Domination, γ −Domination Topological Indices and φP −Polynomial of Some Chemical Structures Applied for the Treatment of COVID-19 Patients

Hanan Ahmed [1],* iD **, Anwar Alwardi** [2] iD **, Ruby Salestina M** [1]**, Soner Nandappa D** [3] iD

[1]   University of Mysore, Mysuru, India; hananahmed1a@gmail.com (H.A.); ruby.salestina@gmail.com (R.S.M.);
[2]   University of Aden, Yemen; a_wardi@hotmail.com (A.A.);
[3]   University of Mysore, Manasagangotri, Mysuru, India; e-mail: ndsoner@yahoo.co.in (S.N.D);
*   Correspondence: hananahmed1a@gmail.com;

Abstract: In medical science, pharmacology, chemical, biological, pharmaceutical properties of molecular structure are essential for drug preparation and design. These properties can be studied by using topological indices calculation. In this research work, we establish the topological properties of some chemical structures that have been applied for the treatment of COVID-19 patients by using the domination of topological indices and γ −domination indices. We determine the φP − polynomial for the antiviral chemical structures. The results obtained can help study the chemical properties of chemical structures that have been applied for the treatment of COVID-19 patients.

Keywords: COVID-19; chloroquine; hydroxy-chloroquine; domination indices; γ −domination indices; φP −polynomial.

1. Introduction

Historically, many infectious diseases have been recorded, and because of them, millions have died in the past few centuries. The most common infectious diseases were the plague, cholera, etc. In the later part of 2019, a new virus(COVID-19) began to multiply and spread, which disrupted the global economy and human health worldwide. So far, there is no specific vaccine available for this disease. Accordingly, it is necessary to determine the appropriate antiviral agents to control the pathogen. The existing antiviral drug test is an important experiment to test whether these drugs are useful in treating and combating related viral diseases [1-4]. Some of the antiviral compounds include chloroquine and hydroxy-chloroquine. Chloroquine is considered n antiviral drug [5-6] and is used to prevent and treat malaria and is also used to treat autoimmune diseases. Many experiments have been conducted to evaluate chloroquine's role and effect in treating COVID-19, and results of clinical trials have been reported in terms of controlling fever and delaying disease progression. Hydroxy-chloroquine has an antiviral effect that is broadly similar to that of chloroquine. More information on a comprehensive review has been carried out to conscripting the available knowledge about discovery, genomic structure, infection mechanism, and clinical features of SARS-CoV-2 see [7]. As per the Forbes report of 30 March 2020, FDA approves chloroquine and hydroxy-chloroquine for emergency corona-virus treatment. Information regarding the chemical, biological, and physical properties of compounds is important and useful in drug design. These characteristics can be predicted by the topological indices of the structure of

molecular graphs. A variety of topological indicators have been created and developed, and many studies have been conducted on them in various fields of molecular graphs and networks [8-19]. A set $D \subseteq V$ is said to be a dominating set of a graph G, if for any vertex $v \in V - D$, there is a vertex $u \in D$ such that u and v are adjacent. The domination number $\gamma(G)$ of a graph G is the minimum cardinality of a minimal dominating set in G. For more details on domination in graphs, see [20-24]. A dominating set $D = \{v_1, v_2, \ldots, v_r\}$ is minimal if $D - v_i$ is not a dominating set [25]. A dominating set of G of minimum cardinality is said to be a minimum dominating set. Topological indices are numerical parameters of a graph, and these parameters are the same for isomorphic graphs.

2. Materials and Methods

The main results obtained in this paper are based on domination topological indices of some drug structures that are considered antiviral, namely, chloroquine and hydroxy-chloroquine, with the help of φ_P-polynomials. In the partial diagram (fig.1 and fig. 3), we consider all vertices except for those vertices, representing the hydrogen atom, as the hydrogen atom does not contribute. We have used harmonic arithmetic, an edge segmentation method, analytical methods, and a score-counting method in the process of concluding. Here we have counted all minimal dominating sets and minimum dominating sets, and through these sets, the domination degree and the domination value were calculated for all vertices. The domination degree of a vertex v is equal to the number of minimal dominating sets containing v [26]. The domination value of v is the number of minimum dominating sets containing v [27]. And based on dividing the edges according to the new degrees of the vertices, φ_P-polynomials were calculated. Using these partitions, we have derived some closed forms of φ_P-polynomials. These polynomials give us the domination and $\gamma-$domination indices, which are calculated with some mathematical operators and Table 2. The numerical results were compared graphically using MATLAB.

3. Results and Discussion

3.1. Basic definitions.

In [26] Hanan Ahmed *et al*. have introduced new degree-based topological indices called domination topological indices, which are based on the domination degree defined as:

Definition 3.1.1. For each vertex $v \in V(G)$, the domination degree denotes by $d_d(v)$ and defined as the number of minimal dominating sets of G which contains v.

The first and second domination Zagreb indices and modified first Zagreb domination indices are defined as:

$DM_1(G) = \sum_{v \in V(G)} d_d^2(v)$,

$DM_2(G) = \sum_{uv \in E(G)} d_d(u)d_d(v)$,

$DM_1^* = \sum_{uv \in E(G)} [d_d(u) + d_d(v)]$

where $d_d(v)$ is the domination degree of the vertex v. The minimum and maximum domination degree of G are denoted by $\delta_d(G) = \delta_d$ and $\Delta_d(G) = \Delta_d$, respectively. In which $\delta_d = \min\{d_d(v): v \in V(G)\}$ and $\Delta_d = \max\{d_d(v): v \in V(G)\}$. In [26], the total number of minimal dominating sets of G is denoted as $T_m(G)$. The forgotten domination, hyper domination, and modified forgotten domination indices of graphs [26] are defined as:

$DF(G) = \sum_{v \in V(G)} d_d^3(v)$,

$$DH(G) = \sum_{uv \in E(G)} [d_d(u) + d_d(v)]^2 ,$$

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

Definition 3.1.2. For each vertex $v \in V(G)$, the domination value of v is defined as [27]:

$$d_\gamma(v) = |\{S \subseteq V(G): S \text{ is a minimum dominating set and } v \in S\}|.$$

We denote the minimum and maximum domination value of a graph G by
$$\delta_\gamma(G) = \delta_\gamma = \min\{d_\gamma(v): v \in V(G)\} \text{ and } \Delta_\gamma(G) = \Delta_\gamma = \max\{d_\gamma(v): v \in V(G)\} \text{ respectively.}$$
We introduce new degree-based topological indices that depend on domination value.

