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**INTERNATIONAL JOURNAL OF ENGINEERING SCIENCES & RESEARCH  
 TECHNOLOGY**
**DOMINATION ATOM BOND SUM CONNECTIVITY INDICES OF CERTAIN  
 NANOSTRUCTURES**
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**ABSTRACT**

In this paper, we introduce the domination atom bond sum connectivity index, multiplicative domination atom bond sum connectivity index and domination atom bond sum connectivity exponential of a graph. Also we determine these newly defined domination atom bond sum connectivity indices for some chemical drugs such as chloroquine and hydroxychloroquine.

**Keywords:** domination atom bond sum connectivity index, multiplicative domination atom bond sum connectivity index, drug.

Mathematics Subject Classification: 05C10, 05C69.

**1. INTRODUCTION**

Let  $G = (V, E)$  be a finite, simple connected graph. Let  $d_G(u)$  denote the degree of a vertex  $u$  in a graph  $G$ . For undefined terms and notations, we refer [1, 2].

In the modeling of Mathematics, a molecular 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. Topological indices are useful for finding correlations between the structure of a chemical compound and its physicochemical properties. Numerous topological indices have been considered in Theoretical Chemistry and have found some applications, especially in QSPR/QSAR research, see [3, 4].

In [5], the domination atom bond sum connectivity index of a graph  $G$  is defined as

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

Very recently, some domination indices have been researched in [6, 7, 8, 9, 10, 11, 12] and some atom bond connectivity indices studied in [13, 14, 15].

We introduce the domination atom bond sum connectivity index of a graph  $G$ , defined as

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

Considering the domination atom bond sum connectivity index, we define the domination atom bond sum connectivity exponential of a graph as



$$DABS(G, x) = \sum_{uv \in E(G)} x^{\sqrt{\frac{d_d(u) + d_d(v) - 2}{d_d(u) + d_d(v)}}}$$

We define the multiplicative domination atom bond sum connectivity index of a graph as

$$DABSH(G) = \prod_{uv \in E(G)} \sqrt{\frac{d_d(u) + d_d(v) - 2}{d_d(u) + d_d(v)}}$$

Recently, some domination parameters were studied, for example, in [16, 17, 18, 19, 20, 21, 22, 23, 24, 25].

In this paper, we compute the domination atom bond sum connectivity index and multiplicative domination atom bond sum connectivity index of chloroquine and hydroxychloroquine.

## 2. RESULTS FOR CHLOROQUINE

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

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

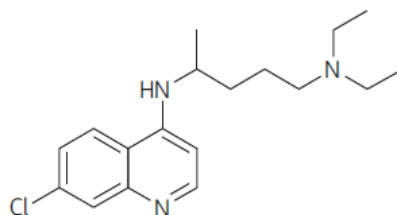


Figure 1. Chemical structure of chloroquine

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

Table 1. [26] Edge partition based on the domination degree of end vertices of each edge of chloroquine.

Table 1. Edge set partitions of chloroquine

$d_d(u), d_d(v) \mid uv \in E(G)$	(216,288)	(216,264)	(216,216)	(324,324)	(297,324)
Number of edges	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 atom bond sum connectivity index of chloroquine as follows:

**Theorem 1.** The domination atom bond sum connectivity index of chloroquine is given by

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[10]



