International Journal of Mathematics Trends and Technology
ISSN: 2231-5373/ https://doi.org/10.14445/22315373/IJMTT-V69I9P501

Volume 69 Issue 9, 1-7, September 2023
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Original Article

Modified Domination and Domination Banhatti Indices of Some Chemical Drugs

V. R. Kulli

Department of Mathematics, Gulbarga University, Gulbarga, India.

Corresponding Author : vrkulli@gmail.com

Received: 12 July 2023 Revised: 17 August 2023 Accepted: 03 September 2023 Published: 22 September 2023

Abstract *- Define the modified domination and domination Banhatti indices of a graph. Here we compute these indices of chloroquine and hydroxychloroquine.*

Keywords - *Modified domination index, Domination Banhatti index, Chloroquine, Hydroxychloroquine.*

Mathematics Subject Classification *- 05C10, 05C69.*

1. Introduction

The graph $G = (V(G), E(G))$, where $V(G)$ vertex set and $E(G)$) edge set. We refer to [1-3], for other definitions.

Topological indices are numerical values obtained from chemical structures. It is very important to determine topological indices of chloroquine hydroxychloroquine to compare physicochemical properties using QSAR models. Some topological indices were studied in [4-13].

The domination degree $d_d(u)$ of a vertex u in a graph G is defined as the number of minimal dominating sets of G which contains u.

mDM_1 (first modified domination) index is defined as

$$mDM_1(G) = \sum_{uv\in E(G)} \frac{1}{d_d(u)+d_d(v)}$$

mDM_2 (second modified domination) index is defined as

$$mDM_2(G) = \sum_{uv\in E(G)} \frac{1}{d_d(u)d_d(v)}$$

DB_1 (first domination Banhatti) index is defined as

$$DB_1(G) = \sum_{uv\in E(G)} \frac{d_d(u)+d_d(v)}{2}$$

DB_2 (second domination Banhatti) index is defined as

$$DB_2(G) = \sum_{uv\in E(G)} \frac{d_d(u)d_d(v)}{2}$$

DB_3 (third domination Banhatti) index is defined as

$$DB_3(G) = \sum_{uv\in E(G)} \left(\frac{d_d(u)+d_d(v)}{2}\right)^2$$

Some domination indices were studied in [14- 29].

In this paper, we determine the modified domination indices and domination Banhatti indices of some standard graphs, two chemical drugs, chloroquine hydroxychloroquine.

2. Results for Some Standard Graphs

Proposition 1. If K_n it is a complete graph with n vertices, then

(i) $mDM_1(K_n) = \frac{n(n-1)}{4}$. (ii) $mDM_1(K_n) = \frac{n(n-1)}{2}$. (iii) $DB_1(K_n) = \frac{n(n-1)}{2}$. (iv) $DB_2(K_n) = \frac{n(n-1)}{4}$.
(v) $DB_3(K_n) = \frac{n(n-1)}{2}$.

Proof: If K_n is a complete graph, then $d_d(u) = 1$. From definitions, we have

(i) $mDM_1(K_n) = \frac{n(n-1)}{2}\frac{1}{(1+1)} = \frac{n(n-1)}{4}$.

(ii) $mDM_2(K_n) = \frac{n(n-1)}{2}\frac{1}{(1\times 1)} = \frac{n(n-1)}{2}$.

(iii) $DB_1(K_n) = \frac{n(n-1)}{2}\left(\frac{1+1}{2}\right) = \frac{n(n-1)}{2}$.

(iv) $DB_2(K_n) = \frac{n(n-1)}{2}\frac{(1\times 1)}{2} = \frac{n(n-1)}{4}$.

(v) $DB_3(K_n) = \frac{n(n-1)}{2}\left(\frac{1+1}{2}\right)^2 = \frac{n(n-1)}{2}$.

Proposition 2. If S_{n+1} is a star graph with $d_d(u)$ =1, then

(i) $mDM_1(S_{n+1}) = \frac{n}{2}$. (ii) $mDM_2(S_{n+1}) = n$. (iii) $DB_1(S_{n+1}) = n$. (iv) $DB_2(S_{n+1}) = \frac{n}{2}$.

(v) $DB_1(S_{n+1}) = n$.