Definition 3.1.3. Let $G = (V, E)$ be any graph. we give the following definition
(i) First and second γ −domination Zagreb indices

$$\gamma M_1(G) = \sum_{v \in V(G)} d_\gamma^2(v) \quad , \quad \gamma M_2(G) = \sum_{uv \in E(G)} d_\gamma(u)d_\gamma(v) ,$$

(ii) Forgotten γ −domination and hyper γ −domination indices

$$\gamma F(G) = \sum_{v \in V(G)} d_\gamma^3(v) \quad , \quad \gamma H(G) = \sum_{uv \in E(G)} [d_\gamma(u) + d_\gamma(v)]^2 ,$$

(iii) Modified first γ −domination Zagreb and modified forgotten γ −domination indices

$$\gamma M_1^* = \sum_{uv \in E(G)} d_\gamma(u) + d_\gamma(v) \quad , \quad \gamma F^*(G) = \sum_{uv \in E(G)} d_\gamma^2(u) + d_\gamma^2(v) .$$

Definition 3.1.4. Let $G = (V, E)$ be a graph, $d_P(v)$ be the P set degree of the vertex v define as

$$d_P(v) = |\{S \subseteq V(G): S \text{ has property } P \text{ and } v \in S\}|.$$

We denote the minimum and maximum P set the degree of G as $\delta_P(G) = \delta_P$ and $\Delta_P(G) = \Delta_P$ respectively. Where $\delta_P = \min\{d_P(v): v \in V(G)\}$ and $\Delta_P = \max\{d_P(v): v \in V(G)\}$

Let $d_p m_{i,j}(G) = |\{e = uv: d_P(u) = i, d_P(v) = j\}|$. We now define φ_P-Polynomial as

$$\varphi_P(G, x, y) = \sum_{\delta_P \leq i \leq j \leq \Delta_P} d_p m_{i,j}(G) x^i y^j .$$

Table 1. The description of some domination and γ −domination topological indices.

D indices	$f(d_d(u), d_d(v))$	γD indices	$f(d_\gamma(u), d_\gamma(v))$
$DM_1^*(G)$	$d_d(u) + d_d(v)$	$\gamma M_1^*(G)$	$d_\gamma(u) + d_\gamma(v)$
$DF^*(G)$	$d_d^2(u) + d_d^2(v)$	$\gamma F^*(G)$	$d_\gamma^2(u) + d_\gamma^2(v)$
$DM_2(G)$	$d_d(u) + d_d(v)$	$\gamma M_2(G)$	$d_\gamma(u)d_\gamma(v)$
$HD(G)$	$d_d^2(u) + d_d^2(v) + 2d_d(u)d_d(v)$	$\gamma H(G)$	$d_d^2(u) + d_d^2(v) + 2d_d(u)d_d(v)$

Domination (D) and γ −Domination (γD) indices defined on E(G) can be written as in Table1.
And

$$D(G) = \sum_{uv \in E(G)} f(d_d(u), d_d(v)), \quad \gamma D(G) = \sum_{uv \in E(G)} f(d_\gamma(u), d_\gamma(v)) .$$

Table 2. Derivation of domination and γ −domination topological indices from φ_P −polynomials.

D indices	Derivation from $\varphi_d(G)$	γD indices	Derivation from $\varphi_\gamma(G)$
$DM_1^*(G)$	$(D_x + D_y)(\varphi_d(G))|_{x=y=1}$	$\gamma M_1^*(G)$	$(D_x + D_y)(\varphi_\gamma(G))|_{x=y=1}$
$DF^*(G)$	$(D_x^2 + D_y^2)(\varphi_d(G))|_{x=y=1}$	$\gamma F^*(G)$	$(D_x^2 + D_y^2)(\varphi_\gamma(G))|_{x=y=1}$
$DM_2(G)$	$(D_x D_y)(\varphi_d(G))|_{x=y=1}$	$\gamma M_2(G)$	$(D_x D_y)(\varphi_\gamma(G))|_{x=y=1}$
$HD(G)$	$(D_x + D_y)^2(\varphi_d(G))|_{x=y=1}$	$\gamma H(G)$	$(D_x + D_y)^2(\varphi_\gamma(G))|_{x=y=1}$

Here, $D_x(f(x, y)) = x\frac{\partial(f(x,y))}{\partial x} \quad , \quad D_y(f(x, y)) = y\frac{\partial(f(x,y))}{\partial y}$

3.2. Discussion.

Suppose G is the molecular graph of chloroquine as in Figure 1. This graph is of order 22 and size 23. We find the minimal dominating sets and determine the domination degree and domination value of all vertices of G. Using this new degree, we calculate domination and γ −domination topological indices and φ_P −polynomial of the molecular structure of chloroquine.
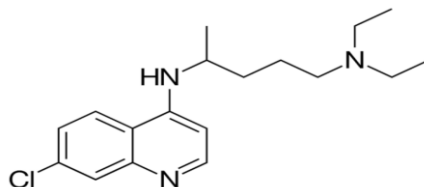

Figure 1. Chemical structure of chloroquine.

