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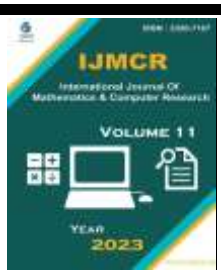

Domination Augmented Banhatti, Domination Augmented Banhatti Sum Indices of Certain Chemical Drugs

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ABSTRACT
In this study, we introduce the domination augmented Banhatti index, domination augmented Banhatti sum index and their corresponding polynomials of a graph. We compute these newly defined domination augmented Banhatti indices for some important chemical drugs such as chloroquine and hydroxychloroquine which are appeared in medical science.

KEYWORDS: domination augmented Banhatti index, domination augmented Banhatti sum index, nanostructure.

I. INTRODUCTION

The simple, connected graph G is with vertex set $V(G)$ and edge set $E(G)$. The number of vertices adjacent to the vertex u is called degree of u, denoted by $d_G(u)$. For other graph terminologies and notions, the readers are referred to books [1, 2]. The 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 [3] have been considered in Chemistry and have found some applications, especially in QSPR/QSAR research [4, 5].Furtula et al. [6], introduced the augmented Zagreb index of a graph G and it is defined as

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

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 [6].

Recently, some augmented indices were studied, for example, in [7, 8, 9, 10, 11, 12, 13, 14]. The domination degree $d_d(u)$ [15] of a vertex u in a graph G is defined as the number of minimal dominating sets of G which contains u. Recently, some domination indices were studied, for example, in [16, 17, 18, 19, 20].

We introduce the domination augmented Banhatti index of a graph G and it is defined as

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

Considering the domination augmented Banhatti index, we define the domination augmented Banhatti polynomial as

$$DABI(G,x)=\sum_{uv\in E(G)}x^{\left(\frac{d_d(u)d_d(v)}{d_d(u)+d_d(v)-2}\right)^3}.$$

We define the domination augmented Banhatti sum index of a graph G as

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

Considering the domination augmented Banhatti sum index, we define the domination augmented Banhatti sum polynomial as

$$DABSI(G,x)=\sum_{uv\in E(G)}x^{\left(\frac{d_d(u)+d_d(v)}{d_d(u)+d_d(v)-2}\right)^3}.$$

Recently, some domination parameters were studied, for example, in [21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33]

In this paper, we compute the domination augmented Banhatti index, domination augmented Banhatti sum index and their corresponding polynomials of chloroquine and hydroxychloroquine.

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

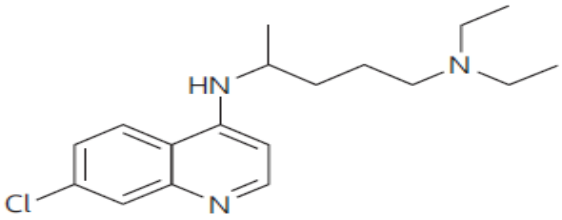

Figure 1. Chemical structure of chloroquine

From Figure 1, we obtain that $\{(d_d(u), d_d(v)) \setminus uv \in E(G)\}$ has 16 bond set partitions.

Table 1. [34] Bond partition based on the domination degreof end atoms of each bond of chloroquine

Table 1. Bond set partitions of chloroquine

$d(u), d(v) \setminus uv \in E(G)$	(216,288)	(216,264)	(216,216)	(324,324)	(297,324)
Number of bonds	2	2	2	4	2
	(240,408)	(240,264)	(144,204)	(246,288)	(144,384)
	1	1	1	1	1
	(288,384)	(216,384)	(216,240)	(240,324)	(216,324)
	1	1	1	1	1
	(216,297)				
	1				

We calculate the domination augmented Banhatti index of chloroquine as follows:

Theorem 1. The domination augmented Banhatti index of chloroquine is given by DABI (G)=100046694-062

