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DIFFERENT VERSIONS OF ATOM BOND SUM CONNECTIVITY INDEX

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ABSTRACT

We introduce some new atom bond sum connectivity indices: second, third and fourth atom bond sum connectivity indices of a graph. In this paper, we compute the atom bond sum connectivity index, the second, third and fourth atom bond sum connectivity indices and neighborhood sum atom bond connectivity index of some important chemical drugs such as chloroquine, hydroxychloroquine and remdesivir.

Keywords: atom bond sum connectivity index, neighborhood sum atom bond connectivity index, drug

1. INTRODUCTION

Let *G* = *(V, E)* be a simple connected graph. 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 or a chemical 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 numerical parameter mathematically derived from the graph structure. These topological indices are useful for establishing correlations between the structure of a molecular compound and its physicochemical properties, see [2].

The atom bond sum connectivity index [3] is

$$ABS(G)=\sum_{uv\in E(G)}\sqrt{\frac{d(u)+d(v)-2}{d(u)+d(v)}}.$$

We introduce the second, third, fourth atom bond sum connectivity indices and the neighborhood sum atom bond connectivity index of a graph as follows:

The second atom bond sum connectivity index of a molecular graph *G* is defined as

$$ABS_2(G)=\sum_{uv\in E(G)}\sqrt{\frac{n(u)+n(v)-2}{n(u)+n(v)}}$$

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 atom bond sum connectivity index of a graph *G* is defined as

$$ABS_3(G)=\sum_{uv\in E(G)}\sqrt{\frac{m(u)+m(v)-2}{m(u)+m(v)}}$$

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.

The fourth atom bond sum connectivity index of a graph G is defined as

$$ABS_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{\varepsilon(u)+\varepsilon(v)-2}{\varepsilon(u)+\varepsilon(v)}}$$

where the number □(u) is the eccentricity of all vertices adjacent a vertex u.

The neighborhood sum atom bond connectivity index [4] is

$$NSA(G) = \sum_{uv \in E(G)} \sqrt{\frac{s(u)+s(v)-2}{s(u)+s(v)}}$$

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

Recently, some atom bond connectivity indices were studied in [5, 6, 7. 8, 9, 10, 11, 12, 13, 14, 15, 16, 17].

In this paper, we compute the atom bond sum connectivity index, the second, third, fourth atom bond sum connectivity indices and the neighborhood sum atom bond connectivity index of some important chemical drugs.

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 A be the chemical structure of chloroquine. This structure has 21 vertices and 23 edges, see Figure 1.

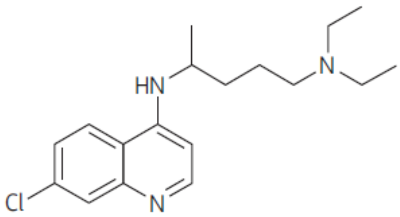

Figure 1. Chemical structure of chloroquine

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

Table 1. Edge set partitions of chloroquine

$d(u),d(v) \setminus uv \in E(A)$	(1, 2)	(1,3)	(2, 2)	(2, 3)	(3, 3)
Number of edges	2	2	5	12	2

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

We compute the different versions of the atom bond sum connectivity index of chloroquine.

Theorem 1. Let *A* be the chemical structure of chloroquine. Then

(i) $ABS(A)=\frac{2}{\sqrt{3}}+\frac{7}{\sqrt{2}}+\frac{12\sqrt{3}}{\sqrt{5}}+\frac{2\sqrt{2}}{\sqrt{3}}.$

(ii) $ABS_2(A)=\frac{57}{\sqrt{10}}+\frac{4\sqrt{19}}{\sqrt{21}}.$

(iii) $ABS_3(A)=4\sqrt{\frac{10}{11}}+4\sqrt{\frac{21}{23}}+12\sqrt{\frac{19}{21}}+\frac{9}{\sqrt{10}}.$