Theorem 3.2.1. The total number of minimal and minimum dominating sets in the molecular graph of chloroquine is 648 and 6, respectively.

Proof. Let G be the molecular graph of chloroquine. We first divide G into four components A_1, A_2, A_3 and A_4. We calculate the minimal dominating sets of each component so that we get $T_m(A_1) = 8$, $T_m(A_2) = 5$, $T_m(A_3) = 7$ and $T_m(A_4) = 4$.

Every minimal dominating set of A_2 is added to each minimal dominating set of A_1 and we check for the minimality of the resulting dominating sets. As a result, we get 27 minimal dominating sets.

Next, every minimal dominating set of A_3 is added to each of these 27 minimal dominating sets, and we check for the minimality of the resulting dominating sets. Here, we get $27 \times 7 = 189$ minimal dominating sets.

Again, every minimal dominating set of A_4 is added to each of the 189 minimal dominating sets, and we check for the minimality of the resulting dominating sets. In this case, we get a total of $4 \times 189 = 756$ minimal dominating sets, of which 108 are repeated.

In all, there is 648 minimal dominating set of G. Note that $\gamma(G) = 7$. We have the fact that every minimum dominating set is a minimal dominating set. Out of 648 minimal dominating sets, there are exactly 6 sets whose cardinality is equal to the domination number of G. Hence G has 6 minimum dominating sets.

Table 3. The domination degrees of all vertices of the molecular graph of chloroquine.

$d_d(v)$	324	216	240	264	288	408	384	144	297
Number of the vertices	7	5	2	2	2	1	1	1	1

Table 4. The domination value of the vertices of the molecular graph of chloroquine

$d_\gamma(v)$	0	2	3	4	6
Number of the vertices	12	2	2	2	4

Theorem 3.2.2. If G is the molecular graph of chloroquine, then

$$\varphi_d(G, x, y) = x^{144}[y^{384} + y^{240}] + x^{216}[2y^{264} + 2y^{288} + 2y^{216} + y^{324} + y^{240} + y^{297} + y^{384}]$$

$$+ x^{240}[y^{264} + y^{324} + y^{408}] + x^{264}y^{288} + x^{288}y^{384} + 2y^{324}[x^{297} + 2x^{324}],$$

$$\varphi_\gamma(G, x, y) = 5 + 2y^3 + 2y^4 + 11y^6 + 2x^2y^4 + x^3y^3.$$

Proof. Case 1. Let $d_d m_{ij}(G) = |\{e = uv: d_d(u) = i, d_d(v) = j\}|$. The edge set of G can be divided into sixteen partitions based on the domination degree of end vertices of each edge as given in Table 5.

Table 5. Edge partition based on the domination degree of the end vertices of each edge.

(i,j)	(216,288)	(216,264)	(216,216)	(324,324)	(297,324)	(240,408)	(240,264)
$d_d m_{i,j}$	2	2	2	4	2	1	1
(i,j)	(144,204)	(246,288)	(144,384)	(288,384)	(216,384)	(216,240)	(240,324)
$d_d m_{i,j}$	1	1	1	1	1	1	1
(i,j)	(216,324)	(216,297)	.	.	.	.	.
$d_d m_{i,j}$	1	1	.	.	.	.	.

Hence from the Table 5, we get:

$$\varphi_d(G, x, y) = \sum_{\delta_d \le i \le j \le \Delta_d} d_d m_{ij}(G)x^i y^j = x^{144}[y^{384} + y^{240}]$$
$$+x^{216}[2y^{264} + 2y^{288} + 2y^{216} + y^{324} + y^{240} + y^{297} + y^{384}]$$
$$+x^{240}[y^{264} + y^{324} + y^{408}] + x^{264}y^{288} + x^{288}y^{384} + 2y^{324}[x^{297} + 2x^{324}]$$

Case 2.

The edge partition depends on the domination value of each edge's end vertices, as given in Table 6.

Table 6. Edge partition depends on the domination value of end vertices of each edge.

(i,j)	(0,0)	(0,3)	(0,6)	(3,3)	(0,4)	(2,4)
$|d_\gamma m_{i,j}|$	5	2	11	1	2	2

So, from Table 6, we get

$$\varphi_\gamma(G, x, y) = \sum_{\delta_\gamma \le i \le j \le \Delta_\gamma} d_\gamma m_{ij}(G)x^i y^j = 5 + 2y^3 + 2y^4 + 11y^6 + 2x^2y^4 + x^3y^3 .$$

In Figure 2, we plotting φ_d −polynomial and and φ_γ −Polynomial of Chloroquine.
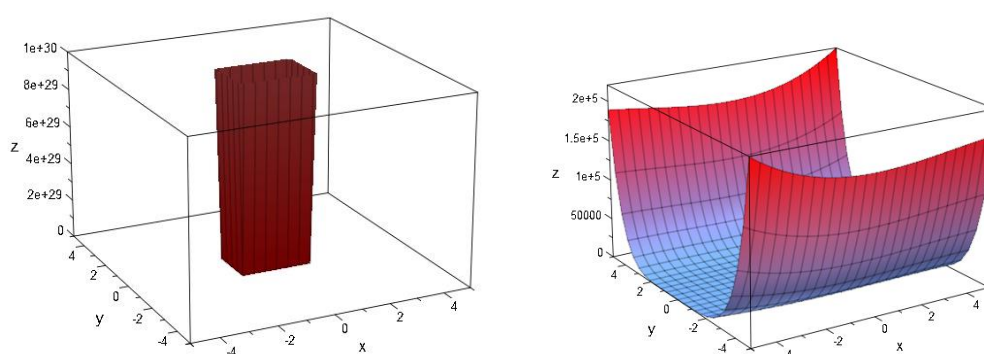
Figure 2. Plotting of (a) φ_d −polynomial and (b) φ_γ −Polynomial of Chloroquine.

