

IRREGULARITY DOMINATION NIRMALA AND DOMINATION SOMBOR INDICES OF CERTAIN DRUGS

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ABSTRACT

In this paper, we introduce the irregularity domination Nirmala index, the irregularity domination Sombor index and their corresponding exponentials of a graph. Also we compute these newly defined irregularity domination indices and their corresponding exponentials for some important chemical drugs which are appeared in medical science.

Keywords: *irregularity domination Nirmala index, irregularity domination Sombor index, chemical drug.*

Mathematics Subject Classification: 05C10, 05C69.

1. 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 called degree of u , denoted by $d_G(u)$. For other graph terminologies and notions, the readers are referred to books [1, 2].

A chemical graph is a graph whose vertices correspond to the atoms and edges to the bonds. Mathematical Chemistry is very useful in the study of Chemical Sciences. We have found many applications in Mathematical Chemistry by using graph indices, especially in QSPR/QSAR research [3, 4].

In [5], the domination Nirmala index of a graph G was introduced and it is defined as

$$DN(G) = \sum_{uv \in E(G)} \sqrt{d_d(u) + d_d(v)}.$$

Recently, some domination indices were studied, for example, in [6, 7, 8, 9, 10, 11, 12] and some Nirmala indices were studied, for example, in [13, 14, 15, 16, 17, 18, 19, 20].

We introduce the irregularity domination Nirmala index of a graph G and it is defined as

$$IDN(G) = \sum_{uv \in E(G)} \sqrt{|d_d(u) - d_d(v)|}.$$

We introduce the irregularity domination Nirmala exponential of a graph G and it is defined as

$$IDN(G, x) = \sum_{uv \in E(G)} x^{\sqrt{|d_d(u) - d_d(v)|}}.$$

Recently, some irregularity indices were studied, for example, in [21, 22, 23, 24, 25, 16, 27, 28].

In [29], the domination Sombor index of a graph G was introduced and it is defined as

$$DSO(G) = \sum_{uv \in E(G)} \sqrt{d_d(u)^2 + d_d(v)^2}.$$

We introduce the irregularity domination Sombor index of a graph G and it is defined as

$$IDSO(G) = \sum_{uv \in E(G)} \sqrt{|d_d(u)^2 - d_d(v)^2|}.$$

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We define the irregularity domination Sombor exponential of a graph G as

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

Recently, some Sombor indices were studied, for example, in [30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42].

In this paper, the irregularity domination Nirmala index, the irregularity domination Sombor index and their corresponding exponentials for chloroquine and hydroxychloroquine are determined.

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

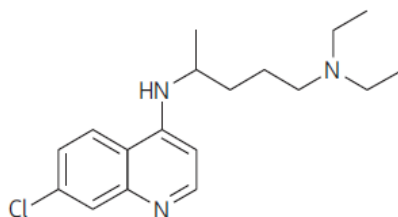


Figure-1: Chemical structure of chloroquine

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

Table 2. [43] Edge partition based on the domination degree of end vertices of each edge of chloroquine

Table-1: Edge set partitions of chloroquine

	(216,288)	(216,264)	(216,216)	(324,324)	(297,324)
$d_d(u), d_d(v) \mid uv \in E(G)$	2	2	2	4	2
Number of edges	(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				

In the following theorem, we compute the irregularity domination Nirmala index of chloroquine.

Theorem 1: The irregularity domination Nirmala index of chloroquine is given by

$$IDN(G) = 145.014251801$$

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

$$\begin{aligned}
 IDN(G) &= \sum_{uv \in E(G)} \sqrt{d_d(u) - d_d(v)} \\
 &= 2\sqrt{216-288} + 2\sqrt{216-264} + 2\sqrt{216-216} + 4\sqrt{324-324} + 2\sqrt{297-324} \\
 &\quad + 1\sqrt{240-408} + 1\sqrt{240-264} + 1\sqrt{144-204} + 1\sqrt{246-288} + 1\sqrt{144-384} \\
 &\quad + 1\sqrt{288-384} + 1\sqrt{216-384} + 1\sqrt{216-240} + 1\sqrt{240-324} + 1\sqrt{216-324} \\
 &\quad + 1\sqrt{216-297} \\
 &= 2\sqrt{72} + 2\sqrt{48} + 0 + 0 + 2\sqrt{27} + 1\sqrt{168} + 1\sqrt{24} + 1\sqrt{60} + 1\sqrt{42} + 1\sqrt{240} \\
 &\quad + 1\sqrt{96} + 1\sqrt{168} + 1\sqrt{24} + 1\sqrt{84} + 1\sqrt{108} + 1\sqrt{81}.
 \end{aligned}$$