(iv) $ABS_4(A)=\sqrt{\frac{6}{7}}+3\sqrt{\frac{13}{15}}+3\sqrt{\frac{15}{17}}+4\sqrt{\frac{17}{19}}+5\sqrt{\frac{19}{21}}+4\sqrt{\frac{21}{23}}+\frac{3\sqrt{23}}{5}.$

(v) $NSA(A)=2\sqrt{\frac{2}{3}}+\sqrt{3}+\frac{4\sqrt{7}}{3}+\frac{10}{\sqrt{5}}+\frac{9}{\sqrt{11}}+2\sqrt{\frac{5}{6}}+3\sqrt{\frac{11}{13}}+2\sqrt{\frac{13}{15}}.$

Proof: Applying definition and edge partition of chloroquine,we conclude

(i) $ABS(A)=\sum_{uv\in E(A)}\sqrt{\frac{d(u)+d(v)-2}{d(u)+d(v)}}$

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

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

(ii) $ABS_2(A)=\sum_{uv\in E(A)}\sqrt{\frac{n(u)+n(v)-2}{n(u)+n(v)}}$

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

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

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

(iii) $$ABS_3(A)=\sum_{uv\in E(A)}\sqrt{\frac{m(u)+m(v)-2}{m(u)+m(v)}}$$

$$=2\left(\sqrt{\frac{1+21-2}{1+21}}\right)+4\left(\sqrt{\frac{1+22-2}{1+22}}\right)+2\left(\sqrt{\frac{2+19-2}{2+19}}\right)+4\left(\sqrt{\frac{3+18-2}{3+18}}\right)+1\left(\sqrt{\frac{4+17-2}{4+17}}\right)+3\left(\sqrt{\frac{5+15-2}{5+15}}\right)$$

$$+1\left(\sqrt{\frac{5+16-2}{5+16}}\right)+1\left(\sqrt{\frac{6+15-2}{6+15}}\right)+2\left(\sqrt{\frac{7+14-2}{7+14}}\right)+1\left(\sqrt{\frac{8+13-2}{8+13}}\right)+1\left(\sqrt{\frac{9+13-2}{9+13}}\right)+1\left(\sqrt{\frac{10+12-2}{10+12}}\right).$$

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

(iv) $$ABS_4(A)=\sum_{uv\in E(A)}\sqrt{\frac{\varepsilon(u)+\varepsilon(v)-2}{\varepsilon(u)+\varepsilon(v)}}$$

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

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

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

(v) $$NSA(A)=\sum_{uv\in E(A)}\sqrt{\frac{s(u)+s(v)-2}{s(u)+s(v)}}$$

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

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

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 vertices and 24 edges, see Figure 2.

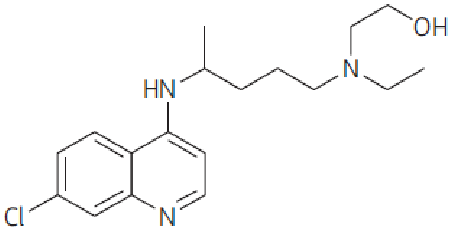

Figure 2. Chemical structure of hydroxychloroquine

From Figure 2, we obtain that

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

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

We determine the different versions of atom bond sum connectivity index of hydroxychloroquine.

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

(i) $ABS(H)=\frac{2}{\sqrt{3}}+\frac{8}{\sqrt{2}}+\frac{12\sqrt{3}}{\sqrt{5}}+\frac{2\sqrt{2}}{\sqrt{3}}.$

(ii) $ABS_2(H)=20\sqrt{\frac{19}{21}}+4\sqrt{\frac{10}{11}}.$

(iii) $ABS_3(H)=5\sqrt{\frac{21}{23}}+4\sqrt{\frac{11}{12}}+12\sqrt{\frac{10}{11}}+3\sqrt{\frac{19}{21}}.$

(iv) $ABS_4(H)=3\sqrt{\frac{13}{15}}+2\sqrt{\frac{15}{17}}+3\sqrt{\frac{17}{19}}+4\sqrt{\frac{19}{21}}+6\sqrt{\frac{21}{23}}+\frac{4\sqrt{23}}{5}+\frac{10}{\sqrt{27}}.$