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

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

$$= 2\left(\frac{216\times 288}{216+288-2}\right)^3 + 2\left(\frac{216\times 264}{216+264-2}\right)^3 + 2\left(\frac{216\times 216}{216+216-2}\right)^3 + 4\left(\frac{324\times 324}{324+324-2}\right)^3$$

$$+2\left(\frac{297\times 324}{297+324-2}\right)^3 + 1\left(\frac{240\times 408}{240+408-2}\right)^3 + 1\left(\frac{240\times 264}{240+264-2}\right)^3 + 1\left(\frac{144\times 204}{144+204-2}\right)^3$$

$$+1\left(\frac{246\times 288}{246+288-2}\right)^3 + 1\left(\frac{144\times 384}{144+384-2}\right)^3 + 1\left(\frac{288\times 384}{288+384-2}\right)^3 + 1\left(\frac{216\times 384}{216+384-2}\right)^3$$

$$+1\left(\frac{216\times 240}{216+240-2}\right)^3 + 1\left(\frac{240\times 324}{240+324-2}\right)^3 + 1\left(\frac{216\times 324}{216+324-2}\right)^3 + 1\left(\frac{216\times 297}{216+297-2}\right)^3$$

$$= 2\left(\frac{62208}{502}\right)^3 + 2\left(\frac{57024}{478}\right)^3 + 2\left(\frac{46656}{430}\right)^3 + 4\left(\frac{104976}{646}\right)^3 + 2\left(\frac{96228}{619}\right)^3 + 1\left(\frac{97920}{646}\right)^3$$

$$+1\left(\frac{63360}{502}\right)^3 + 1\left(\frac{29376}{346}\right)^3 + 1\left(\frac{70848}{532}\right)^3 + 1\left(\frac{55296}{526}\right)^3 + 1\left(\frac{110592}{670}\right)^3 + 1\left(\frac{82944}{598}\right)^3$$

$$+1\left(\frac{51840}{454}\right)^3 + 1\left(\frac{77760}{562}\right)^3 + 1\left(\frac{69984}{538}\right)^3 + 1\left(\frac{64152}{511}\right)^3.$$

By solving the above equation, we get the desired result. We calculate the domination augmented Banhatti sum index of chloroquine as follows:

Theorem 2. The domination augmented Banhatti sum index of chloroquine is given by

$$DABSI(G) = 23.2615101447$$

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

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

$$= 2\left(\frac{216+288}{216+288-2}\right)^3 + 2\left(\frac{216+264}{216+264-2}\right)^3 + 2\left(\frac{216+216}{216+216-2}\right)^3 + 4\left(\frac{324+324}{324+324-2}\right)^3$$
$$+2\left(\frac{297+324}{297+324-2}\right)^3 + 1\left(\frac{240+408}{240+408-2}\right)^3 + 1\left(\frac{240+264}{240+264-2}\right)^3 + 1\left(\frac{144+204}{144+204-2}\right)^3$$
$$+1\left(\frac{246+288}{246+288-2}\right)^3 + 1\left(\frac{144+384}{144+384-2}\right)^3 + 1\left(\frac{288+384}{288+384-2}\right)^3 + 1\left(\frac{216+384}{216+384-2}\right)^3$$
$$+1\left(\frac{216+240}{216+240-2}\right)^3 + 1\left(\frac{240+324}{240+324-2}\right)^3 + 1\left(\frac{216+324}{216+324-2}\right)^3 + 1\left(\frac{216+297}{216+297-2}\right)^3$$
$$= 2\left(\frac{504}{502}\right)^3 + 2\left(\frac{480}{478}\right)^3 + 2\left(\frac{432}{430}\right)^3 + 4\left(\frac{648}{646}\right)^3 + 2\left(\frac{621}{619}\right)^3 + 1\left(\frac{648}{646}\right)^3$$
$$+1\left(\frac{504}{502}\right)^3 + 1\left(\frac{348}{346}\right)^3 + 1\left(\frac{534}{532}\right)^3 + 1\left(\frac{528}{526}\right)^3 + 1\left(\frac{672}{670}\right)^3 + 1\left(\frac{600}{598}\right)^3$$
$$+1\left(\frac{456}{454}\right)^3 + 1\left(\frac{564}{562}\right)^3 + 1\left(\frac{540}{538}\right)^3 + 1\left(\frac{513}{511}\right)^3.$$

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

In the following theorem, by using definitions, we obtain the domination augmented Banhatti polynomial and domination augmented Banhatti sum polynomial of chloroquine.