Theorem 3.2.3. Suppose G is the molecular graph of chloroquine. Then

1. $DM_1^*(G) = 12627, \gamma M_1^*(G) = 98,$

2. $DM_2(G) = 1728576, \quad \gamma M_2(G) = 25,$

3. $DF^*(G) = 3633075, \quad \gamma F^*(G) = 504,$

4. $DH(G) = 7090227, \quad \gamma H(G) = 554,$

5. $DM_1(G) = 1811457, \quad \gamma M_1(G) = 202,$

6. $DF(G) = 554421762, \quad \gamma F(G) = 1062.$

Proof. We have,

$$\varphi_d(G, x, y) = x^{144}[y^{384} + y^{240}] + x^{216}[2y^{264} + 2y^{288} + 2y^{216} + y^{324} + y^{240} + y^{297} + y^{384}]$$

$$+ x^{240}[y^{264} + y^{324} + y^{408}] + x^{264}y^{288} + x^{288}y^{384} + 2y^{324}[x^{297} + 2x^{324}].$$

Then

$$(D_x + D_y)(\varphi_d(G, x, y)) = x^{144}[528y^{384} + 384y^{240}] + x^{216}[960y^{264} + 1008y^{288} + 864y^{216}$$

$$+ 540y^{324} + 456y^{240} + 513y^{297} + 600y^{384}] + 552x^{264}y^{288} + 672x^{288}y^{384}$$

$$+ x^{240}[504y^{264} + 564y^{324} + 648y^{408}] + y^{324}[1242x^{297} + 2592x^{324}],$$

$$(D_x D_y)(\varphi_d(G, x, y))$$
$$= 144x^{144}[384y^{384} + 240y^{240}] + 216x^{216}[528y^{264} + 567y^{288} + 432y^{216}$$

$$+ 324y^{324} + 240y^{240} + 297y^{297} + 384y^{384}] + 240x^{240}[264y^{264} + 324y^{324}$$

$$+ 408y^{408}] + 76032x^{264}y^{288} + 110592x^{288}y^{384} + 648y^{324}[297x^{297} + 648x^{324}],$$

$$(D_x^2 + D_y^2)(\varphi_d(G, x, y))$$
$$= x^{144}[168192y^{384} + 78336y^{240}] + x^{216}[232704y^{264} + 259200y^{288} + 186624y^{216}$$

$$+ 151632y^{324} + 104256y^{240} + 134865y^{297} + 194112y^{384}] + x^{240}[127296y^{264}$$

$$+ 162576y^{324} + 224064y^{408}] + 152640x^{264}y^{288} + 230400x^{288}y^{384}$$

$$+ y^{324}[386370x^{297} + 839808x^{324}],$$

$$(D_x^2 + D_y^2)(\varphi_d(G, x, y))$$
$$= x^{144}[168192y^{384} + 78336y^{240}] + x^{216}[232704y^{264} + 259200y^{288} + 186624y^{216}$$

$$+ 151632y^{324} + 104256y^{240} + 134865y^{297} + 194112y^{384}] + x^{240}[127296y^{264}$$

$$+ 162576y^{324} + 224064y^{408}] + 152640x^{264}y^{288} + 230400x^{288}y^{384}$$

$$+ y^{324}[386370x^{297} + 839808x^{324}],$$

$$(D_x^2 + D_y^2 + 2D_x D_y)(\varphi_d(G, x, y))$$
$$= x^{144}[278784y^{384} + 147456y^{240}] + x^{216}[460800y^{264} + 508032y^{288}$$

$$+373248y^{216} + 291600y^{324} + 207936y^{240} + 263169y^{297} + 360000y^{384}]$$

$$+x^{240}[254016y^{264} + 318096y^{324} + 419904y^{408}] + 304704x^{246}y^{288}$$

$$+451584x^{288}y^{384} + y^{324}[771282x^{297} + 1679616x^{324}].$$

By using Table 2, we get

$$DM_1^*(G) = x^{144}[528y^{384} + 384y^{240}] + x^{216}[960y^{264} + 1008y^{288} + 864y^{216}$$

$$+540y^{324} + 456y^{240} + 513y^{297} + 600y^{384}] + 552x^{264}y^{288} + 672x^{288}y^{384}$$

$$x^{240}[504y^{264} + 564y^{324} + 648y^{408}] + y^{324}[1242x^{297} + 2592x^{324}]|_{x=y=1} = 12627,$$

$$DM_2(G) = 144x^{144}[384y^{384} + 240y^{240}] + 216x^{216}[528y^{264} + 567y^{288} + 432y^{216}$$

$$+324y^{324} + 240y^{240} + 297y^{297} + 384y^{384}] + 240x^{240}[264y^{264} + 324y^{324}$$

$$+408y^{408}] + 76032x^{264}y^{288} + 110592x^{288}y^{384} + 648y^{324}[297x^{297}$$

$$+648x^{324}]|_{x=y=1} = 1728576,$$

$$DF^*(G) = x^{144}[168192y^{384} + 78336y^{240}] + x^{216}[232704y^{264} + 259200y^{288}$$
$$+ 186624y^{216}$$

$$+151632y^{324} + 104256y^{240} + 134865y^{297} + 194112y^{384}] + x^{240}[127296y^{264}$$

$$+162576y^{324} + 224064y^{408}] + 152640x^{264}y^{288} + 230400x^{288}y^{384}$$

$$+y^{324}[386370x^{297} + 839808x^{324}]|_{x=y=1} = 3633075,$$

$$DH(G) = x^{144}[278784y^{384} + 147456y^{240}] + x^{216}[460800y^{264} + 508032y^{288}$$

$$+373248y^{216} + 291600y^{324} + 207936y^{240} + 263169y^{297} + 360000y^{384}]$$

$$+x^{240}[254016y^{264} + 318096y^{324} + 419904y^{408}] + 304704x^{246}y^{288}$$

$$+451584x^{288}y^{384} + y^{324}[771282x^{297} + 1679616x^{324}]|_{x=y=1} = 7090227.$$