Proposition 3. If $S_{p+1,q+1}$ is a double star graph with $d_d(u)$ =2, then

(i) $mDM_1(S_{p+1,q+1}) = \frac{p+q+1}{4}$. (ii) $mDM_2(S_{p+1,q+1}) = \frac{p+q+1}{4}$. (iii) $DB_1(S_{p+1,q+1}) = 2(p+q+1)$.

(iv) $DB_2(S_{p+1,q+1}) = 2(p+q+1)$. (iv) $DB_3(S_{p+1,q+1}) = 4(p+q+1)$.

Proposition 4. Let $K_{m,n}$ be a complete bipartite graph with $2 \leq m \leq n$. Then

(i) $mDM_1(K_{m,n}) = \frac{mn}{m+n+2}$. (ii) $mDM_2(K_{m,n}) == \frac{mn}{(m+1)(n+1)}$

(iii) $DB_1(K_{m,n}) = \frac{mn(m+n+2)}{2}$. (iv) $DB_2(K_{m,n}) = \frac{mn(m+1)(n+1)}{2}$.

(v) $DB_3(K_{m,n}) = \frac{mn(m+n+2)^2}{4}$.

Proof: Let $G=K_{m,n}$, $m, n \geq 2$ with $d_d(u)= m+1$

$= n+1$, for all $u \in V(G)$.

From the definition, we have

(i) $mDM_1(K_{m,n}) = \frac{mn}{m+1+n+1} = \frac{mn}{m+n+2}$

(ii) $mDM_2(K_{m,n}) == \frac{mn}{(m+1)(n+1)}$

(iii) $DB_1(K_{m,n}) = \frac{mn(m+1+n+1)}{2} = \frac{mn(m+n+2)}{2}$.

(iv) $DB_2(K_{m,n}) = \frac{mn(m+1)(n+1)}{2}$.

(v) $DB_3(K_{m,n}) = \frac{mn(m+1+n+1)^2}{2^2} = \frac{mn(m+n+2)^2}{4}$.

3. Results for Chloroquine

Chloroquine is a drug used to prevent and treat malaria. The graph G of chloroquine has 21 atoms and 23 bonds; see Figure 1.

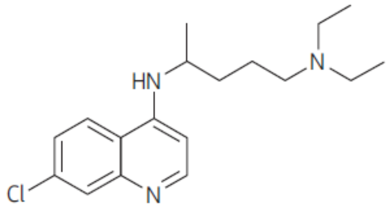

Fig. 1 Chemical structure of chloroquine

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

Table 1. Bond set partitions of chloroquine

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

Theorem 1. mDM_1 index of chloroquine is

$$mDM_1(G) = 0.04324746393$$

Proof: From definition,

$$mDM_1(G) = \sum_{uv\in E(G)} \frac{1}{d_d(u)+d_d(v)}$$

$$= \frac{2}{216+288} + \frac{2}{216+264} + \frac{2}{216+216} + \frac{4}{324+324} + \frac{2}{297+324} + \frac{1}{240+408}$$
$$+ \frac{1}{240+264} + \frac{1}{144+204} + \frac{1}{246+288} + \frac{1}{144+384} + \frac{1}{288+384} + \frac{1}{216+384}$$
$$+ \frac{1}{216+240} + \frac{1}{240+324} + \frac{1}{216+324} + \frac{1}{216+297}$$
$$= \frac{2}{504} + \frac{2}{480} + \frac{2}{432} + \frac{4}{648} + \frac{2}{621} + \frac{1}{648} + \frac{1}{504} + \frac{1}{348} + \frac{1}{534} + \frac{1}{528} + \frac{1}{672} + \frac{1}{600}$$
$$+ \frac{1}{456} + \frac{1}{564} + \frac{1}{540} + \frac{1}{513}$$

=0.04324746393

Theorem 2.mDM_2 index of chloroquine is

$$mDM_2(G) = 0.00034430832$$

Proof: From definition,

$$mDM_2(G) = \sum_{uv\in E(G)} \frac{1}{d_d(u)d_d(v)}$$

$$= \frac{2}{216\times288} + \frac{2}{216\times264} + \frac{2}{216\times216} + \frac{4}{324\times324} + \frac{2}{297\times324} + \frac{1}{240\times408}$$
$$+ \frac{1}{240\times264} + \frac{1}{144\times204} + \frac{1}{246\times288} + \frac{1}{144\times384} + \frac{1}{288\times384} + \frac{1}{216\times384}$$
$$+ \frac{1}{216\times240} + \frac{1}{240\times324} + \frac{1}{216\times324} + \frac{1}{216\times297}$$
$$= \frac{2}{62208} + \frac{2}{57024} + \frac{2}{46656} + \frac{4}{104976} + \frac{2}{96228} + \frac{1}{97920} + \frac{1}{63360} + \frac{1}{29376}$$
$$+ \frac{1}{70848} + \frac{1}{55296} + \frac{1}{110076} + \frac{1}{82944} + \frac{1}{51840} + \frac{1}{77760} + \frac{1}{69984} + \frac{1}{64152}$$

