\sqrt{21\times22}}{21+22}\right)^{2}.$$

After simplification, we get the desired result.

(iv) $GA_4II(G_3)=\prod_{uv\in E(G_3)}\frac{2\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)}$

$$=\left(\frac{2\sqrt{9\times10}}{9+10}\right)^{2}\times\left(\frac{2\sqrt{10\times11}}{10+11}\right)^{4}\times\left(\frac{2\sqrt{11\times12}}{11+12}\right)^{4}\times\left(\frac{2\sqrt{12\times13}}{12+13}\right)^{7}\times\left(\frac{2\sqrt{13\times13}}{13+13}\right)^{1}$$

$$\times\left(\frac{2\sqrt{13\times14}}{13+14}\right)^{7}\times\left(\frac{2\sqrt{14\times15}}{14+15}\right)^{5}\times\left(\frac{2\sqrt{15\times16}}{15+16}\right)^{4}\times\left(\frac{2\sqrt{16\times16}}{16+16}\right)^{1}\times\left(\frac{2\sqrt{16\times17}}{16+17}\right)^{4}$$

$$\times\left(\frac{2\sqrt{17\times18}}{17+18}\right)^{5}.$$

After simplification, we get the desired result.

(v) $GA_5II(G_3)=\prod_{uv\in E(G_3)}\frac{2\sqrt{s(u)s(v)}}{s(u)+s(v)}$

$$=\left(\frac{2\sqrt{2\times4}}{2+4}\right)^{2}\times\left(\frac{2\sqrt{3\times6}}{3+6}\right)^{3}\times\left(\frac{2\sqrt{3\times7}}{3+7}\right)^{1}\times\left(\frac{2\sqrt{3\times8}}{3+8}\right)^{1}\times\left(\frac{2\sqrt{4\times4}}{4+4}\right)^{2}$$

$$\times\left(\frac{2\sqrt{4\times5}}{4+5}\right)^{4}\times\left(\frac{2\sqrt{4\times6}}{4+6}\right)^{2}\times\left(\frac{2\sqrt{4\times7}}{4+7}\right)^{1}\times\left(\frac{2\sqrt{4\times9}}{4+9}\right)^{1}\times\left(\frac{2\sqrt{5\times5}}{5+5}\right)^{2}$$

$$\times\left(\frac{2\sqrt{5\times6}}{5+6}\right)^{6}\times\left(\frac{2\sqrt{5\times7}}{5+7}\right)^{1}\times\left(\frac{2\sqrt{5\times8}}{5+8}\right)^{2}\times\left(\frac{2\sqrt{5\times9}}{5+9}\right)^{1}\times\left(\frac{2\sqrt{6\times6}}{6+6}\right)^{1}$$

$$\times\left(\frac{2\sqrt{6\times7}}{6+7}\right)^{3}\times\left(\frac{2\sqrt{6\times8}}{6+8}\right)^{1}\times\left(\frac{2\sqrt{7\times7}}{7+7}\right)^{4}\times\left(\frac{2\sqrt{7\times8}}{7+8}\right)^{1}\times\left(\frac{2\sqrt{7\times9}}{7+9}\right)^{1}$$

$$\times\left(\frac{2\sqrt{8\times8}}{8+8}\right)^{1}\times\left(\frac{2\sqrt{8\times9}}{8+9}\right)^{2}\times\left(\frac{2\sqrt{9\times9}}{9+9}\right)^{1}.$$

After simplification, we get the desired result.

4. CONCLUSION

In this study, we have computed the first, second, third, fourth and fifth multiplicative geometric-arithmetic indices of some important chemical structures.

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