By using Table 3, and the definition of first domination Zagreb and forgotten domination indices we get, $DM_1(G) = 1811457$ and $DF(G) = 554421762$

For γ −domination indices, we have

$$\varphi_\gamma(G, x, y) = \sum_{\delta_\gamma \leq i \leq j \leq \Delta_\gamma} d_\gamma m_{ij}(G)x^i y^j = 5 + 2y^3 + 2y^4 + 11y^6 + 2x^2 y^4 + x^3 y^3$$

Then

$$(D_x + D_y)(\varphi_\gamma(G, x, y)) = 12x^2 y^4 + 6x^3 y^3 + 6y^3 + 8y^4 + 66y^6,$$

$$(D_x D_y)(\varphi_\gamma(G, x, y)) = 16x^2y^4 + 9x^3y^3,$$

$$(D_x^2 + D_y^2)(\varphi_\gamma(G, x, y)) = 40x^2y^4 + 18x^3y^3 + 18y^3 + 32y^4 + 396y^6,$$

$$(D^2 + x + D_y^2 + 2D_xD_y)(\varphi_\gamma(G, x, y)) = 72x^2y^4 + 36x^3y^3 + 18y^3 + 32y^4 + 396y^6.$$

By using Table 2, we get

$$\gamma M_1^*(G) = 12x^2y^4 + 6x^3y^3 + 6y^3 + 8y^4 + 66y^6|_{x=y=1} = 98,$$

$$\gamma M_2(G) = 16x^2y^4 + 9x^3y^3|_{x=y=1} = 25,$$

$$\gamma F^*(G) = 40x^2y^4 + 18x^3y^3 + 18y^3 + 32y^4 + 396y^6|_{x=y=1} = 504,$$

$$\gamma H(G) = 72x^2y^4 + 36x^3y^3 + 18y^3 + 32y^4 + 396y^6|_{x=y=1} = 554.$$

Finally, by using Table 4, we get $\gamma M_1(G) = 202$ and $\gamma F(G) = 1062$.

Suppose H is the molecular graph of hydroxy-chloroquine as in Figure 3. This graph has an order 23 and size 24. We find the minimal dominating sets and determine the domination degree and domination value of all vertices of H. Using this new degree, we calculate domination and γ −domination topological indices and φ_P −polynomial of the molecular structure of hydroxy-chloroquine.
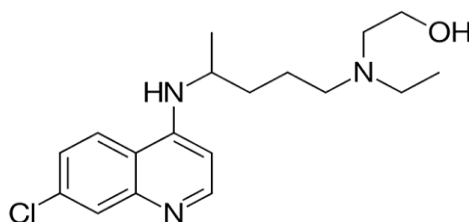

Figure 3. Chemical structure of hydroxy-chloroquine.

Theorem 3.2.4. The total number of minimal dominating and minimum dominating sets of the molecular graph of hydroxy-chloroquine is 945 and 2, respectively.

Proof. Proof of this theorem is on the same line as that of Theorem 3.2.1.

To obtain φ_d and φ_γ polynomials of H, Table 7 and 8, are essential.

Table 7. Domination degrees of vertices of H.

$d_d(v)$	459	324	385	315	420	486	621	567
Number of vertices	3	3	2	2	2	2	1	1
$d_d(v)$	297	340	317	210	425	350	595	.
Number of vertices	1	1	1	1	1	1	1	.

Table 8. Domination value of vertices of H.

$d_\gamma(v)$	0	1	2
Number of vertices	16	2	5

Theorem 3.2.5. Suppose H is the molecular structure of hydroxy-chloroquine. Then,

$$\varphi_d(H, x, y) = x^{210}[y^{350} + y^{425}] + x^{297}[y^{324} + y^{567}] + x^{315}[y^{317} + y^{385} + 2y^{420} + y^{425}]$$

$$+x^{317}[y^{340} + y^{385}] + x^{324}[y^{324} + y^{459} + y^{567} + y^{621}] + x^{340}y^{486}$$

$$+x^{350}[y^{385} + y^{595}] + x^{385}y^{420} + x^{420}y^{425} + 3x^{459}y^{486} + x^{486}y^{567},$$

$$\varphi_\gamma(H, x, y) = 15y^2 + 2y + xy + 6.$$

Proof.   Case 1. Let $d_d m_{ij}(G) = |\{e = uv: d_d(u) = i, d_d(v) = j\}|$.

Table 9. Edges partition based on the domination degree of the end vertices of each edge.

(i,j)	(210,350)	(210,425)	(297,324)	(297,567)	(315,317)	(315,385)	(315,420)
$d_d m_{i,j}$	1	1	1	1	1	1	2
(i,j)	(315,425)	(317,340)	(317,385)	(324,324)	(324,459)	(324,567)	(324,621)
$d_d m_{i,j}$	1	1	1	1	1	1	1
(i,j)	(340,486)	(350,385)	(350,595)	(385,420)	(420,425)	(459,486)	(486,567)
$d_d m_{i,j}$	1	1	1	1	1	3	1

So, from Table 9, we get

$$\varphi_d(H, x, y) = x^{210}[y^{350} + y^{425}] + x^{297}[y^{324} + y^{567}] + x^{315}[y^{317} + y^{385} + 2y^{420} + y^{425}]$$

$$+x^{317}[y^{340} + y^{385}] + x^{324}[y^{324} + y^{459} + y^{567} + y^{621}] + x^{340}y^{486}$$

$$+x^{350}[y^{385} + y^{595}] + x^{385}y^{420} + x^{420}y^{425} + 3x^{459}y^{486} + x^{486}y^{567}.$$