=0.00034430832

Theorem 3. DB_1 index of chloroquine is

$$DB_1(G) = 6283.5$$

Proof: From definition,

$$DB_1(G) = \sum_{uv\in E(G)} \frac{d_d(u)+d_d(v)}{2}$$

$$= \frac{2(216+288)}{2} + \frac{2(216+264)}{2} + \frac{2(216+216)}{2} + \frac{4(324+324)}{2} + \frac{2(297+324)}{2} + \frac{1(240+408)}{2}$$
$$+ \frac{1(240+264)}{2} + \frac{1(144+204)}{2} + \frac{1(246+288)}{2} + \frac{1(144+384)}{2} + \frac{1(288+384)}{2} + \frac{1(216+384)}{2}$$
$$+ \frac{1(216+240)}{2} + \frac{1(240+324)}{2} + \frac{1(216+324)}{2} + \frac{1(216+297)}{2}$$
$$= \frac{2(504)}{2} + \frac{2(480)}{2} + \frac{2(432)}{2} + \frac{4(648)}{2} + \frac{2(621)}{2} + \frac{648}{2} + \frac{504}{2} + \frac{348}{2} + \frac{534}{2} + \frac{528}{2} + \frac{672}{2} + \frac{600}{2}$$
$$+ \frac{456}{2} + \frac{564}{2} + \frac{540}{2} + \frac{513}{2}$$

=6283.5

Theorem 4. DB_2 index of chloroquine is

$$DB_2(G) = 859296$$

Proof: From definition,

$$DB_2(G) = \sum_{uv\in E(G)} \frac{d_d(u)d_d(v)}{2}$$

$$= \frac{2(216\times288)}{2} + \frac{2(216\times264)}{2} + \frac{2(216\times216)}{2} + \frac{4(324\times324)}{2} + \frac{2(297\times324)}{2} + \frac{1(240\times408)}{2}$$

$$+ \frac{1(240\times264)}{2} + \frac{1(144\times204)}{2} + \frac{1(246\times288)}{2} + \frac{1(144\times384)}{2} + \frac{1(288\times384)}{2} + \frac{1(216\times384)}{2}$$

$$+ \frac{1(216\times240)}{2} + \frac{1(240\times324)}{2} + \frac{1(216\times324)}{2} + \frac{1(216\times297)}{2}$$

$$= \frac{2(62208)}{2} + \frac{2(57024)}{2} + \frac{2(46656)}{2} + \frac{4(104976)}{2} + \frac{2(96228)}{2} + \frac{1(97920)}{2} + \frac{1(63360)}{2} + \frac{1(29376)}{2}$$

$$+ \frac{1(70848)}{2} + \frac{1(55296)}{2} + \frac{1(110076)}{2} + \frac{1(82944)}{2} + \frac{1(51840)}{2} + \frac{1(77760)}{2} + \frac{1(69984)}{2} + \frac{1(64152)}{2}$$

=859206

Theorem 5. DB_3 index of chloroquine is

$$DB_3(G) = 1761081.75$$

Proof: From definition,

$$DB_3(G) = \sum_{uv\in E(G)} \left(\frac{d_d(u)+d_d(v)}{2}\right)^2 = \frac{2(216+288)^2}{4} + \frac{2(216+264)^2}{4} + \frac{2(216+216)^2}{4} + \frac{4(324+324)^2}{4} + \frac{2(297+324)^2}{4} +$$

$$\frac{1(240+408)^2}{4} + \frac{1(240+264)^2}{4} + \frac{1(144+204)^2}{4} + \frac{1(246+288)^2}{4} + \frac{1(144+384)^2}{4} + \frac{1(288+384)^2}{4} + \frac{1(216+384)^2}{4}$$