Theorem 3. (i) The domination augmented Banhatti polynomial of chloroquine is given by

$$DABI(G,x) = 2x^{\left(\frac{31104}{251}\right)^3} + 2x^{\left(\frac{28512}{239}\right)^3} + 2x^{\left(\frac{23328}{215}\right)^3} + 4x^{\left(\frac{52488}{323}\right)^3} + 2x^{\left(\frac{96228}{619}\right)^3} + x^{\left(\frac{2880}{19}\right)^3}$$
$$+x^{\left(\frac{31680}{251}\right)^3} + x^{\left(\frac{14688}{173}\right)^3} + x^{\left(\frac{17712}{133}\right)^3} + x^{\left(\frac{27648}{263}\right)^3} + x^{\left(\frac{55296}{335}\right)^3} + x^{\left(\frac{41472}{299}\right)^3}$$
$$+x^{\left(\frac{25920}{227}\right)^3} + x^{\left(\frac{38880}{281}\right)^3} + x^{\left(\frac{34992}{269}\right)^3} + x^{\left(\frac{64152}{511}\right)^3}.$$

(ii) The domination augmented Banhatti sum polynomial chloroquine is given by

$$DABI(G,x) = 2x^{\left(\frac{252}{251}\right)^3} + 2x^{\left(\frac{240}{239}\right)^3} + 2x^{\left(\frac{216}{215}\right)^3} + 4x^{\left(\frac{324}{323}\right)^3} + 2x^{\left(\frac{621}{619}\right)^3} + x^{\left(\frac{324}{323}\right)^3}$$
$$+x^{\left(\frac{252}{251}\right)^3} + x^{\left(\frac{174}{173}\right)^3} + x^{\left(\frac{267}{266}\right)^3} + x^{\left(\frac{264}{263}\right)^3} + x^{\left(\frac{336}{335}\right)^3} + x^{\left(\frac{300}{299}\right)^3}$$
$$+x^{\left(\frac{278}{277}\right)^3} + x^{\left(\frac{282}{281}\right)^3} + x^{\left(\frac{270}{269}\right)^3} + x^{\left(\frac{513}{511}\right)^3}.$$

III. 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.

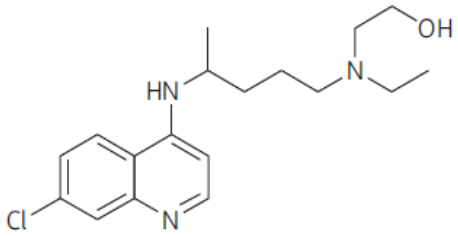

Figure 2. Chemical structure of hydroxychloroquine

From Figure 2, we obtain that $\{(d_d(u), d_d(v)) \setminus uv \in E(H)\}$ has 21 bond set partition

Table 2. [34] Bond partition based on the domination degree of end atoms of each bond of hydroxychloroquine.

$d_d(u), d_d(v) \setminus uv \in E(H)$	(210,350)	(210,425)	(207,324)	(207,567)	(315,317)
Number of bonds	1	1	1	1	1
	(315,385)	(315,420)	(315,425)	(317,340)	(317,385)
	1	2	1	1	1
	(324,324)	(324,459)	(324,567)	(324,621)	(340,486)
	1	1	1	1	1
	(350,385)	(350,595)	(385,420)	(420,425)	(459,486)
	1	1	1	1	3
	(486,567)				
	1				

We calculate the domination augmented Banhatti index of hydroxychloroquine as follows:

Theorem 4. The domination augmented Banhatti index of hydroxychloroquine is given by

$$DABI(H) = 177527870.256$$

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

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

$$= 1\left(\frac{210\times 350}{558}\right)^3 + 1\left(\frac{210\times 425}{633}\right)^3 + 1\left(\frac{207\times 324}{529}\right)^3 + 1\left(\frac{207\times 567}{772}\right)^3$$

$$+1\left(\frac{315\times 317}{630}\right) + 1\left(\frac{315\times 385}{698}\right)^3 + 2\left(\frac{315\times 420}{733}\right)^3 + 1\left(\frac{315\times 425}{738}\right)^3$$

$$+1\left(\frac{317\times 340}{655}\right)^3 + 1\left(\frac{317\times 385}{700}\right)^3 + 1\left(\frac{324\times 324}{646}\right)^3 + 1\left(\frac{324\times 459}{781}\right)^3$$

$$+1\left(\frac{324\times 567}{889}\right)^3 + 1\left(\frac{324\times 621}{943}\right)^3 + 1\left(\frac{340\times 486}{824}\right)^3 + 1\left(\frac{350\times 385}{733}\right)^3$$

$$+1\left(\frac{350\times 595}{943}\right)^3 + 1\left(\frac{385\times 420}{803}\right)^3 + 1\left(\frac{420\times 425}{843}\right)^3 + 3\left(\frac{459\times 486}{943}\right)^3$$

$$+1\left(\frac{486\times 567}{1051}\right)^3.$$

$$=1\left(\frac{73500}{558}\right)^3+1\left(\frac{89250}{633}\right)^3+1\left(\frac{67068}{529}\right)^3+1\left(\frac{117369}{772}\right)^3$$
$$+1\left(\frac{99855}{630}\right)+1\left(\frac{121275}{698}\right)^3+2\left(\frac{132300}{733}\right)^3+1\left(\frac{133875}{738}\right)^3$$
$$+1\left(\frac{107780}{655}\right)^3+1\left(\frac{122045}{700}\right)^3+1\left(\frac{104976}{646}\right)^3+1\left(\frac{148716}{781}\right)^3$$
$$+1\left(\frac{183708}{889}\right)^3+1\left(\frac{201204}{943}\right)^3+1\left(\frac{165240}{824}\right)^3+1\left(\frac{134750}{733}\right)^3$$
$$+1\left(\frac{208250}{943}\right)^3+1\left(\frac{161700}{803}\right)^3+1\left(\frac{178500}{843}\right)^3+3\left(\frac{223074}{943}\right)^3$$
$$+1\left(\frac{275562}{1051}\right)^3.$$

By solving the above equation, we get the desired result.We calculate the domination augmented Banhatti sum index of hydroxychloroquine as follows:

Theorem 5. The domination augmented Banhatti sum index of hydroxychloroquine is given by

$$DABSI(H)=24.1915199653$$

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

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

$$=1\left(\frac{210+350}{210+350-2}\right)^3+1\left(\frac{210+425}{210+425-2}\right)^3+1\left(\frac{207+324}{207+324-2}\right)^3+1\left(\frac{207+567}{207+567-2}\right)^3$$
$$+1\left(\frac{315+317}{315+317-2}\right)+1\left(\frac{315+385}{315+385-2}\right)^3+2\left(\frac{315+420}{315+420-2}\right)^3+1\left(\frac{315+425}{315+425-2}\right)^3$$
$$+1\left(\frac{317+340}{317+340-2}\right)^3+1\left(\frac{317+385}{317+385-2}\right)^3+1\left(\frac{324+324}{324+324-2}\right)^3+1\left(\frac{324+459}{324+459-2}\right)^3$$
$$+1\left(\frac{324+567}{324+567-2}\right)^3+1\left(\frac{324+621}{324+621-2}\right)^3+1\left(\frac{340+486}{340+486-2}\right)^3+1\left(\frac{350+385}{350+385-2}\right)^3$$
$$+1\left(\frac{350+595}{350+595-2}\right)^3+1\left(\frac{385+420}{385+420-2}\right)^3+1\left(\frac{420+425}{420+425-2}\right)^3+3\left(\frac{459+486}{459+486-2}\right)^3$$
$$+1\left(\frac{486+567}{486+567-2}\right)^3.$$