Case 2: The partition of edges depending on the domination value of the vertices give $d_\gamma m_{0,0} = 5$, $d_\gamma m_{0,3} = 2$, $d_\gamma m_{0,6} = 11$, $d_\gamma m_{3,3} = 1$, $d_\gamma m_{2,4} = 2$ and $d_\gamma m_{0,4} = 2$.

$$\varphi_\gamma(H, x, y) = d_\gamma m_{0,0} + d_\gamma m_{0,3}y^3 + d_\gamma m_{0,6}y^6 + d_\gamma m_{3,3}x^3y^3 + d_\gamma m_{2,4}x^2y^2 + d_\gamma m_{0,4}y^4$$

Substituting the values of $d_\gamma m_{i,j}$ we get,

$$\varphi_\gamma(H, x, y) = 15y^2 + 2y + xy + 6.$$

In Figure 4, we present the 3D representation of φ_d −polynomial and φ_γ −Polynomial of Hydroxy-chloroquine.
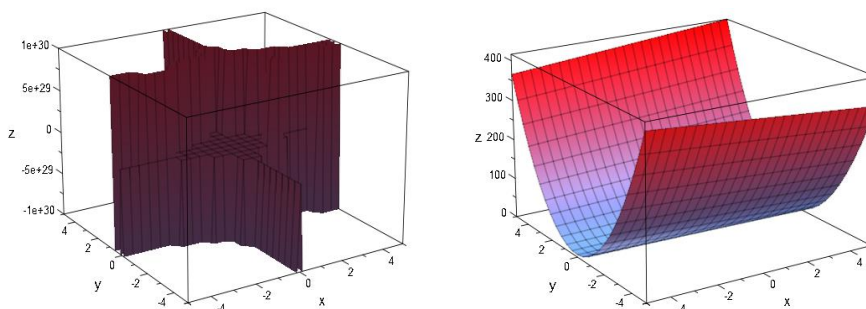
Figure 4. Plotting of (a)φ_d −polynomial and (b) φ_γ −Polynomial of Hydroxy-chloroquine.

Theorem 3.2.6. Suppose H is the molecular graph of hydroxy-chloroquine. Then
1. $DM_1^*(H) = 18892$, $\gamma M_1^*(H) = 34$,

2. $DM_2(H) = 3708635, \quad \gamma M_2(H) = 1,$

3. $DF^*(H) = 7858978, \quad \gamma F^*(H) = 64,$

4. $DH(H) = 15276248, \quad \gamma H(H) = 66,$

5. $DM_1(H) = 4003420, \gamma M_1(H) = 22,$

6. $DF(H) = 1820798614, \gamma F(H) = 42.$

Proof. We have,

$$\varphi_d(H, x, y) = x^{210}[y^{350} + y^{425}] + x^{297}[y^{324} + y^{567}] + x^{315}[y^{317} + y^{385} + 2y^{420} + y^{425}]$$

$$+ x^{317}[y^{340} + y^{385}] + x^{324}[y^{324} + y^{459} + y^{567} + y^{621}] + x^{340}y^{486}$$

$$+ x^{350}[y^{385} + y^{595}] + x^{385}y^{420} + x^{420}y^{425} + 3x^{459}y^{486} + x^{486}y^{567}.$$

Then,

$$(D_x + D_y)(\varphi_d(H, x, y)) = x^{210}[560y^{350} + 635y^{425}] + x^{297}[621y^{324} + 864y^{567}]$$

$$+ x^{315}[632y^{317} + 700y^{385} + 1470y^{420} + 740y^{425}]$$

$$+ x^{317}[657y^{340} + 702y^{385}] + x^{324}[648y^{324} + 783y^{459} + 891y^{567} + 945y^{621}]$$

$$+ 826x^{340}y^{486} + x^{350}[735y^{385} + 945x^{595}] + 805x^{385}y^{420} + 845x^{420}y^{425}$$

$$+ 2835x^{459}y^{486} + 1053x^{486}y^{567},$$

$(D_xD_y)(\varphi_d(H, x, y)) = 210x^{210}[350y^{350} + 425y^{425}] + 297x^{297}[324y^{324} + 567y^{567}] + 315x^{314}[317y^{317} + 385y^{385} + 840y^{420} + 425y^{425}] + 317x^{317}[340y^{340} + 385y^{385}] + 324x^{324}[324y^{324} + 459y^{459} + 567y^{567} + 621y^{621}] + 165240x^{340}y^{486} + 350x^{350}[385y^{385} + 595y^{595}] + 161700x^{385}y^{420} + 178500x^{420}y^{425} + 669222x^{459}y^{486} + 275562x^{486}y^{567},$

$(D_x^2 + D_y^2)(\varphi_d(H, x, y))$
$$= x^{210}[166600y^{350} + 224725y^{425}] + x^{297}[193185y^{324} + 409698y^{567}]$$

$$+ x^{315}[199714y^{317} + 247450y^{385} + 551250y^{240} + 279850y^{425}]$$

$$+ x^{317}[216089y^{340} + 248714y^{385}] + x^{324}[209952y^{324} + 315657y^{459} + 426465y^{567}$$

$$+ 490617y^{621}] + 351796x^{340}y^{486} + x^{350}[270725y^{385} + 476525y^{595}]$$

$$+ 324625x^{385}y^{425} + 357025x^{420}y^{425} + 1340631x^{459}y^{486} + 557685x^{486}y^{567},$$