$$+ \frac{1(216+240)^2}{4} + \frac{1(240+324)^2}{4} + \frac{1(216+324)^2}{4} + \frac{1(216+297)^2}{4}$$

$$= \frac{2(504)^2}{4} + \frac{2(480)^2}{4} + \frac{2(432)^2}{4} + \frac{4(648)^2}{4} + \frac{2(621)^2}{4} + \frac{(648)^2}{4} + \frac{(504)^2}{4} + \frac{(348)^2}{4}$$

$$+ \frac{(534)^2}{4} + \frac{(528)^2}{4} + \frac{(672)^2}{4} + \frac{(600)^2}{4} + \frac{(456)^2}{4} + \frac{(564)^2}{4} + \frac{(540)^2}{4} + \frac{(513)^2}{4}$$

=1761081.75

4. Results for Hydroxychloroquine

Hydroxychloroquine is another drug which has antiviral activity very similar to that of chloroquine. The graph *H* of hydroxychloroquine has 22 atoms and 24 bonds, see Figure 2.

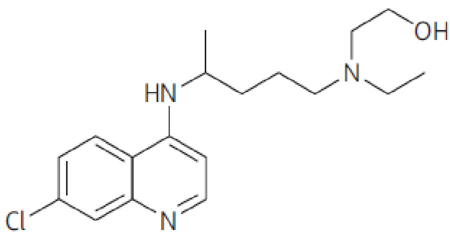

Fig. 2 Chemical structure of hydroxychloroquine

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

Table 2. Edge 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				

Theorem 6. mDM_1 index of hydroxychloroquine is

$$mDM_1(H) = 0.03163257708$$

Proof: From definition,

$$mDM_1(H) = \sum_{uv\in E(H)} \frac{1}{d_d(u)+d_d(v)}$$

$$= \frac{1}{210+350} + \frac{1}{210+425} + \frac{1}{207+324} + \frac{1}{207+567} + \frac{1}{315+317} + \frac{1}{315+385}$$
$$+ \frac{2}{315+420} + \frac{1}{315+425} + \frac{1}{317+340} + \frac{1}{317+385} + \frac{1}{324+324} + \frac{1}{324+459}$$
$$+ \frac{1}{324+567} + \frac{1}{324+621} + \frac{1}{340+486} + \frac{1}{350+385} + \frac{1}{350+595} + \frac{1}{385+420}$$
$$+ \frac{1}{420+425} + \frac{3}{459+486} + \frac{1}{486+567}$$
$$= \frac{1}{560} + \frac{1}{635} + \frac{1}{531} + \frac{1}{774} + \frac{1}{632} + \frac{1}{700} + \frac{2}{735} + \frac{1}{740} + \frac{1}{657} + \frac{1}{702} + \frac{1}{648}$$
$$+ \frac{1}{783} + \frac{1}{991} + \frac{1}{945} + \frac{1}{826} + \frac{1}{735} + \frac{1}{945} + \frac{1}{805} + \frac{1}{845} + \frac{3}{945} + \frac{1}{1053}$$

=0.03163257708

Theorem 7. mDM_2 index of hydroxychloroquine is

$$mDM_2(H) = 0.00018036173$$

Proof: From definition,

$$mDM_2(H) = \sum_{uv\in E(H)} \frac{1}{d_d(u)d_d(v)}$$

$$= \frac{1}{210\times350} + \frac{1}{210\times425} + \frac{1}{207\times324} + \frac{1}{207\times567} + \frac{1}{315\times317} + \frac{1}{315\times385}$$
$$+ \frac{2}{315\times420} + \frac{1}{315\times425} + \frac{1}{317\times340} + \frac{1}{317\times385} + \frac{1}{324\times324} + \frac{1}{324\times459}$$
$$+ \frac{1}{324\times567} + \frac{1}{324\times621} + \frac{1}{340\times486} + \frac{1}{350\times385} + \frac{1}{350\times595} + \frac{1}{385\times420}$$
$$+ \frac{1}{420\times425} + \frac{3}{459\times486} + \frac{1}{486\times567}$$