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

We calculate the irregularity domination Nirmala exponential of chloroquine as follows:

Theorem 2: The irregularity domination Nirmala exponential of chloroquine is given by

$$IDN(G, x) = 2x^{\sqrt{72}} + 2x^{\sqrt{48}} + 6 + 2x^{\sqrt{27}} + 2x^{\sqrt{168}} + 2x^{\sqrt{24}} + x^{\sqrt{60}} + x^{\sqrt{42}} + x^{\sqrt{240}} \\ + x^{\sqrt{96}} + x^{\sqrt{84}} + x^{\sqrt{108}} + x^{\sqrt{81}}.$$

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

$$IDN(G, x) = \sum_{uv \in E(G)} x^{\sqrt{|d_d(u) - d_d(v)|}} \\ = 2x^{\sqrt{216-288}} + 2x^{\sqrt{216-264}} + 2x^{\sqrt{216-216}} + 4x^{\sqrt{324-324}} + 2x^{\sqrt{297-324}} + 1x^{\sqrt{240-408}} \\ + 1x^{\sqrt{240-264}} + 1x^{\sqrt{144-204}} + 1x^{\sqrt{246-288}} + 1x^{\sqrt{144-384}} + 1x^{\sqrt{288-384}} + 1x^{\sqrt{216-384}} \\ + 1x^{\sqrt{216-240}} + 1x^{\sqrt{240-324}} + 1x^{\sqrt{216-324}} + 1x^{\sqrt{216-297}}. \\ = 2x^{\sqrt{72}} + 2x^{\sqrt{48}} + 2x^0 + 4x^0 + 2x^{\sqrt{27}} + 1x^{\sqrt{168}} + 1x^{\sqrt{24}} + 1x^{\sqrt{60}} + 1x^{\sqrt{42}} + 1x^{\sqrt{240}} \\ + 1x^{\sqrt{96}} + 1x^{\sqrt{168}} + 1x^{\sqrt{24}} + 1x^{\sqrt{84}} + 1x^{\sqrt{108}} + 1x^{\sqrt{81}}.$$

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

In the following theorem, we compute the irregularity domination Sombor index of chloroquine.

Theorem 3: The irregularity domination Sombor index of chloroquine is given by

$$IDSO(G) = 3372.80249809$$

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

$$IDSO(G) = \sum_{uv \in E(G)} \sqrt{|d_d(u)^2 - d_d(v)^2|} \\ = 2\sqrt{216^2 - 288^2} + 2\sqrt{216^2 - 264^2} + 2\sqrt{216^2 - 216^2} + 4\sqrt{324^2 - 324^2} + 2\sqrt{297^2 - 324^2} \\ + 1\sqrt{240^2 - 408^2} + 1\sqrt{240^2 - 264^2} + 1\sqrt{144^2 - 204^2} + 1\sqrt{246^2 - 288^2} + 1\sqrt{144^2 - 384^2} \\ + 1\sqrt{288^2 - 384^2} + 1\sqrt{216^2 - 384^2} + 1\sqrt{216^2 - 240^2} + 1\sqrt{240^2 - 324^2} + 1\sqrt{216^2 - 324^2} \\ + 1\sqrt{216^2 - 297^2}. \\ = 2\sqrt{36288} + 2\sqrt{23040} + 0 + 0 + 2\sqrt{16767} + 1\sqrt{108864} + 1\sqrt{12096} + 1\sqrt{20880} \\ + 1\sqrt{22428} + 1\sqrt{126720} + 1\sqrt{64512} + 1\sqrt{100800} + 1\sqrt{10944} + 1\sqrt{47376} + 1\sqrt{58320} + 1\sqrt{41553}.$$

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

We compute the irregularity domination Sombor exponential of chloroquine as follows:

