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DIFFERRENT VERSIONS OF SUM AUGMENTED BANHATTI INDEX OF CERTAIN CHEMICAL STRUCTURES

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ABSTRACT

A novel degree based topological index was introduced, the so called sum augmented Banhatti index. We introduce the second, third, fourth and neighborhood sum augmented Banhatti indices of a graph. Also we compute the sum augmented Banhatti index, second, third, fourth and neighborhood sum augmented Banhatti indices for some important chemical structures such as chloroquine, hydroxychloroquine and remdesivir.

Keywords: *sum augmented Banhatti index, second, third, fourth and neighborhood sum augmented Banhatti indices, chemical structure.*

Mathematics Subject Classification: *05C05, 05C07, 05C09, 05C92.*

1. INTRODUCTION

Let G be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. Let $d(u)$ be the degree of a vertex u in a graph G. For undefined terms and notations, we refer [1].

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

Furtula *et al.* [5] defined the augmented Zagreb index as

$$AZI(G)=\sum_{uv\in E(G)}\left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^3.$$

This topological index has proved to a valuable predictive index in the study of the heat formation in octanes and heptanes, whose prediction power is better than atom bond connectivity index, see [5].

Recently, some augmented Zagreb indices were studied, for example, in [6, 7, 8, 9, 10, 11].

The sum augmented index [12] of a graph G is

$$SAI(G)=\sum_{uv\in E(G)}\left(\frac{d(u)+d(v)}{d(u)+d(v)-2}\right)^3.$$

Now we call this index as sum augmented Banhatti index and it is denoted by $SABI(G)$.

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We now introduce the second, third, fourth and neighborhood sum augmented Banhatti indices of a graph as follows:

The second sum augmented Banhatti index of a graph G is defined as

$$SABI_2(G) = \sum_{uv \in E(G)} \left(\frac{n(u)+n(v)}{n(u)+n(v)-2} \right)^3$$

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 sum augmented Banhatti index of a graph G is defined as

$$SABI_3(G) = \sum_{uv \in E(G)} \left(\frac{m(u)+m(v)}{m(u)+m(v)-2} \right)^3$$

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 sum augmented Banhatti index of a graph G is defined as

$$SABI_4(G) = \sum_{uv \in E(G)} \left(\frac{\varepsilon(u)+\varepsilon(v)}{\varepsilon(u)+\varepsilon(v)-2} \right)^3$$

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

The neighborhood sum augmented Banhatti index of a graph G is defined as

$$NSAB(G) = \sum_{uv \in E(G)} \left(\frac{s(u)+s(v)}{s(u)+s(v)-2} \right)^3$$

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

Recently, some topological indices were studied, for example, in [13, 14, 15].

In this paper, we compute the sum augmented Banhatti index and the second, third, fourth and neighborhood sum augmented Banhatti indices of some significant molecular structures of drugs such as chloroquine, hydroxychloroquine, remdesivir. For molecular structures, see [16, 17].

2. RESULTS FOR CHLOROQUINE

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

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

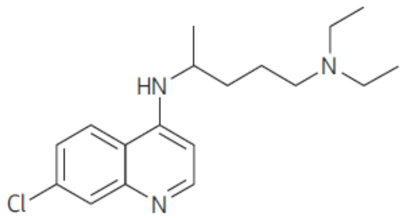

Figure-1: Chemical structure of chloroquine

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

Table-1: Bond set partitions of chloroquine

$d(u), d(v) \setminus uv \in E(G)$	(1, 2)	(1,3)	(2, 2)	(2, 3)	(3, 3)	
Number of bonds	2	2	5	12	2	
$n(u), n(v) \setminus uv \in E(G)$	(1,19)	(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	
$m(u), m(v) \setminus uv \in E(G)$	(1,21)	(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
$\varepsilon(u), \varepsilon(v) \setminus uv \in E(G)$	(7,7)	(8,7)	(8,9)	(9,10)	(10,11)	
Number of bonds	1	3	3	4	5	
	(11,12)	(12,13)				
	4	3				
$s(u), s(v) \setminus uv \in E(G)$	(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	

We calculate the different versions of sum augmented Banhatti index of chloroquine.