$$DABS(G) = 22.9567105385$$

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

$$\begin{aligned} DABS(G) &= \sum_{uv \in E(G)} \sqrt{\frac{d_d(u) + d_d(v) - 2}{d_d(u) + d_d(v)}} \\ &= 2 \left( \sqrt{\frac{216+288-2}{216+288}} \right) + 2 \left( \sqrt{\frac{216+264-2}{216+264}} \right) + 2 \left( \sqrt{\frac{216+216-2}{216+216}} \right) + 4 \left( \sqrt{\frac{324+324-2}{324+324}} \right) \\ &\quad + 2 \left( \sqrt{\frac{297+324-2}{297+324}} \right) + 1 \left( \sqrt{\frac{240+408-2}{240+408}} \right) + 1 \left( \sqrt{\frac{240+264-2}{240+264}} \right) + 1 \left( \sqrt{\frac{144+204-2}{144+204}} \right) \\ &\quad + 1 \left( \sqrt{\frac{246+288-2}{246+288}} \right) + 1 \left( \sqrt{\frac{144+384-2}{144+384}} \right) + 1 \left( \sqrt{\frac{288+384-2}{288+384}} \right) + 1 \left( \sqrt{\frac{216+384-2}{216+384}} \right) \\ &\quad + 1 \left( \sqrt{\frac{216+240-2}{216+240}} \right) + 1 \left( \sqrt{\frac{240+324-2}{240+324}} \right) + 1 \left( \sqrt{\frac{216+324-2}{216+324}} \right) + 1 \left( \sqrt{\frac{216+297-2}{216+297}} \right) \\ &= 2 \left( \sqrt{\frac{502}{504}} \right) + 2 \left( \sqrt{\frac{478}{480}} \right) + 2 \left( \sqrt{\frac{430}{432}} \right) + 4 \left( \sqrt{\frac{646}{648}} \right) + 2 \left( \sqrt{\frac{619}{621}} \right) + 1 \left( \sqrt{\frac{646}{648}} \right) \\ &\quad + 1 \left( \sqrt{\frac{502}{504}} \right) + 1 \left( \sqrt{\frac{346}{348}} \right) + 1 \left( \sqrt{\frac{532}{534}} \right) + 1 \left( \sqrt{\frac{526}{528}} \right) + 1 \left( \sqrt{\frac{670}{672}} \right) + 1 \left( \sqrt{\frac{598}{600}} \right) \\ &\quad + 1 \left( \sqrt{\frac{454}{456}} \right) + 1 \left( \sqrt{\frac{562}{564}} \right) + 1 \left( \sqrt{\frac{538}{540}} \right) + 1 \left( \sqrt{\frac{511}{513}} \right). \end{aligned}$$

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

We calculate the domination atom bond sum connectivity exponential of chloroquine as follows:

**Theorem 2.** The domination atom bond sum connectivity exponential of chloroquine is given by

$$\begin{aligned} DABS(G, x) &= 3x \sqrt{\frac{251}{252}} + 2x \sqrt{\frac{239}{240}} + 2x \sqrt{\frac{215}{216}} + 5x \sqrt{\frac{323}{324}} + 2x \sqrt{\frac{619}{621}} + x \sqrt{\frac{173}{174}} + x \sqrt{\frac{266}{267}} \\ &\quad + x \sqrt{\frac{263}{264}} + x \sqrt{\frac{335}{336}} + x \sqrt{\frac{299}{300}} + x \sqrt{\frac{227}{228}} + x \sqrt{\frac{281}{282}} + x \sqrt{\frac{269}{270}} + x \sqrt{\frac{511}{513}}. \end{aligned}$$

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

$$\begin{aligned} DABS(G, x) &= \sum_{uv \in E(G)} x \sqrt{\frac{d_d(u) + d_d(v) - 2}{d_d(u) + d_d(v)}} \\ &= 2x \sqrt{\frac{216+288-2}{216+288}} + 2x \sqrt{\frac{216+264-2}{216+264}} + 2x \sqrt{\frac{216+216-2}{216+216}} + 4x \sqrt{\frac{324+324-2}{324+324}} \\ &\quad + 2x \sqrt{\frac{297+324-2}{297+324}} + 1x \sqrt{\frac{240+408-2}{240+408}} + 1x \sqrt{\frac{240+264-2}{240+264}} + 1x \sqrt{\frac{144+204-2}{144+204}} \\ &\quad + 1x \sqrt{\frac{246+288-2}{246+288}} + 1x \sqrt{\frac{144+384-2}{144+384}} + 1x \sqrt{\frac{288+384-2}{288+384}} + 1x \sqrt{\frac{216+384-2}{216+384}} \\ &\quad + 1x \sqrt{\frac{216+240-2}{216+240}} + 1x \sqrt{\frac{240+324-2}{240+324}} + 1x \sqrt{\frac{216+324-2}{216+324}} + 1x \sqrt{\frac{216+297-2}{216+297}} \end{aligned}$$