Theorem 4: The irregularity domination Sombor exponential of chloroquine is given by

$$IDSO(G, x) = 2x^{\sqrt{36288}} + 2x^{\sqrt{23040}} + 6 + 2x^{\sqrt{16767}} + x^{\sqrt{108864}} + x^{\sqrt{12096}} + x^{\sqrt{20880}} \\ + x^{\sqrt{22428}} + x^{\sqrt{126720}} + x^{\sqrt{64512}} + x^{\sqrt{100800}} + x^{\sqrt{10944}} + x^{\sqrt{47376}} + x^{\sqrt{58320}} + x^{\sqrt{41553}}.$$

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

$$IDSO(G, x) = \sum_{uv \in E(G)} x^{\sqrt{|d_d(u)^2 - d_d(v)^2|}} \\ = 2x^{\sqrt{216^2 - 288^2}} + 2x^{\sqrt{216^2 - 264^2}} + 2x^{\sqrt{216^2 - 216^2}} + 4x^{\sqrt{324^2 - 324^2}} + 2x^{\sqrt{297^2 - 324^2}} + 1x^{\sqrt{240^2 - 408^2}} \\ + 1x^{\sqrt{240^2 - 264^2}} + 1x^{\sqrt{144^2 - 204^2}} + 1x^{\sqrt{246^2 - 288^2}} + 1x^{\sqrt{144^2 - 384^2}} + 1x^{\sqrt{288^2 - 384^2}} + 1x^{\sqrt{216^2 - 384^2}} \\ + 1x^{\sqrt{216^2 - 240^2}} + 1x^{\sqrt{240^2 - 324^2}} + 1x^{\sqrt{216^2 - 324^2}} + 1x^{\sqrt{216^2 - 297^2}}. \\ = 2x^{\sqrt{36288}} + 2x^{\sqrt{23040}} + 2x^0 + 4x^0 + 2x^{\sqrt{16767}} + 1x^{\sqrt{108864}} + 1x^{\sqrt{12096}} + 1x^{\sqrt{20880}} \\ + 1x^{\sqrt{22428}} + 1x^{\sqrt{126720}} + 1x^{\sqrt{64512}} + 1x^{\sqrt{100800}} + 1x^{\sqrt{10944}} + 1x^{\sqrt{47376}} + 1x^{\sqrt{58320}} + 1x^{\sqrt{41553}}.$$

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.

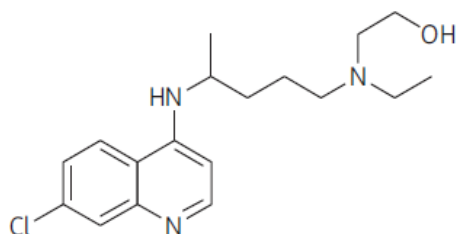


Figure-2: Chemical structure of hydroxychloroquine

From Figure 2, we obtain that $\{(d_d(u), d_d(v)) \mid uv \in E(H)\}$ has 21 edge set partitions,

Table 2. [43] Bond 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				

In the following theorem, we determine the irregularity domination Nirmala index of hydroxychloroquine.

Theorem 5: The irregularity domination Nirmala index of hydroxychloroquine is given by

$$IDN(H) = 220.923506142$$

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

$$\begin{aligned}
 IDN(H) &= \sum_{uv \in E(H)} \sqrt{|d_d(u) - d_d(v)|} \\
 &= 1\sqrt{|210 - 350|} + 1\sqrt{|210 - 425|} + 1\sqrt{|207 - 324|} + 1\sqrt{|207 - 567|} + 1\sqrt{|315 - 317|} \\
 &\quad + 1\sqrt{|315 - 385|} + 2\sqrt{|315 - 420|} + 1\sqrt{|315 - 425|} + 1\sqrt{|317 - 340|} + 1\sqrt{|317 - 385|} \\
 &\quad + 1\sqrt{|324 - 324|} + 1\sqrt{|324 - 459|} + 1\sqrt{|324 - 567|} + 1\sqrt{|324 - 621|} + 1\sqrt{|340 - 486|} \\
 &\quad + 1\sqrt{|350 - 385|} + 1\sqrt{|350 - 595|} + 1\sqrt{|385 - 420|} + 1\sqrt{|420 - 425|} + 3\sqrt{|459 - 486|} \\
 &\quad + 1\sqrt{|486 - 567|}. \\
 &= 1\sqrt{140} + 1\sqrt{215} + 1\sqrt{117} + 1\sqrt{360} + 1\sqrt{2} + 1\sqrt{70} + 2\sqrt{105} \\
 &\quad + 1\sqrt{110} + 1\sqrt{23} + 1\sqrt{68} + 0 + 1\sqrt{135} + 1\sqrt{243} + 1\sqrt{297} \\
 &\quad + 1\sqrt{146} + 1\sqrt{35} + 1\sqrt{245} + 1\sqrt{35} + 1\sqrt{5} + 3\sqrt{27} + 1\sqrt{81}.
 \end{aligned}$$

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

We now compute the irregularity domination Nirmala index of hydroxychloroquine.