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

(i) $SABI(G)=110+\frac{500}{9}+\frac{27}{4}.$

(ii) $SABI_2(G)=19\left(\frac{10}{9}\right)^3+4\left(\frac{21}{19}\right)^3.$

(iii) $SABI_3(G)=4\left(\frac{11}{10}\right)^3+4\left(\frac{23}{21}\right)^3+12\left(\frac{21}{19}\right)^3+3\left(\frac{10}{9}\right)^3.$

(iv) $SABI_4(G)=1\left(\frac{7}{6}\right)^3+3\left(\frac{15}{13}\right)^3+3\left(\frac{17}{15}\right)^3+4\left(\frac{19}{17}\right)^3+5\left(\frac{21}{19}\right)^3+4\left(\frac{23}{21}\right)^3+3\left(\frac{25}{23}\right)^3.$

(v) $NSAB(G)=2\left(\frac{3}{2}\right)^3+2\left(\frac{4}{3}\right)^3+4\left(\frac{9}{7}\right)^3+5\left(\frac{5}{4}\right)^3+3\left(\frac{11}{9}\right)^3+2\left(\frac{6}{5}\right)^3+3\left(\frac{13}{11}\right)^3+2\left(\frac{15}{13}\right)^3.$

Proof: By using the definitions and cardinalities of the bond partition of G, we deduce

(i) $$SABI(G)=\sum_{uv\in E(G)}\left(\frac{d(u)+d(v)}{d(u)+d(v)-2}\right)^3$$

$$=2\left(\frac{1+2}{1+2-2}\right)^3+2\left(\frac{1+3}{1+3-2}\right)^3+5\left(\frac{2+2}{2+2-2}\right)^3+12\left(\frac{2+3}{2+3-2}\right)^3+2\left(\frac{3+3}{3+3-2}\right)^3$$

By solving the above equation, we get the desired result.

(ii) $$SABI_2(G)=\sum_{uv\in E(G)}\left(\frac{n(u)+n(v)}{n(u)+n(v)-2}\right)^3$$

$$=2\left(\frac{1+19}{1+19-2}\right)^3+4\left(\frac{1+20}{1+20-2}\right)^3+2\left(\frac{2+18}{2+18-2}\right)^3+4\left(\frac{3+17}{3+17-2}\right)^3+1\left(\frac{4+16}{4+16-2}\right)^3$$

$$+4\left(\frac{5+15}{5+15-2}\right)^3+1\left(\frac{6+14}{6+14-2}\right)^3+3\left(\frac{7+13}{7+13-2}\right)^3+1\left(\frac{9+11}{9+11-2}\right)^3+1\left(\frac{10+10}{10+10-2}\right)^3$$

By solving the above equation, we get the desired result.

(iii) $SABI_3(G)=\sum_{uv\in E(G)}\left(\frac{m(u)+m(v)}{m(u)+m(v)-2}\right)^3$

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

By solving the above equation, we get the desired result.

(iv) $SABI_4(G)=\sum_{uv\in E(G)}\left(\frac{\varepsilon(u)+\varepsilon(v)}{\varepsilon(u)+\varepsilon(v)-2}\right)^3$

$$=1\left(\frac{7+7}{7+7-2}\right)^3+3\left(\frac{8+7}{8+7-2}\right)^3+3\left(\frac{8+9}{8+9-2}\right)^3+4\left(\frac{9+10}{9+10-2}\right)^3+5\left(\frac{10+11}{10+11-2}\right)^3$$
$$+4\left(\frac{11+12}{11+12-2}\right)^3+3\left(\frac{12+13}{12+13-2}\right)^3$$

By solving the above equation, we obtain the necessary result.

(v) $NSAB(G)=\sum_{uv\in E(G)}\left(\frac{s(u)+s(v)}{s(u)+s(v)-2}\right)^3$

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

By solving the above equation, we get the desired result.

3. RESULTS FOR 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 *H* be the chemical structure of hydroxychloroquine. This structure has 22 atoms and 24 bonds, see Figure 2.