=0.00018036173

Theorem 8. DB_1 index of chloroquine is

$$DB_1(H) = 9406$$

Proof: From definition,

$$DB_1(H) = \sum_{uv\in E(H)} \frac{d_d(u)+d_d(v)}{2}$$

$$= \frac{210+350}{2} + \frac{210+425}{2} + \frac{207+324}{2} + \frac{207+567}{2} + \frac{315+317}{2} + \frac{315+385}{2}$$
$$+ \frac{2(315+420)}{2} + \frac{315+425}{2} + \frac{317+340}{2} + \frac{317+385}{2} + \frac{324+324}{2} + \frac{324+459}{2}$$
$$+ \frac{324+567}{2} + \frac{324+621}{2} + \frac{340+486}{2} + \frac{350+385}{2} + \frac{350+595}{2} + \frac{385+420}{2}$$
$$+ \frac{420+425}{2} + \frac{3(459+486)}{2} + \frac{486+567}{2}$$
$$= \frac{560}{2} + \frac{635}{2} + \frac{531}{2} + \frac{774}{2} + \frac{632}{2} + \frac{700}{2} + \frac{2\times735}{2} + \frac{740}{2} + \frac{657}{2} + \frac{702}{2} + \frac{648}{2}$$
$$+ \frac{783}{2} + \frac{991}{2} + \frac{945}{2} + \frac{826}{2} + \frac{735}{2} + \frac{945}{2} + \frac{805}{2} + \frac{845}{2} + \frac{3\times945}{2} + \frac{1053}{2}.$$

=9406

Theorem 9. DB_2 index of hydroxychloroquine is

$$DB_2(H) = 1814222.5$$

Proof: From definition,

$$DB_2(H) = \sum_{uv\in E(H)} \frac{d_d(u)d_d(v)}{2}$$

$$= \frac{210\times350}{2} + \frac{210\times425}{2} + \frac{207\times324}{2} + \frac{207\times567}{2} + \frac{315\times317}{2} + \frac{315\times385}{2}$$
$$+ \frac{2(315\times420)}{2} + \frac{315\times425}{2} + \frac{317\times340}{2} + \frac{317\times385}{2} + \frac{324\times324}{2} + \frac{324\times459}{2}$$
$$+ \frac{324\times567}{2} + \frac{324\times621}{2} + \frac{340\times486}{2} + \frac{350\times385}{2} + \frac{350\times595}{2} + \frac{385\times420}{2}$$
$$+ \frac{420\times425}{2} + \frac{3(459\times486)}{2} + \frac{486\times567}{2}$$

=1814222.5

Theorem 10. DB_3 index of hydroxychloroquine is

$$DB_3(H) = 3803337$$

Proof: From definition,

$$DB_3(H) = \sum_{uv\in E(H)} \left(\frac{d_d(u)+d_d(v)}{2}\right)^2$$

$$= \frac{(210+350)^2}{4} + \frac{(210+425)^2}{4} + \frac{(207+324)^2}{4} + \frac{(207+567)^2}{4} + \frac{(315+217)^2}{4} + \frac{(315+385)^2}{4}$$

$$+ \frac{2(315+420)^2}{4} + \frac{(315+425)^2}{4} + \frac{(317+340)^2}{4} + \frac{(317+385)^2}{4} + \frac{(324+324)^2}{4} + \frac{(324+459)^2}{4}$$

$$+ \frac{(324+567)^2}{4} + \frac{(324+621)^2}{4} + \frac{(340+486)^2}{4} + \frac{(350+385)^2}{4} + \frac{(350+595)^2}{4} + \frac{(385+420)^2}{4}$$

$$+ \frac{(420+425)^2}{4} + \frac{3(459+486)^2}{4} + \frac{(486+567)^2}{4}$$

$$= \frac{560^2}{4} + \frac{635^2}{4} + \frac{531^2}{4} + \frac{774^2}{4} + \frac{632^2}{4} + \frac{700^2}{4} + \frac{2\times(735)^2}{4} + \frac{740^2}{4} + \frac{657^2}{4} + \frac{702^2}{4} + \frac{648^2}{4}$$

$$+ \frac{783^2}{4} + \frac{991^2}{4} + \frac{945^2}{4} + \frac{826^2}{4} + \frac{735^2}{4} + \frac{945^2}{4} + \frac{805^2}{4} + \frac{845^2}{4} + \frac{3\times(945)^2}{4} + \frac{1053^2}{4}.$$

=3803337

5. Conclusion

Defined modified domination indices and domination Banhatti indices of a chemical graph and obtained computational values of chemical drugs such as chloroquine, hydroxychloroquine. These values can useful in planning the effective use of these two chemical drugs in Medical Science.

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