Theorem 6: The irregularity domination Nirmala exponential of chloroquine is given by

$$IDN(H, x) = x^{\sqrt{140}} + x^{\sqrt{215}} + x^{\sqrt{117}} + x^{\sqrt{360}} + x^{\sqrt{2}} + x^{\sqrt{70}} + 2x^{\sqrt{105}} \\ + x^{\sqrt{110}} + x^{\sqrt{23}} + x^{\sqrt{68}} + 1 + x^{\sqrt{135}} + x^{\sqrt{243}} + x^{\sqrt{297}} \\ + x^{\sqrt{146}} + 2x^{\sqrt{35}} + x^{\sqrt{245}} + x^{\sqrt{5}} + 3x^{\sqrt{27}} + x^{\sqrt{81}}.$$

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

$$IDN(H, x) = \sum_{uv \in E(H)} x^{\sqrt{d_d(u) - d_d(v)}} \\ = 1x^{\sqrt{210-350}} + 1x^{\sqrt{210-425}} + 1x^{\sqrt{207-324}} + 1x^{\sqrt{207-567}} + 1x^{\sqrt{315-317}} \\ + 1x^{\sqrt{315-385}} + 2x^{\sqrt{315-420}} + 1x^{\sqrt{315-425}} + 1x^{\sqrt{317-340}} + 1x^{\sqrt{317-385}} \\ + 1x^{\sqrt{324-324}} + 1x^{\sqrt{324-459}} + 1x^{\sqrt{324-567}} + 1x^{\sqrt{324-621}} + 1x^{\sqrt{340-486}} \\ + 1x^{\sqrt{350-385}} + 1x^{\sqrt{350-595}} + 1x^{\sqrt{385-420}} + 1x^{\sqrt{420-425}} + 3x^{\sqrt{459-486}} + 1x^{\sqrt{486-567}}. \\ = 1x^{\sqrt{140}} + 1x^{\sqrt{215}} + 1x^{\sqrt{117}} + 1x^{\sqrt{360}} + 1x^{\sqrt{2}} + 1x^{\sqrt{70}} + 2x^{\sqrt{105}} \\ + 1x^{\sqrt{110}} + 1x^{\sqrt{23}} + 1x^{\sqrt{68}} + 1x^0 + 1x^{\sqrt{135}} + 1x^{\sqrt{243}} + 1x^{\sqrt{297}} \\ + 1x^{\sqrt{146}} + 1x^{\sqrt{35}} + 1x^{\sqrt{245}} + 1x^{\sqrt{5}} + 3x^{\sqrt{27}} + 1x^{\sqrt{81}}.$$

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

In the following theorem, we calculate the irregularity domination Sombor index of hydroxychloroquine.

Theorem 7: The irregularity domination Sombor index of hydroxychloroquine is given by

$$IDSO(H) = 6258.46669388$$

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

$$IDSO(H) = \sum_{uv \in E(H)} \sqrt{d_d(u)^2 - d_d(v)^2} \\ = 1\sqrt{210^2 - 350^2} + 1\sqrt{210^2 - 425^2} + 1\sqrt{207^2 - 324^2} + 1\sqrt{207^2 - 567^2} + 1\sqrt{315^2 - 317^2} \\ + 1\sqrt{315^2 - 385^2} + 2\sqrt{315^2 - 420^2} + 1\sqrt{315^2 - 425^2} + 1\sqrt{317^2 - 340^2} + 1\sqrt{317^2 - 385^2} \\ + 1\sqrt{324^2 - 324^2} + 1\sqrt{324^2 - 459^2} + 1\sqrt{324^2 - 567^2} + 1\sqrt{324^2 - 621^2} + 1\sqrt{340^2 - 486^2} \\ + 1\sqrt{350^2 - 385^2} + 1\sqrt{350^2 - 595^2} + 1\sqrt{385^2 - 420^2} + 1\sqrt{420^2 - 425^2} + 3\sqrt{459^2 - 486^2} \\ + 1\sqrt{486^2 - 567^2}. \\ = 1\sqrt{78400} + 1\sqrt{140224} + 1\sqrt{64575} + 1\sqrt{281088} + 1\sqrt{1264} + 1\sqrt{49000} + 2\sqrt{77175} \\ + 1\sqrt{81400} + 1\sqrt{15111} + 1\sqrt{47736} + 0 + 1\sqrt{23905} + 1\sqrt{216513} + 1\sqrt{280665} \\ + 1\sqrt{120596} + 1\sqrt{104125} + 1\sqrt{309925} + 1\sqrt{28175} + 1\sqrt{4225} + 3\sqrt{25515} + 1\sqrt{85293}.$$

