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M-Polynomials and Degree-Based Topological Indices of Dexamethasone, Chloroquine and Hydroxychloroquine; using in COVID-19

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Abstract— *The molecular structure is base in drug making. It shows chemical and biological attributes, these attributes can be determined by topological index. In this article we extract certain topological properties of Dexamethasone, Chloroquine and Hydroxychloroquine molecular structures. We calculate M-polynomials and some connectivity indices like Randić index, Zagreb index, augmented Zagreb index, inverse sum index, harmonic index and symmetric division index of these antiviral drugs.*

Keywords— *M-polynomial, Antiviral durgs, Zagreb index, Randić index, inverse sum index, harmonic index and symmetric division index, COVID-19.*

I. Introduction

A cell is the base of life, but a virus not contain any cell. It can not reproduce itself, it reproduce only in the living cell with RNA. There is no drug to kill the viruses, the only our immune system is the way to fight against viruses. The antiviral drugs are used to trap it inside the cell and it from coping, to give the time to immune system for preparation against viruses.

In the last month of 2019, a number of pneumonia cases were reported in Wuhan China, because of a novel coronavirus (COVID 19). Its spread rate is very high and now on 9th July 2020, 11.9 million confirmed cases reported, 54700 deaths and 6.53 million recovered worldwide [Acc. to Wikipedia]. Effective medicine with less side effect is required on the urgent bases unless its vaccine is arrived. Here we study three drugs Dexamethasone, Chloroquine and Hydroxychloroquine.

Dexamethasone can be used to cure diseases like of immune disorders, allergy, certain skin condition, respiratory issues and in cancer []. It is a steriod also use for asthma and is using in COVID 19, it reduced the death rate about 33% [1]. Chloroquine and Hydroxychloroquine are used to treat malaria. These are also used in auto-immune diseases including HIV [8]. In chemical graph theory, we study the molecular structure by using a graph. In this graph we represent atoms by vertices and bonds by edges. "Every number which is uniquely determined by a graph is called a graph invariant. These invariant of molecular graph which are used for structure-property or structure-activity correlations are usually called topological indices" [5].

Let G is combination of vertices $V(G)$ and edges $E(G)$ and d_u is degree of vertex u and is the number of edges incident with u. For molecular structure we usually take simple undirected graph. In 2015, Klavzor et al. [2] introduced degree dependent M-polynomial, that has similar the role distance based Hosoya polynomial.

In present study, we calculate distance based topological indices with the help of M-polynomials.

II. Basic Definitions and Literature Review

In this article, G be connected simple graph, with $V(G)$ vertices set and $E(G)$ edges set. Degree of any vertex u is d_u.

Definition: The M-polynomial of G is [2]

$$M(G;x,y) = \sum_{(\delta \le i \le j \le 4)} m_{ij}\, x^i y^j$$

where $\delta = min\{d(v)/v \in V(G)\}$, $4 = max\{d(v)/v \in V(G)\}$ and $m_{ij}(G)$ is the edge $uv \in E(G)$ s.t. $\{d(u),d(v)\} = \{i,j\}$.

The topological index began from Wiener index, in 1945, Wiener defined them while studying alkane's boiling point [12]. The first degree based topological index is Randić index which presented by Milan Randić [10] and defined as

$$R_{-\frac{1}{2}} = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

Generalized Randić index is

$$R_\alpha = \sum_{uv \in E(G)} \frac{1}{\left(\sqrt{d_u d_v}\right)^\alpha}$$

Inverse generalized Randić index is

$$RR_\alpha = \sum_{uv \in E(G)} (d_u d_v)^\alpha$$

The first and second Zagreb indices were defined by Gutman and Trinajstić [4,6,11] and defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$$

$$M_2(G) = \sum_{uv \in E(G)} (d_u d_v)$$

The second modified Zagreb index defined as

$$mM_2(G) = \sum_{uv \in E(G)} \frac{1}{(d_u d_v)}$$

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The symmetric division index defined [3] used for surface determination of polychlorobiphenyls [9] and formulated as

$$SDD(G) = \sum_{uv\in E(G)} \frac{min(d_u, d_v)}{max(d_u, d_v)} + \frac{max(d_u, d_v)}{min(d_u, d_v)}$$