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

We calculate the multiplicative domination atom bond sum connectivity index of chloroquine as follows:

**Theorem 3.** The multiplicative domination atom bond sum connectivity index of chloroquine is given by

$$DABSII(G) = 0.95759388043$$

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

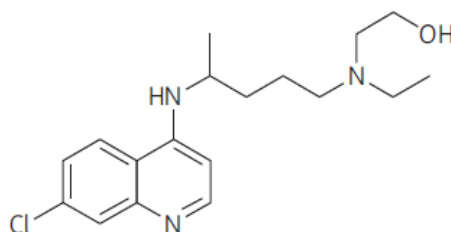
$$\begin{aligned}
 DABSII(G) &= \prod_{uv \in E(G)} \sqrt{\frac{d_d(u) + d_d(v) - 2}{d_d(u) + d_d(v)}} \\
 &= \left( \sqrt{\frac{216 + 288 - 2}{216 + 288}} \right)^2 \times \left( \sqrt{\frac{216 + 264 - 2}{216 + 264}} \right)^2 \times \left( \sqrt{\frac{216 + 216 - 2}{216 + 216}} \right)^2 \times \left( \sqrt{\frac{324 + 324 - 2}{324 + 324}} \right)^4 \\
 &\times \left( \sqrt{\frac{297 + 324 - 2}{297 + 324}} \right)^2 \times \left( \sqrt{\frac{240 + 408 - 2}{240 + 408}} \right)^1 \times \left( \sqrt{\frac{240 + 264 - 2}{240 + 264}} \right)^1 \times \left( \sqrt{\frac{144 + 204 - 2}{144 + 204}} \right)^1 \\
 &\times \left( \sqrt{\frac{246 + 288 - 2}{246 + 288}} \right)^1 \times \left( \sqrt{\frac{144 + 384 - 2}{144 + 384}} \right)^1 \times \left( \sqrt{\frac{288 + 384 - 2}{288 + 384}} \right)^1 \times \left( \sqrt{\frac{216 + 384 - 2}{216 + 384}} \right)^1 \\
 &\times \left( \sqrt{\frac{216 + 240 - 2}{216 + 240}} \right)^1 \times \left( \sqrt{\frac{240 + 324 - 2}{240 + 324}} \right)^1 \times \left( \sqrt{\frac{216 + 324 - 2}{216 + 324}} \right)^1 \times \left( \sqrt{\frac{216 + 297 - 2}{216 + 297}} \right)^1 \\
 &= \left( \sqrt{\frac{502}{504}} \right)^2 \times \left( \sqrt{\frac{478}{480}} \right)^2 \times \left( \sqrt{\frac{430}{432}} \right)^2 \times \left( \sqrt{\frac{646}{648}} \right)^4 \times \left( \sqrt{\frac{619}{621}} \right)^2 \times \left( \sqrt{\frac{646}{648}} \right)^1 \\
 &\times \left( \sqrt{\frac{502}{504}} \right)^1 \times \left( \sqrt{\frac{346}{348}} \right)^1 \times \left( \sqrt{\frac{532}{534}} \right)^1 \times \left( \sqrt{\frac{526}{528}} \right)^1 \times \left( \sqrt{\frac{670}{672}} \right)^1 \times \left( \sqrt{\frac{598}{600}} \right)^1 \\
 &\times \left( \sqrt{\frac{454}{456}} \right)^1 \times \left( \sqrt{\frac{562}{564}} \right)^1 \times \left( \sqrt{\frac{538}{540}} \right)^1 \times \left( \sqrt{\frac{511}{513}} \right)^1
 \end{aligned}$$

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  $\{(d_d(u), d_d(v)) \mid uv \in E(H)\}$  has 21 edge set partitions,

**Table 2. [26] Edge partition based on the domination degree of end vertices of each edge of hydroxychloroquine**

$d_d(u), d_d(v) \mid uv \in E(H)$	(210,350)	(210,425)	(207,324)	(207,567)	(315,317)
Number of edges	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 compute the domination atom bond sum connectivity index of hydroxychloroquine.