$$=1\left(\frac{560}{558}\right)^3+1\left(\frac{635}{633}\right)^3+1\left(\frac{531}{529}\right)^3+1\left(\frac{774}{772}\right)^3+1\left(\frac{632}{630}\right)+1\left(\frac{700}{698}\right)^3+2\left(\frac{735}{733}\right)^3$$
$$+1\left(\frac{740}{738}\right)^3+1\left(\frac{657}{655}\right)^3+1\left(\frac{702}{700}\right)^3+1\left(\frac{648}{646}\right)^3+1\left(\frac{783}{781}\right)^3+1\left(\frac{891}{889}\right)^3+1\left(\frac{945}{943}\right)^3$$
$$+1\left(\frac{826}{824}\right)^3+1\left(\frac{735}{733}\right)^3+1\left(\frac{945}{943}\right)^3+1\left(\frac{805}{803}\right)^3+1\left(\frac{845}{843}\right)^3+3\left(\frac{945}{943}\right)^3+1\left(\frac{1053}{1051}\right)^3.$$

By solving the above equation, we get the desired result. In the following theorem, by using definitions, we obtain the domination augmented Banhatti polynomial and domination augmented Banhatti sum polynomial of hydroxychloroquine.

Theorem 6. (i) The domination augmented Banhatti polynomial of hydroxychloroquine is given by

$$DABI(H,x) = x^{\left(\frac{73500}{558}\right)^3} + x^{\left(\frac{89250}{633}\right)^3} + x^{\left(\frac{67068}{529}\right)^3} + x^{\left(\frac{117369}{772}\right)^3} + x^{\left(\frac{99855}{630}\right)^3} + x^{\left(\frac{121275}{698}\right)^3} + 2x^{\left(\frac{132300}{733}\right)^3}$$
$$+x^{\left(\frac{133875}{738}\right)^3} + x^{\left(\frac{107780}{655}\right)^3} + x^{\left(\frac{122045}{700}\right)^3} + x^{\left(\frac{104976}{646}\right)^3} + x^{\left(\frac{148716}{781}\right)^3} + x^{\left(\frac{183708}{889}\right)^3} + x^{\left(\frac{201204}{943}\right)^3}$$
$$+x^{\left(\frac{165240}{824}\right)^3} + x^{\left(\frac{134750}{733}\right)^3} + x^{\left(\frac{208250}{943}\right)^3} + x^{\left(\frac{161700}{803}\right)^3} + x^{\left(\frac{178500}{843}\right)^3} + 3x^{\left(\frac{223074}{943}\right)^3} + x^{\left(\frac{275562}{1051}\right)^3}.$$

(ii) The domination augmented Banhatti sum polynomial hydroxychloroquine is given by

$$DABSI(H,x) = x^{\left(\frac{280}{279}\right)^3} + x^{\left(\frac{635}{633}\right)^3} + x^{\left(\frac{531}{529}\right)^3} + x^{\left(\frac{387}{386}\right)^3} + x^{\left(\frac{316}{315}\right)^3} + x^{\left(\frac{350}{349}\right)^3} + 2x^{\left(\frac{735}{733}\right)^3}$$
$$+x^{\left(\frac{370}{369}\right)^3} + x^{\left(\frac{657}{655}\right)^3} + x^{\left(\frac{351}{350}\right)^3} + x^{\left(\frac{324}{323}\right)^3} + x^{\left(\frac{783}{781}\right)^3} + x^{\left(\frac{891}{889}\right)^3} + x^{\left(\frac{945}{943}\right)^3}$$
$$+x^{\left(\frac{413}{412}\right)^3} + x^{\left(\frac{735}{733}\right)^3} + x^{\left(\frac{945}{943}\right)^3} + x^{\left(\frac{805}{803}\right)^3} + x^{\left(\frac{845}{843}\right)^3} + 3x^{\left(\frac{945}{943}\right)^3} + x^{\left(\frac{1053}{1051}\right)^3}.$$

IV. CONCLUSION

In this study, we have determined the domination augmented Banhatti index and domination augmented Banhatti sum index and their corresponding polynomials for some important drugs such as chloroquine and hydroxychloroquine which are appeared in medical science.

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