Hormonic index [13]

$$H(G) = \sum_{uv\in E(G)} \frac{2}{(d_u + d_v)}$$

Inverse sum index

$$I(G) = \sum_{uv\in E(G)} \frac{d_u d_v}{(d_u + d_v)}$$

Augmented Zagreb index [7]

$$A(G) = \sum_{uv\in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3$$

We can also compute these topological indices with this following table

TABLE I. Derivation of topological indices from M-polynomial

Topological Index	$f(x,y)$	Derivative from
First Zagreb Index	$x+y$	$(D_x + D_y)(M(G;x,y))\|_{x=y=1}$
Second Zagreb Index	xy	$(D_x D_y)(M(G;x,y))\|_{x=y=1}$
modified second Zagreb Index	$\frac{1}{xy}$	$(S_x S_y)(M(G;x,y))\|_{x=y=1}$
Randić index	xy^α	$(D_x^\alpha D_y^\alpha)(M(G;x,y))\|_{x=y=1}$
Inverse Randić index	$\frac{1}{xy^\alpha}$	$(S_x^\alpha S_y^\alpha)(M(G;x,y))\|_{x=y=1}$
Symmetric index	$\frac{x^2+y^2}{xy}$	$(D_x S_y + S_x D_y)(M(G;x,y))\|_{x=y=1}$
Harmonic index	$\frac{2}{x+y}$	$(2S_x J)(M(G;x,y))\|_{x=1}$
Inverse sum index	$\frac{xy}{x+y}$	$(S_x J D_x D_y)(M(G;x,y))\|_{x=1}$
Augmented Zagreb index	$\left(\frac{xy}{x+y-2}\right)^3$	$S_x^3 Q_{-2} J D_x^3 D_y^3 (M(G;x,y))\|_{x=1}$

Where

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

$$S_x f(x,y) = \int \frac{f(x,y)}{x} dx, \qquad S_y f(x,y) = \int \frac{f(x,y)}{y} dy$$

$$Jf(x,y) = f(x,x), \qquad Q_\alpha f(x,y) = x^\alpha f(x,y)$$

III. MAIN RESULTS

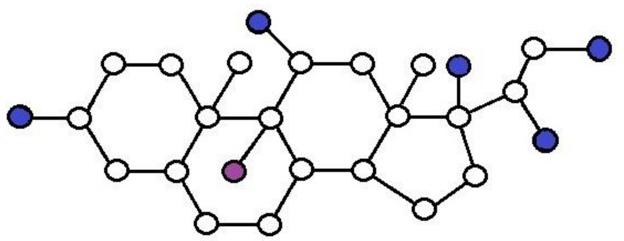

Fig. 1. Dexamethasone 2D molecular graph

Number of edges	(1,2)	(1,3)	(1,4)	(2,2)	(2,3)
Frequency	1	3	4	3	8
Number of edges	(2,4)	(3,3)	(3,4)	(4,4)	
Frequency	3	1	5	2	

Theorem 1: *The M-polynomial of Dexamethasone graph G is*

$$M(G;x,y) = xy^2 + 3xy^3 + 4xy^4 + 3x^2y^2 + 8x^2y^3 + 3x^2y^4 + x^3y^3 + 5x^3y^4 + 2x^4y^4$$

Proof: From Fig. 1, we can see that edge set of Dexamethasone has nine edge partitions,

$E_{\{1,2\}} = \{e = uv \in E(G) | d_u = 1, d_v = 2\}$
$E_{\{1,3\}} = \{e = uv \in E(G) | d_u = 1, d_v = 3\}$
$E_{\{1,4\}} = \{e = uv \in E(G) | d_u = 1, d_v = 4\}$
$E_{\{2,2\}} = \{e = uv \in E(G) | d_u = 2, d_v = 2\}$
$E_{\{2,3\}} = \{e = uv \in E(G) | d_u = 2, d_v = 3\}$
$E_{\{2,4\}} = \{e = uv \in E(G) | d_u = 2, d_v = 4\}$
$E_{\{3,3\}} = \{e = uv \in E(G) | d_u = 3, d_v = 3\}$
$E_{\{3,4\}} = \{e = uv \in E(G) | d_u = 3, d_v = 4\}$
$E_{\{4,4\}} = \{e = uv \in E(G) | d_u = 4, d_v = 4\}$

Such that

$|E_{\{1,2\}}| = 1$, $|E_{\{1,3\}}| = 3$, $|E_{\{1,4\}}| = 4$
$|E_{\{2,2\}}| = 3$, $|E_{\{2,3\}}| = 8$, $|E_{\{2,4\}}| = 3$
$|E_{\{3,3\}}| = 1$, $|E_{\{3,4\}}| = 5$, $|E_{\{4,4\}}| = 2$