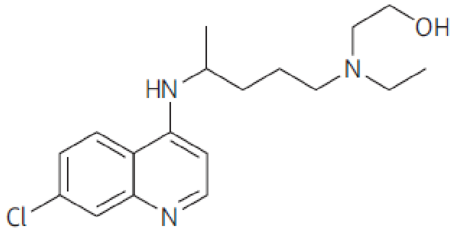

Figure-2: Chemical structure of hydroxychloroquine

From Figure 2, we obtain that
(i) $\{(d(u), d(v)) \setminus uv \in E(H)\}$ has 5 bond set partitions,
(ii)$\{(n(u), n(v)) \setminus uv \in E(H)\}$ has 9 bond set partitions,
(iii)$\{(m(u), m(v)) \setminus uv \in E(H)\}$ has 12 bond set partitions,
(iv) $\{(\varepsilon(u), \varepsilon(v)) \setminus uv \in E(H)\}$ has 7 bond set partitions,
(iv) $\{(s(u), s(v)) \setminus uv \in E(H)\}$ has 11 bond set partitions.

Table-2: Bond set partitions of hydroxychloroquine

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

We compute the different versions of sum augmented Banhatti index of hydroxychloroquine.

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

(i) $SABI(H) = 55 + 12\left(\frac{5}{3}\right)^3 + 2\left(\frac{2}{3}\right)^3.$

(ii) $SABI_2(H) = 20\left(\frac{21}{19}\right)^3 + 4\left(\frac{11}{10}\right)^3.$

(iii) $SABI_3(H) = 5\left(\frac{23}{21}\right)^3 + 4\left(\frac{12}{11}\right)^3 + 12\left(\frac{11}{10}\right)^3 + 3\left(\frac{21}{19}\right)^3.$

(iv) $SABI_4(H) = 3\left(\frac{15}{13}\right)^3 + 2\left(\frac{17}{15}\right)^3 + 3\left(\frac{19}{17}\right)^3 + 4\left(\frac{21}{19}\right)^3 + 6\left(\frac{23}{21}\right)^3 + 4\left(\frac{25}{23}\right)^3 + 2\left(\frac{27}{25}\right)^3.$

(v) $NSAB(H) = 1\left(\frac{5}{3}\right)^3 + 1\left(\frac{3}{2}\right)^3 + 3\left(\frac{4}{3}\right)^3 + 4\left(\frac{9}{7}\right)^3 + 4\left(\frac{5}{4}\right)^3 + 4\left(\frac{11}{9}\right)^3 + 2\left(\frac{6}{5}\right)^3 + 3\left(\frac{13}{11}\right)^3 + 2\left(\frac{15}{13}\right)^3.$

Proof: By using the definitions and cardinalities of the bond partition of *H*, we deduce

(i) $$SABI(H) = \sum_{uv \in E(H)} \left(\frac{d(u)+d(v)}{d(u)+d(v)-2}\right)^3$$

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

By solving the above equation, we obtain the desired result.

(ii) $$SABI_2(H) = \sum_{uv \in E(H)} \left(\frac{n(u)+n(v)}{n(u)+n(v)-2}\right)^3$$

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

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

By solving the above equation, we get the necessary result.

(iii) $$SABI_3(H)=\sum_{uv\in E(H)}\left(\frac{m(u)+m(v)}{m(u)+m(v)-2}\right)^3$$

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

By solving the above equation, we get the desired result.

(iv) $$SABI_4(H)=\sum_{uv\in E(H)}\left(\frac{\varepsilon(u)+\varepsilon(v)}{\varepsilon(u)+\varepsilon(v)-2}\right)^3$$

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

gives the desired result by solving the above equation

(v) $$NSAB(H)=\sum_{uv\in E(H)}\left(\frac{s(u)+s(v)}{s(u)+s(v)-2}\right)^3$$

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

By solving the above equation, we get the desired result.

4. RESULTS FOR REMDESIVIR

Remdesivir is an antiviral drug which was developed by the biopharmaceutical company Gilead Sciences. Let *R* be the molecular graph of remdesivir. This graph has 41 atoms and 44 bonds.

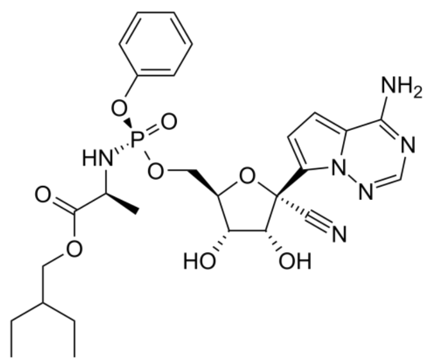

Figure-3: Chemical structure of remdesivir

Table-3: Bond set partitions of remdesivir

$d(u), d(v) \backslash uv \in E(R)$	(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
$n(u), n(v) \backslash uv \in E(R)$	(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							
$m(u), m(v) \backslash uv \in E(R)$	(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	
$\varepsilon(u), \varepsilon(v) \backslash uv \in E(R)$	(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					
$s(u), s(v) \backslash uv \in E(R)$	(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	

We determine the different versions of sum augmented Banhatti index of remdesivir.