**Theorem 4.** The domination atom bond sum connectivity index of hydroxychloroquine is given by

$$DABS(H) = 23.9682324713$$

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

$$\begin{aligned}
 DABS(H) &= \sum_{uv \in E(H)} \sqrt{\frac{d_d(u) + d_d(v) - 2}{d_d(u) + d_d(v)}} \\
 &= 1 \left( \sqrt{\frac{210 + 350 - 2}{210 + 350}} \right) + 1 \left( \sqrt{\frac{210 + 425 - 2}{210 + 425}} \right) + 1 \left( \sqrt{\frac{207 + 324 - 2}{207 + 324}} \right) + 1 \left( \sqrt{\frac{207 + 567 - 2}{207 + 567}} \right) \\
 &+ 1 \left( \sqrt{\frac{315 + 317 - 2}{315 + 317}} \right) + 1 \left( \sqrt{\frac{315 + 385 - 2}{315 + 385}} \right) + 2 \left( \sqrt{\frac{315 + 420 - 2}{315 + 420}} \right) + 1 \left( \sqrt{\frac{315 + 425 - 2}{315 + 425}} \right) \\
 &+ 1 \left( \sqrt{\frac{317 + 340 - 2}{317 + 340}} \right) + 1 \left( \sqrt{\frac{317 + 385 - 2}{317 + 385}} \right) + 1 \left( \sqrt{\frac{324 + 324 - 2}{324 + 324}} \right) + 1 \left( \sqrt{\frac{324 + 459 - 2}{324 + 459}} \right) \\
 &+ 1 \left( \sqrt{\frac{324 + 567 - 2}{324 + 567}} \right) + 1 \left( \sqrt{\frac{324 + 621 - 2}{324 + 621}} \right) + 1 \left( \sqrt{\frac{340 + 486 - 2}{340 + 486}} \right) + 1 \left( \sqrt{\frac{350 + 385 - 2}{350 + 385}} \right) \\
 &+ 1 \left( \sqrt{\frac{350 + 595 - 2}{350 + 595}} \right) + 1 \left( \sqrt{\frac{385 + 420 - 2}{385 + 420}} \right) + 1 \left( \sqrt{\frac{420 + 425 - 2}{420 + 425}} \right) + 3 \left( \sqrt{\frac{459 + 486 - 2}{459 + 486}} \right) \\
 &+ 1 \left( \sqrt{\frac{486 + 567 - 2}{486 + 567}} \right).
 \end{aligned}$$

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

We compute the domination atom bond sum connectivity exponential of hydroxychloroquine.

**Theorem 5.** The domination atom bond sum connectivity exponential of hydroxychloroquine is given by

$$\begin{aligned}
 DABS(H, x) = & 1x\sqrt{\frac{279}{280}} + 1x\sqrt{\frac{633}{635}} + 1x\sqrt{\frac{529}{531}} + 1x\sqrt{\frac{386}{387}} + 1x\sqrt{\frac{315}{316}} + 1x\sqrt{\frac{349}{350}} \\
 & + 2x\sqrt{\frac{733}{735}} + 1x\sqrt{\frac{369}{370}} + 1x\sqrt{\frac{655}{657}} + 1x\sqrt{\frac{350}{351}} + 1x\sqrt{\frac{323}{324}} + 1x\sqrt{\frac{781}{783}} \\
 & + 1x\sqrt{\frac{889}{891}} + 1x\sqrt{\frac{943}{945}} + 1x\sqrt{\frac{412}{413}} + 1x\sqrt{\frac{733}{735}} + 1x\sqrt{\frac{943}{945}} + 1x\sqrt{\frac{803}{805}} \\
 & + 1x\sqrt{\frac{843}{845}} + 3x\sqrt{\frac{943}{945}} + x\sqrt{\frac{1051}{1053}}.
 \end{aligned}$$