(v) $NSA(H)=\sqrt{\frac{3}{5}}+\sqrt{\frac{2}{3}}+\frac{3\sqrt{3}}{2}+\frac{4\sqrt{7}}{3}+4\sqrt{\frac{4}{5}}+\frac{12}{\sqrt{11}}+2\sqrt{\frac{5}{6}}+3\sqrt{\frac{11}{13}}+2\sqrt{\frac{13}{15}}.$

Proof: Applying definition and edge partition of hydroxychloroquine,we conclude

(i) $ABS(H)=\sum_{uv\in E(H)}\sqrt{\frac{d(u)+d(v)-2}{d(u)+d(v)}}$

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

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

(ii) $ABS_2(H)=\sum_{uv\in E(H)}\sqrt{\frac{n(u)+n(v)-2}{n(u)+n(v)}}$

$$=2\left(\sqrt{\frac{1+20-2}{1+20}}\right)+4\left(\sqrt{\frac{1+21-2}{1+21}}\right)+3\left(\sqrt{\frac{2+19-2}{2+19}}\right)+4\left(\sqrt{\frac{3+18-2}{3+18}}\right)+4\left(\sqrt{\frac{5+16-2}{5+16}}\right)$$
$$+3\left(\sqrt{\frac{6+15-2}{6+15}}\right)+2\left(\sqrt{\frac{7+14-2}{7+14}}\right)+1\left(\sqrt{\frac{10+11-2}{10+11}}\right)+1\left(\sqrt{\frac{8+13-2}{8+13}}\right).$$

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

(iii) $ABS_3(H)=\sum_{uv\in E(H)}\sqrt{\frac{m(u)+m(v)-2}{m(u)+m(v)}}$

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

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

(iv) $ABS_4(H)=\sum_{uv\in E(H)}\sqrt{\frac{\varepsilon(u)+\varepsilon(v)-2}{\varepsilon(u)+\varepsilon(v)}}$

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

gives the desired result by solving the above equation

(v) $NSA(H)=\sum_{uv\in E(H)}\sqrt{\frac{s(u)+s(v)-2}{s(u)+s(v)}}$

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

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 vertices and 44 edges.

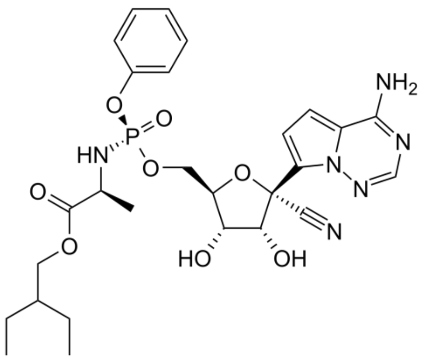

Figure 3. Chemical structure of remdesivir

From Figure 3, we obtain that

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

Table 3. Edge set partitions of remdesivir

$d(u), d(v)\setminus uv\in E(R)$	(1,2)	(1, 3)	(1, 4)	(2, 2)	(2, 3)	(2, 4)	(3, 3)	(3, 4)
Number of edges	2	5	2	9	14	4	6	2
$n(u), n(v)\setminus uv\in E(R)$	(1,6)	(1,34)	(1,38)	(1,39)	(2,37)	(3,12)	(3,23)	(3,36)
Number of edges	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							
$m(u),m(v)\setminus uv\in E(R)$	(1,42)	(1,43)	(2,8)	(2,32)	(2,40)	(2,41)	(3,39)	(4,15)
Number of edges	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 edges	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 edges	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 compute the different versions of atom bond sum connectivity index of remdesivir.