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

(i) $SABI(R) = 166 + 16\left(\frac{5}{3}\right)^3 + 10\left(\frac{3}{2}\right)^3 + 2\left(\frac{7}{5}\right)^3.$

(ii) $SABI_2(R) = 1\left(\frac{7}{5}\right)^3 + 1\left(\frac{35}{33}\right)^3 + 2\left(\frac{39}{37}\right)^3 + 9\left(\frac{20}{19}\right)^3 + 1\left(\frac{15}{13}\right)^3 + 1\left(\frac{13}{12}\right)^3 + 2\left(\frac{18}{17}\right)^3 + 2\left(\frac{37}{35}\right)^3 + 3\left(\frac{19}{18}\right)^3.$

(iii) $SABI_3(R) = 22\left(\frac{43}{41}\right)^3 + 9\left(\frac{22}{21}\right)^3 + 1\left(\frac{5}{4}\right)^3 + 1\left(\frac{17}{16}\right)^3 + 8\left(\frac{21}{20}\right)^3 + 1\left(\frac{19}{17}\right)^3 + 1\left(\frac{15}{14}\right)^3 + 1\left(\frac{41}{39}\right)^3.$

(iv) $SABI_4(R) = 2\left(\frac{19}{17}\right)^3 + 4\left(\frac{21}{19}\right)^3 + 4\left(\frac{23}{21}\right)^3 + 7\left(\frac{25}{23}\right)^3 + 1\left(\frac{13}{12}\right)^3 + 7\left(\frac{27}{25}\right)^3$

$+5\left(\frac{29}{27}\right)^3 + 4\left(\frac{31}{29}\right)^3 + 1\left(\frac{16}{15}\right)^3 + 4\left(\frac{33}{31}\right)^3 + 5\left(\frac{35}{33}\right)^3.$

(v) $NSAB(R) = 2\left(\frac{3}{2}\right)^3 + 7\left(\frac{9}{7}\right)^3 + 5\left(\frac{5}{4}\right)^3 + 8\left(\frac{11}{9}\right)^3 + 2\left(\frac{4}{3}\right)^3 + 6\left(\frac{13}{11}\right)^3$

$+2\left(\frac{6}{5}\right)^3 + 6\left(\frac{7}{6}\right)^3 + 1\left(\frac{15}{13}\right)^3 + 1\left(\frac{8}{7}\right)^3 + 3\left(\frac{17}{15}\right)^3 + 1\left(\frac{9}{8}\right)^3.$

Proof: Applying definitions and bond partition of remdesivir, we conclude

(i) $SABI(R) = \sum_{uv \in E(R)} \left(\frac{d(u)+d(v)}{d(u)+d(v)-2}\right)^3$

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

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

By solving the above equation, we get the desired result.

(ii) $SABI_2(R)=\sum_{uv\in E(R)}\left(\frac{n(u)+n(v)}{n(u)+n(v)-2}\right)^3$

$$=1\left(\frac{1+6}{1+6-2}\right)^3+1\left(\frac{1+34}{1+34-2}\right)^3+2\left(\frac{1+38}{1+38-2}\right)^3+9\left(\frac{1+39}{1+39-2}\right)^3+8\left(\frac{2+37}{2+37-2}\right)^3$$

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

$$+1\left(\frac{4+34}{4+34=2}\right)^3+1\left(\frac{4+35}{4+35=2}\right)^3+2\left(\frac{5+34}{5+34=2}\right)^3+1\left(\frac{6+32}{6+32-2}\right)^3+2\left(\frac{6+33}{6+33-2}\right)^3$$

$$+1\left(\frac{8+31}{8+31-2}\right)^3+1\left(\frac{9+30}{9+30-2}\right)^3+1\left(\frac{10+29}{10+29-2}\right)^3+1\left(\frac{11+28}{11+28-2}\right)^3+1\left(\frac{12+24}{12+24-2}\right)^3$$

$$+1\left(\frac{13+24}{13+24-2}\right)^3+1\left(\frac{13+25}{13+25-2}\right)^3+1\left(\frac{17+22}{17+22-2}\right)^3+1\left(\frac{18+21}{18+21-2}\right)^3+1\left(\frac{19+20}{19+20-2}\right)^3.$$

By solving the above equation, we obtain the desired result.