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

$$\begin{aligned}
 DABS(H, x) &= \sum_{uv \in E(H)} x^{\sqrt{\frac{d_d(u)+d_d(v)-2}{d_d(u)+d_d(v)}}} \\
 &= 1x\sqrt{\frac{210+350-2}{210+350}} + 1x\sqrt{\frac{210+425-2}{210+425}} + 1x\sqrt{\frac{207+324-2}{207+324}} + 1x\sqrt{\frac{207+567-2}{207+567}} + 1x\sqrt{\frac{315+317-2}{315+317}} + 1x\sqrt{\frac{315+385-2}{315+385}} \\
 &+ 2x\sqrt{\frac{315+420-2}{315+420}} + 1x\sqrt{\frac{315+425-2}{315+425}} + 1x\sqrt{\frac{317+340-2}{317+340}} + 1x\sqrt{\frac{317+385-2}{317+385}} + 1x\sqrt{\frac{324+324-2}{324+324}} + 1x\sqrt{\frac{324+459-2}{324+459}} \\
 &+ 1x\sqrt{\frac{324+567-2}{324+567}} + 1x\sqrt{\frac{324+621-2}{324+621}} + 1x\sqrt{\frac{340+486-2}{340+486}} + 1x\sqrt{\frac{350+385-2}{350+385}} + 1x\sqrt{\frac{350+595-2}{350+595}} + 1x\sqrt{\frac{385+420-2}{385+420}} \\
 &+ 1x\sqrt{\frac{420+425-2}{420+425}} + 3x\sqrt{\frac{459+486-2}{459+486}} + 1x\sqrt{\frac{486+567-2}{486+567}}.
 \end{aligned}$$

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

We compute the multiplicative domination atom bond sum connectivity index of hydroxychloroquine.

**Theorem 6.** The multiplicative domination atom bond sum connectivity index of hydroxychloroquine is given by

$$DABSII(H) = 0.9687107182$$

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

$$\begin{aligned}
 DABSII(H) &= \prod_{uv \in E(H)} \sqrt{\frac{d_d(u)+d_d(v)-2}{d_d(u)+d_d(v)}} \\
 &= \left( \sqrt{\frac{210+350-2}{210+350}} \right)^1 \times \left( \sqrt{\frac{210+425-2}{210+425}} \right)^1 \times \left( \sqrt{\frac{207+324-2}{207+324}} \right)^1 \times \left( \sqrt{\frac{207+567-2}{207+567}} \right)^1 \\
 &\times \left( \sqrt{\frac{315+317-2}{315+317}} \right)^1 \times \left( \sqrt{\frac{315+385-2}{315+385}} \right)^1 \times \left( \sqrt{\frac{315+420-2}{315+420}} \right)^2 \times \left( \sqrt{\frac{315+425-2}{315+425}} \right)^1 \\
 &\times \left( \sqrt{\frac{317+340-2}{317+340}} \right)^1 \times \left( \sqrt{\frac{317+385-2}{317+385}} \right)^1 \times \left( \sqrt{\frac{324+324-2}{324+324}} \right)^1 \times \left( \sqrt{\frac{324+459-2}{324+459}} \right)^1
 \end{aligned}$$

$$\begin{aligned} & \times \left( \sqrt{\frac{324+567-2}{324+567}} \right)^1 \times \left( \sqrt{\frac{324+621-2}{324+621}} \right)^1 \times \left( \sqrt{\frac{340+486-2}{340+486}} \right)^1 \times \left( \sqrt{\frac{350+385-2}{350+385}} \right)^1 \\ & \times \left( \sqrt{\frac{350+595-2}{350+595}} \right)^1 \times \left( \sqrt{\frac{385+420-2}{385+420}} \right)^1 \times \left( \sqrt{\frac{420+425-2}{420+425}} \right)^1 \times \left( \sqrt{\frac{459+486-2}{459+486}} \right)^3 \\ & \times \left( \sqrt{\frac{486+567-2}{486+567}} \right)^1. \end{aligned}$$

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

#### 4. CONCLUSION

In this paper, we have computed the domination atom bond sum connectivity index and multiplicative domination atom bond sum connectivity index of two chemical drugs such as chloroquine and hydroxychloroquine.

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