Theorem 3. Let$R$ be the chemical structure of hydroxychloroquine. Then

(i) $ABS(R)=\frac{2}{\sqrt{3}}+\frac{14}{\sqrt{2}}+16\sqrt{\frac{3}{5}}+10\sqrt{\frac{2}{3}}+2\sqrt{\frac{5}{7}}.$

(ii) $ABS_2(R)=\sqrt{\frac{5}{7}}+\sqrt{\frac{33}{35}}+24\sqrt{\frac{37}{39}}+9\sqrt{\frac{19}{20}}+\sqrt{\frac{13}{15}}+\sqrt{\frac{12}{13}}+\frac{\sqrt{34}}{3}+2\sqrt{\frac{35}{37}}+\frac{18}{\sqrt{38}}.$

(iii) $ABS_3(R)=22\sqrt{\frac{41}{43}}+9\sqrt{\frac{21}{22}}+\frac{2}{\sqrt{5}}+\frac{4}{\sqrt{17}}+8\sqrt{\frac{20}{21}}+\sqrt{\frac{17}{19}}+\sqrt{\frac{14}{15}}+\sqrt{\frac{39}{41}}.$

(iv) $ABS_4(R)=2\sqrt{\frac{17}{19}}+4\sqrt{\frac{19}{21}}+4\sqrt{\frac{21}{23}}+\frac{7\sqrt{23}}{5}+\sqrt{\frac{12}{13}}+\frac{35}{\sqrt{27}}+5\sqrt{\frac{27}{29}}+4\sqrt{\frac{29}{31}}+\frac{\sqrt{15}}{4}+4\sqrt{\frac{31}{33}}+5\sqrt{\frac{33}{35}}.$

(v) $NSA(R)=2\sqrt{\frac{2}{3}}+\frac{7\sqrt{7}}{3}+\frac{10}{\sqrt{5}}+\frac{24}{\sqrt{11}}+\sqrt{3}+6\sqrt{\frac{11}{13}}+2\sqrt{\frac{5}{6}}+6\sqrt{\frac{6}{7}}+\sqrt{\frac{13}{15}}+\frac{\sqrt{14}}{4}+3\sqrt{\frac{15}{17}}+\frac{4}{\sqrt{18}}.$

Proof: Applying definition and edge partition of remdesivir, we conclude

(i) $ABS(R)=\sum_{uv\in E(R)}\sqrt{\frac{d(u)+d(v)-2}{d(u)+d(v)}}$

$$=2\left(\sqrt{\frac{1+2-2}{1+2}}\right)+5\left(\sqrt{\frac{1+3-2}{1+3}}\right)+2\left(\sqrt{\frac{1+4-2}{1+4}}\right)+9\left(\sqrt{\frac{2+2-2}{2+2}}\right)+14\left(\sqrt{\frac{2+3-2}{2+3}}\right)$$
$$+4\left(\sqrt{\frac{2+4-2}{2+4}}\right)+6\left(\sqrt{\frac{3+3-2}{3+3}}\right)+2\left(\sqrt{\frac{3+4-2}{3+4}}\right).$$

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

(ii) $ABS_2(R)=\sum_{uv\in E(R)}\sqrt{\frac{n(u)+n(v)-2}{n(u)+n(v)}}$

$$=1\sqrt{\frac{1+6-2}{1+6}}+1\sqrt{\frac{1+34-2}{1+34}}+2\sqrt{\frac{1+38-2}{1+38}}+9\sqrt{\frac{1+39-2}{1+39}}+8\sqrt{\frac{2+37-2}{2+37}}$$
$$+1\sqrt{\frac{3+12-2}{3+12}}+1\sqrt{\frac{3+23-2}{3+23}}+2\sqrt{\frac{3+36-2}{3+36}}+1\sqrt{\frac{4+32-2}{4+32}}+1\sqrt{\frac{4+33-2}{4+33}}$$
$$+1\sqrt{\frac{4+34-2}{4+34}}+1\sqrt{\frac{4+35-2}{4+35}}+2\sqrt{\frac{5+34-2}{5+34}}+1\sqrt{\frac{6+32-2}{6+32}}+2\sqrt{\frac{6+33-2}{6+33}}$$