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

In the following theorem, we compute the irregularity domination Sombor exponential of chloroquine.

Theorem 8: The irregularity domination Sombor exponential of chloroquine is given by

$$IDSO(H, x) = x^{\sqrt{78400}} + x^{\sqrt{140224}} + x^{\sqrt{64575}} + x^{\sqrt{281088}} + x^{\sqrt{1264}} + x^{\sqrt{49000}} + 2x^{\sqrt{77175}} \\ + x^{\sqrt{81400}} + x^{\sqrt{15111}} + x^{\sqrt{15111}} + x^0 + x^{\sqrt{23905}} + x^{\sqrt{216513}} + x^{\sqrt{280665}} \\ + x^{\sqrt{120596}} + x^{\sqrt{104125}} + x^{\sqrt{309925}} + x^{\sqrt{28175}} + x^{\sqrt{4225}} + 3x^{\sqrt{25515}} + x^{\sqrt{85293}}.$$

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

$$\begin{aligned}
 IDSO(H, x) &= \sum_{uv \in E(H)} x^{\sqrt{d_d(u)^2 - d_d(v)^2}} \\
 &= 1x^{\sqrt{210^2 - 350^2}} + 1x^{\sqrt{210^2 - 425^2}} + 1x^{\sqrt{207^2 - 324^2}} + 1x^{\sqrt{207^2 - 567^2}} + 1x^{\sqrt{315^2 - 317^2}} \\
 &\quad + 1x^{\sqrt{315^2 - 385^2}} + 2x^{\sqrt{315^2 - 420^2}} + 1x^{\sqrt{315^2 - 425^2}} + 1x^{\sqrt{317^2 - 340^2}} + 1x^{\sqrt{317^2 - 385^2}} \\
 &\quad + 1x^{\sqrt{324^2 - 324^2}} + 1x^{\sqrt{324^2 - 459^2}} + 1x^{\sqrt{324^2 - 567^2}} + 1x^{\sqrt{324^2 - 621^2}} + 1x^{\sqrt{340^2 - 486^2}} \\
 &\quad + 1x^{\sqrt{350^2 - 385^2}} + 1x^{\sqrt{350^2 - 595^2}} + 1x^{\sqrt{385^2 - 420^2}} + 1x^{\sqrt{420^2 - 425^2}} + 3x^{\sqrt{459^2 - 486^2}} \\
 &\quad + 1x^{\sqrt{486^2 - 567^2}}. \\
 &= 1x^{\sqrt{78400}} + 1x^{\sqrt{140224}} + 1x^{\sqrt{64575}} + 1x^{\sqrt{281088}} + 1x^{\sqrt{1264}} + 1x^{\sqrt{49000}} + 2x^{\sqrt{77175}} \\
 &\quad + 1x^{\sqrt{81400}} + 1x^{\sqrt{15111}} + 1x^{\sqrt{1511}} + x^0 + 1x^{\sqrt{23905}} + 1x^{\sqrt{216513}} + 1x^{\sqrt{280665}} \\
 &\quad + 1x^{\sqrt{120596}} + 1x^{\sqrt{104125}} + 1x^{\sqrt{309925}} + 1x^{\sqrt{28175}} + 1x^{\sqrt{4225}} + 3x^{\sqrt{25515}} + 1x^{\sqrt{85293}}.
 \end{aligned}$$

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

4. CONCLUSION

In this study, we have determined the irregularity domination Nirmala index, the irregularity domination Sombor index and their corresponding exponentials for some important drugs such as chloroquine, hydroxychloroquine which are appeared in medical science.

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