$(D_x^2 + D_y^2 + 2D_xD_y)(\varphi_d(H, x, y))$
$$= x^{210}[313600y^{350} + 403225y^{425}] + x^{297}[385641y^{324} + 746496y^{567}]$$

$$+x^{315}[399424y^{317} + 490000y^{385} + 1080450y^{240} + 547600y^{425}]$$

$$+x^{317}[431649y^{340} + 492804y^{385}] + x^{324}[419904y^{324} + 613089y^{459}$$

$$+793881y^{567} + 893025y^{621}] + 682276x^{340}y^{486} + x^{350}[540225y^{385}$$

$$+893025y^{495}] + 648025x^{385}y^{420} + 714025x^{420}y^{425} + 2679075x^{459}y^{486}$$

$$+1108809x^{486}y^{567}.$$

Hence,

$$DM_1^*(H) = x^{210}[560y^{350} + 635y^{425}] + x^{297}[621y^{324} + 864y^{567}] + x^{315}[632y^{317} + 700y^{385}$$

$$+1470y^{420} + 740y^{425}] + x^{317}[657y^{340} + 702y^{385}] + x^{324}[648y^{324} + 783y^{459} + 891y^{567}$$

$$+945y^{621}] + 826x^{340}y^{486} + x^{350}[735y^{385} + 945x^{595}] + 805x^{385}y^{420} + 845x^{420}y^{425} + 2835x^{459}y^{486} + 1053x^{486}y^{567}|_{x=y=1} = 18892,$$

$$DM_2(H) = 210x^{210}[350y^{350} + 425y^{425}] + 297x^{297}[324y^{324} + 567y^{567}] + 315x^{314}[317y^{317}$$

$$+385y^{385} + 840y^{420} + 425y^{425}] + 317x^{317}[340y^{340} + 385y^{385}] + 324x^{324}[324y^{324}$$

$$+459y^{459} + 567y^{567} + 621y^{621}] + 165240x^{340}y^{486} + 350x^{350}[385y^{385} + 595y^{595}]$$

$$+161700x^{385}y^{420} + 178500x^{420}y^{425} + 669222x^{459}y^{486} + 275562x^{486}y^{567}|_{x=y=1}$$
$$= 3708635,$$

$$DF^*(H) = x^{210}[166600y^{350} + 224725y^{425}] + x^{297}[193185y^{324} + 409698y^{567}]$$

$$+x^{315}[199714y^{317} + 247450y^{385} + 551250y^{240} + 279850y^{425}]$$

$$+x^{317}[216089y^{340} + 248714y^{385}] + x^{324}[209952y^{324} + 315657y^{459} + 426465y^{567}$$

$$+490617y^{621}] + 351796x^{340}y^{486} + x^{350}[270725y^{385} + 476525y^{595}]$$

$$+324625x^{385}y^{425} + 357025x^{420}y^{425} + 1340631x^{459}y^{486} + 557685x^{486}y^{567}|_{x=y=1}$$
$$= 7858978,$$

$$DH(H) = x^{210}[313600y^{350} + 403225y^{425}] + x^{297}[385641y^{324} + 746496y^{567}]$$

$$+x^{315}[399424y^{317} + 490000y^{385} + 1080450y^{240} + 547600y^{425}]$$

$$+x^{317}[431649y^{340} + 492804y^{385}] + x^{324}[419904y^{324} + 613089y^{459}$$

$$+793881y^{567} + 893025y^{621}] + 682276x^{340}y^{486} + x^{350}[540225y^{385}$$

$$+893025y^{495}] + 648025x^{385}y^{420} + 714025x^{420}y^{425} + 2679075x^{459}y^{486}$$

$$+1108809x^{486}y^{567}|_{x=y=1} = 15276248.$$

By using the definition of first domination Zagreb and forgotten domination indices we get,

$$DM_1(H) = 4003420 , \quad DF(H) = 1820798614.$$

In the same way, we can calculate the γ −domination indices of H.

4. Conclusions

In this research, we have studied the topological characteristics of some chemical compounds, namely chloroquine and hydroxy-chloroquine, that are used to prevent the spread of the COVID-19 epidemic through some indices based on domination degree and domination value. First, we find φ_d −polynomial and φ_γ −polynomial and their respective 3D graphs. Then we compute the domination and γ −domination indices from these polynomials. It is known that topological indices can predict some different characteristics, such as the central factor, stability of chemical compounds, boiling point, etc., and the results obtained in this research paper have significance in the study of some properties for chemical compounds used to prevent the spread of the COVID-19.

Funding

Acknowledgments

Conflicts of Interest

The authors declare no conflict of interest.

References

1. Schrezenmeier, E.; Dörner, T. Mechanisms of action of hydroxychloroquine and chloroquine: implications for rheumatology. *Nature Reviews Rheumatology* **2020**, *16*, 155-166, https://doi.org/10.1038/s41584-020-0372-x
2. Wang, M.; Cao, R.; Zhang, L.; Yang, X.; Liu, J.; Xu, M.; Shi, Z.; Hu, Z.; Zhong, W.; Xiao, G. Remdesivir and chloroquine effectively inhibit the recently emerged novel coronavirus (2019-nCoV) in vitro. *Cell Research* **2020**, *30*, 269-271, https://doi.org/10.1038/s41422-020-0282-0.
3. Xu, X.; Chen, P.; Wang, J.; Feng, J.; Zhou, H.; Li, X.; Zhong, W.; Hao, P. Evolution of the novel coronavirus from the ongoing Wuhan outbreak and modeling of its spike protein for risk of human transmission. *Science China Life Sciences* **2020**, *63*, 457-460, https://doi.org/10.1007/s11427-020-1637-5.
4. Zhou, D.; Dai, S.-M.; Tong, Q. COVID-19: a recommendation to examine the effect of hydroxychloroquine in preventing infection and progression. *Journal of Antimicrobial Chemotherapy* **2020**, *75*, 1667-1670, https://doi.org/10.1093/jac/dkaa114.
5. Savarino, A.; Di Trani, L.; Donatelli, I.; Cauda, R.; Cassone, A. New insights into the antiviral effects of chloroquine. *The Lancet Infectious Diseases* **2006**, *6*, 67-69, https://doi.org/10.1016/S1473-3099(06)70361-9.
6. Yan, Y.; Zou, Z.; Sun, Y.; Li, X.; Xu, K.-F.; Wei, Y.; Jin, N.; Jiang, C. Anti-malaria drug chloroquine is highly effective in treating avian influenza A H5N1 virus infection in an animal model. *Cell Research* **2013**, *23*, 300-302, https://doi.org/10.1038/cr.2012.165