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$$+1\sqrt{\frac{8+31-2}{8+31}}+1\sqrt{\frac{9+30-2}{9+30}}+1\sqrt{\frac{10+29-2}{10+29}}+1\sqrt{\frac{11+28-2}{11+28}}+1\sqrt{\frac{12+24-2}{12+24}}$$
$$+1\sqrt{\frac{13+24-2}{13+24}}+1\sqrt{\frac{13+25-2}{13+25}}+1\sqrt{\frac{17+22-2}{17+22}}+1\sqrt{\frac{18+21-2}{18+21}}+1\sqrt{\frac{19+20-2}{19+20}}.$$

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

(iii) $$ABS_3(R)=\sum_{uv\in E(R)}\sqrt{\frac{m(u)+m(v)-2}{m(u)+m(v)}}$$

$$=2\sqrt{\frac{1+42-2}{1+42}}+9\sqrt{\frac{1+43-2}{1+43}}+1\sqrt{\frac{2+8-2}{2+8}}+1\sqrt{\frac{2+32-2}{2+32}}+2\sqrt{\frac{2+40-2}{2+40}}$$
$$+6\sqrt{\frac{2+41-2}{2+41}}+2\sqrt{\frac{3+39-2}{3+39}}+1\sqrt{\frac{4+15-2}{4+15}}+1\sqrt{\frac{4+39-2}{4+39}}+1\sqrt{\frac{4+26-2}{4+26}}$$
$$+2\sqrt{\frac{5+37-2}{5+37}}+1\sqrt{\frac{5+38-2}{5+38}}+1\sqrt{\frac{6+35-2}{6+35}}+2\sqrt{\frac{6+37-2}{6+37}}+1\sqrt{\frac{7+36-2}{7+36}}$$
$$+2\sqrt{\frac{8+35-2}{8+35}}+1\sqrt{\frac{10+33-2}{10+33}}+2\sqrt{\frac{11+32-2}{11+32}}+1\sqrt{\frac{15+27-2}{15+27}}+1\sqrt{\frac{16+26-2}{16+26}}$$
$$+1\sqrt{\frac{16+27-2}{16+27}}+1\sqrt{\frac{20+23-2}{20+23}}+2\sqrt{\frac{21+22-2}{21+22}}.$$

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

(iv) $$ABS_4(R)=\sum_{uv\in E(R)}\sqrt{\frac{\varepsilon(u)+\varepsilon(v)-2}{\varepsilon(u)+\varepsilon(v)}}$$

$$=2\sqrt{\frac{9+10-2}{9+10}}+4\sqrt{\frac{10+11-2}{10+11}}+4\sqrt{\frac{11+12-2}{11+12}}+7\sqrt{\frac{12+13-2}{12+13}}+1\sqrt{\frac{13+13-2}{13+13}}+7\sqrt{\frac{13+14-2}{13+14}}$$
$$+5\sqrt{\frac{14+15-2}{14+15}}+4\sqrt{\frac{15+16-2}{15+16}}+1\sqrt{\frac{16+16-2}{16+16}}+4\sqrt{\frac{16+17-2}{16+17}}+5\sqrt{\frac{17+18-2}{17+18}}.$$