(iii) $SABI_3(R)=\sum_{uv\in E(R)}\left(\frac{m(u)+m(v)}{m(u)+m(v)-2}\right)^3$

$$=2\left(\frac{1+42}{1+42-2}\right)^3+9\left(\frac{1+43}{1+43-2}\right)^3+1\left(\frac{2+8}{2+8-2}\right)^3+1\left(\frac{2+32}{2+32-2}\right)^3+2\left(\frac{2+40}{2+40-2}\right)^3$$

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

$$+2\left(\frac{5+37}{5+37-2}\right)^3+1\left(\frac{5+38}{5+38-2}\right)^3+1\left(\frac{6+35}{6+35-2}\right)^3+2\left(\frac{6+37}{6+37-2}\right)^3+1\left(\frac{7+36}{7+36-2}\right)^3$$

$$+2\left(\frac{8+35}{8+35-2}\right)^3+1\left(\frac{10+33}{10+33-2}\right)^3+2\left(\frac{11+32}{11+32-2}\right)^3+1\left(\frac{15+27}{15+27-2}\right)^3+1\left(\frac{16+26}{16+26-2}\right)^3$$

$$+1\left(\frac{16+27}{16+27-2}\right)^3+1\left(\frac{20+23}{20+23-2}\right)^3+2\left(\frac{21+22}{21+22-2}\right)^3.$$

By solving the above equation, we get the necessary result.

(iv) $SABI_4(R)=\sum_{uv\in E(R)}\left(\frac{\varepsilon(u)+\varepsilon(v)}{\varepsilon(u)+\varepsilon(v)-2}\right)^3$

$$=2\left(\frac{9+10}{9+10-2}\right)^3+4\left(\frac{10+11}{10+11-2}\right)^3+4\left(\frac{11+12}{11+12-2}\right)^3+7\left(\frac{12+13}{12+13-2}\right)^3$$

$$+1\left(\frac{13+13}{13+13-2}\right)^3+7\left(\frac{13+14}{13+14-2}\right)^3+5\left(\frac{14+15}{14+15-2}\right)^3+4\left(\frac{15+16}{15+16-2}\right)^3$$

$$+1\left(\frac{16+16}{16+16-2}\right)^3+4\left(\frac{16+17}{16+17-2}\right)^3+5\left(\frac{17+18}{17+18-2}\right)^3.$$

By solving the above equation, we obtain the desired result.

(v) $NSAB(R)=\sum_{uv\in E(R)}\left(\frac{s(u)+s(v)}{s(u)+s(v)-2}\right)^3$

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

$$+4\left(\frac{4+5}{4+5-2}\right)^3+2\left(\frac{4+6}{4+6-2}\right)^3+1\left(\frac{4+7}{4+7-2}\right)^3+1\left(\frac{4+9}{4+9-2}\right)^3+2\left(\frac{5+5}{5+5-2}\right)^3$$
$$+6\left(\frac{5+6}{5+6-2}\right)^3+1\left(\frac{5+7}{5+7-2}\right)^3+2\left(\frac{5+8}{5+8-2}\right)^3+1\left(\frac{5+9}{5+9-2}\right)^3+1\left(\frac{6+6}{6+6-2}\right)^3$$
$$+3\left(\frac{6+7}{6+7-2}\right)^3+1\left(\frac{6+8}{6+8-2}\right)^3+4\left(\frac{7+7}{7+7-2}\right)^3+1\left(\frac{7+8}{7+8-2}\right)^3+1\left(\frac{7+9}{7+9-2}\right)^3$$
$$+1\left(\frac{8+8}{8+8-2}\right)^3+2\left(\frac{8+9}{8+9-2}\right)^3+1\left(\frac{9+9}{9+9-2}\right)^3.$$

By solving the above equation, we get the desired result.

4. CONCLUSION

In this study, we have calculated the sum augmented Banhatti index and the second, third, fourth and neighborhood sum augmented Banhatti indices of some important chemical structures of drugs which are applied to test the chemical, medical and pharmaceutical characteristics.

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