7. Dan, S. Insights into the Origin, Transmission and Outbreak of Coronavirus Disease (Covid 19): A Recent Study. *Asian Journal of Chemistry* **2020**, *32*, 2403-2415, https://doi.org/10.14233/ajchem.2020.22891.
8. De, N. Computing Reformulated First Zagreb Index of Some Chemical Graphs as an Application of Generalized Hierarchical Product of Graphs. **2018**, *2(2018)*, 338-350,
9. Gao, W.; Asif, M.; Nazeer, W. The Study of Honey Comb Derived Network via Topological Indices. *Open Journal of Mathematical Analysis* **2018**, *2*, 10-26, http://dx.doi.org/10.30538/psrp-oma2018.0014.
10. Mondal, S.; De, N.; Pal, A. Topological properties of Graphene using some novel neighborhood degree-based topological indices. *International Journal of Mathematics for Industry* **2019**, *11*, https://doi.org/10.1142/S2661335219500060.
11. Zheng, L.; Wang, Y.; Gao, W. Topological Indices of Hyaluronic Acid-Paclitaxel Conjugates' Molecular Structure in Cancer Treatment. *Open Chemistry* **2019**, *17*, 81-87, https://doi.org/10.1515/chem-2019-0009.
12. Mondal, S.; De, N.; Pal, A. Topological Indices of Some Chemical Structures Applied for the Treatment of COVID-19 Patients. *Polycyclic Aromatic Compounds* **2020**, https://doi.org/10.1080/10406638.2020.1770306.
13. Qing, X.; Wang, Z.; Munir, M.; Ahmad, H. Molecular Irregularity Indices of Nanostar, Fullerene, and Polymer Dendrimers. *Journal of Chemistry* **2020**, *2020*, 1–12, https://doi.org/10.1155/2020/9437612.
14. Hussain, Z.; Munir, M.; Rafique, S.; Hussnain, T.; Ahmad, H.; Chel Kwun, Y.; Min Kang, S. Imbalance-Based Irregularity Molecular Descriptors of Nanostar Dendrimers. *Processes* **2019**, *7*, 517-532, https://doi.org/10.3390/pr7080517.
15. Gao, W.; Iqbal, Z.; Ishaq, M.; Aslam, A.; Sarfraz, R. Topological Aspects of Dendrimers via Distance Based Descriptors. *IEEE Access* **2019**, *7*, 35619-35630, https://doi.org/10.1109/ACCESS.2019.2904736.
16. Imran, M.; Bokhary, S.A.U.H.; Manzoor, S.; Siddiqui, M.K. On molecular topological descriptors of certain families of nanostar dendrimers. *Eurasian Chemical Communications* **2020**, *2*, 680-687, https://doi.org/10.33945/SAMI/ECC.2020.6.5.
17. Kulli, V. On Hyper KV and Square KV Indices and their Polynomials of Certain Families of Dendrimers. *Journal of Computer and Mathematical Sciences* **2019**, *10*, 279-286, https://doi.org/10.29055/jcms/1007.
18. Gao, W.; Iqbal, Z.; Ishaq, M.; Sarfraz, R.; Aamir, M.; Aslam, A. On Eccentricity-Based Topological Indices Study of a Class of Porphyrin-Cored Dendrimers. *Biomolecules* **2018**, *8*, 71-81, https://doi.org/10.3390/biom8030071.
19. Kang, S.M.; Zahid, M.A.; Virk, A.u.R.; Nazeer, W.; Gao, W. Calculating the Degree-based Topological Indices of Dendrimers. *Open Chemistry* **2018**, *16*, 681-688, https://doi.org/10.1515/chem-2018-0071.
20. Berge, C. *Graphs and Hypergraphs*. North-Holland, Amsterdam, **1973**.
21. Berge, C. Theory of Graphs and its Applications. Methuen, London, **1962**.
22. Cockayne, E.J.; Hedetniemi, S.T. Towards a theory of domination in graphs. *Networks* **1977**, *7*, 247-261.
23. Jaeger, F.; Payan, C.J.C.A.S.S.A. Relations du type Nordhaus-Gaddum pour le nombre d'absorption d'un graphe simple. *C. R. Acad. Sci. Paris, Series* **1972**, *274*, 728-730.
24. Ore, O. Theory of Graphs. Amer. Math. Soc. Colloq. Publ., Providence, Volume 38, **1962**.
25. Couturier, J.-F.; Letourneur, R.; Liedloff, M. On the number of minimal dominating sets on some graph classes. *Theoretical Computer Science* **2015**, *562*, 634-642, https://doi.org/10.1016/j.tcs.2014.11.006.
26. Hanan Ahmed, A.M.; Alwardi, A.; Salestina, M. On Domination Topological Indices Of Graphs. *International Journal of Analysis and Applications* **2021**, *19*, 47-64, https://doi.org/10.28924/2291-8639-19-2021-47.
27. Eunjeong, Y. Domination value in graph. *arXiv* **2012**, *7*, 30-43.