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

(v) $$NSA(R)=\sum_{uv\in E(R)}\sqrt{\frac{s(u)+s(v)-2}{s(u)+s(v)}}$$

$$=2\sqrt{\frac{2+4-2}{2+4}}+3\sqrt{\frac{3+6-2}{3+6}}+1\sqrt{\frac{3+7-2}{3+7}}+1\sqrt{\frac{3+8-2}{3+8}}+2\sqrt{\frac{4+4-2}{4+4}}$$
$$+4\sqrt{\frac{4+5-2}{4+5}}+2\sqrt{\frac{4+6-2}{4+6}}+1\sqrt{\frac{4+7-2}{4+7}}+1\sqrt{\frac{4+9-2}{4+9}}+2\sqrt{\frac{5+5-2}{5+5}}$$
$$+6\sqrt{\frac{5+6-2}{5+6}}+1\sqrt{\frac{5+7-2}{5+7}}+2\sqrt{\frac{5+8-2}{5+8}}+1\sqrt{\frac{5+9-2}{5+9}}+1\sqrt{\frac{6+6-2}{6+6}}$$
$$+3\sqrt{\frac{6+7-2}{6+7}}+1\sqrt{\frac{6+8-2}{6+8}}+4\sqrt{\frac{7+7-2}{7+7}}+1\sqrt{\frac{7+8-2}{7+8}}+1\sqrt{\frac{7+9-2}{7+9}}$$
$$+1\sqrt{\frac{8+8-2}{8+8}}+2\sqrt{\frac{8+9-2}{8+9}}+1\sqrt{\frac{9+9-2}{9+9}}.$$

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

5. CONCLUSION

The atom bond sum connectivity index, the second, third, fourth atom bond sum connectivity indices and the neighborhood sum atom bond connectivity index of some important chemical drugs have been computed.

REFERENCES

1. V.R.Kulli, *College Graph Theory,* Vishwa International Publications, Gulbarga, India (2012).
2. I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. Total -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* 17, (1972) 535-538.
3. A.Ali, B.Furtula, I.Redzepovic and I.Gutman, Atom bond sum connectivity indiex, *J. Math. Chem.* in press. DOI: 10.1007/s10910-022-01403-1.
4. V.R.Kulli, Neighborhood sum atom bond connectivity indices of some nanostar dendrimers, *International Journal of Mathematics and Computer Research,* 11(2) (2023) 3230-3235.
5. A.R.Bindsree, V.Lokesha and P.S.Ranjini, ABC index on subdivision graphs and line graphs, *IOSR Journal of Mathematics,* 1-6.
6. K.C.Das, Atom bond connectivity index of graphs, *Discrete Applied Mathematics,* 158 (2010) 1181-1188.
7. E.Estrada, Atom bond connectivity and the energetic of branched alkanes, *Chem. Phys. Lett.* 463 (2008) 422-425.
8. E.Estrada, L.Torres, L.Rodriguez and I.Gutman, An atom bond connectivity index: modeling the enthalpy of formation of alkanes, *Indian J. Chem.*37 (1998) 849-855.
9. B.Furtula, A.Graovac and D.Vukicevic, Atom bond connectivity index of trees, *Discrete Applied Mathematics,* 157 (2009) 2828-2835.
10. V.R.Kulli, Multiplicative connectivity indices of certain nanotubes, *Annals of Pure and Applied Mathematics,* 12(2) (2016) 169-176.
11. V.R.Kulli, Two new multiplicative atom bond connectivity indices, *Annals of Pure and Applied Mathematics,* 13(1) (2017) 1-7.
12. W.Gao, M.K.Jamil, W.Nazeer and M.Amin, Degree based Multiplicative atom bond connectivity index of nanostructures, *IAENG International Journal of Applied Mathematics,* 47:4, *IJAM*-47-4-04 (2017).
13. V.R.Kulli, Product connectivity leap index and *ABC* leap index of helm graphs, *Annals of Pure and Applied Mathematics,* 18(2) (2018) 189-193.
14. N.M.Husin, R.Hasni and N.E.Arif, Atom bond connectivity and geometric-arithmetic indices of dendrimer nanostars, *Australian Journal of Basic and Applied Sciences*, 7(9) (2013) 10-14.
15. V.R.Kulli, *ABC, GA, AG* HDR indices of certain chemical drugs, *International Journal of Mathematics Trends and Technology*, 68(2) (2022) 80-88.
16. V.R.Kulli, Atom bond connectivity E-Banhatti indices, *International Journal of Mathematics and Computer Research,* 11(1) (2023).
17. V.R.Kulli and M.H.Akhabari, Multiplicative atom bond connectivity and multiplicative geometric-arithmetic indices of dendrimer nanostars, *Annals of Pure and Applied Mathematics,* 16(2) (2018) 429-436.