Now

$$M(G;x,y) = \sum_{(i\le j)} m_{ij}\, x^i y^j$$

$$M(G;x,y) = \sum_{(1\le 2)} m_{12}\, x^1y^2 + \sum_{(1\le 3)} m_{13}\, x^1y^3 + \sum_{(1\le 4)} m_{14}\, x^1y^4 + \sum_{(2\le 2)} m_{22}\, x^2y^2 + \sum_{(2\le 3)} m_{23}\, x^2y^3 + \sum_{(2\le 4)} m_{24}\, x^2y^4 + \sum_{(3\le 3)} m_{33}\, x^3y^3 + \sum_{(3\le 4)} m_{34}\, x^3y^4 + \sum_{(4\le 4)} m_{44}\, x^4y^4$$

$$M(G;x,y) = |E_{\{1,2\}}|xy^2 + |E_{\{1,3\}}|xy^3 + |E_{\{1,4\}}|xy^4 + |E_{\{2,2\}}|x^2y^2 + |E_{\{2,3\}}|x^2y^3 + |E_{\{2,4\}}|x^2y^4 + |E_{\{3,3\}}|x^3y^3 + |E_{\{3,4\}}|x^3y^4 + |E_{\{4,4\}}|x^4y^4$$

$$M(G;x,y) = xy^2 + 3xy^3 + 4xy^4 + 3x^2y^2 + 8x^2y^3 + 3x^2y^4 + x^3y^3 + 5x^3y^4 + 2x^4y^4$$

Proposition: Let G be graph of Dexamethasone, we then have following connectivity dependent topological indices.

1. $M_1(G) = 165$
2. $M_2(G) = 212$
3. $mM_2(G) = \frac{101}{18}$
4. $R_\alpha(G) = 2^\alpha + 3^{\alpha+1} + 2^{2\alpha+2} + 3\cdot 2^{2\alpha} + 2^{\alpha+3}\cdot 3^\alpha + 3\cdot 2^{3\alpha} + 3^{2\alpha} + 5\cdot 2^{2\alpha}\cdot 3^\alpha + 2^{4\alpha+1}$
5. $RR_\alpha(G) = \frac{1}{2^\alpha} + \frac{1}{3^{\alpha-1}} + \frac{1}{2^{2\alpha-2}} + \frac{3}{2^{2\alpha}} + \frac{1}{2^{\alpha-3}.3^\alpha} + \frac{3}{2^{3\alpha}} + \frac{1}{3^{2\alpha}} + \frac{5}{2^{2\alpha}.3^\alpha} + \frac{1}{2^{4\alpha-1}}$
6. $SSD(G) = \frac{307}{4}$
7. $H(G) = \frac{821}{70}$

8. $I(G) = \frac{15451}{420}$
9. $A(G) = \frac{11216579}{43200}$

Proof: Now the following calculations are available by using the above formulas.
Let

$$M(G;x,y) = xy^2 + 3xy^3 + 4xy^4 + 3x^2y^2 + 8x^2y^3 + 3x^2y^4 + x^3y^3 + 5x^3y^4 + 2x^4y^4$$

$$D_xM(G;x,y) = xy^2 + 3xy^3 + 4xy^4 + 6x^2y^2 + 16x^2y^3 + 6x^2y^4 + 3x^3y^3 + 15x^3y^4 + 8x^4y^4$$

$$D_yM(G;x,y) = 2xy^2 + 9xy^3 + 16xy^4 + 6x^2y^2 + 24x^2y^3 + 12x^2y^4 + 3x^3y^3 + 20x^3y^4 + 8x^4y^4$$

$$D_xD_yM(G;x,y) = 2xy^2 + 9xy^3 + 16xy^4 + 12x^2y^2 + 48x^2y^3 + 24x^2y^4 + 9x^3y^3 + 60x^3y^4 + 32x^4y^4$$

$$S_xD_yM(G;x,y) = 2xy^2 + 9xy^3 + 16xy^4 + 3x^2y^2 + 12x^2y^3 + 6x^2y^4 + x^3y^3 + \frac{20}{3}x^3y^4 + 2x^4y^4$$

$$S_yM(G;x,y) = \frac{1}{2}xy^2 + 9xy^3 + 16xy^4 + \frac{3}{2}x^2y^2 + \frac{8}{3}x^2y^3 + \frac{3}{4}x^2y^4 + \frac{1}{2}x^3y^3 + \frac{5}{4}x^3y^4 + \frac{1}{2}x^4y^4$$

$$D_xS_yM(G;x,y) = \frac{1}{2}xy^2 + xy^3 + xy^4 + 3x^2y^2 + \frac{16}{3}x^2y^3 + \frac{3}{2}x^2y^4 + x^3y^3 + \frac{15}{4}x^3y^4 + 2x^4y^4$$

$$S_xS_yM(G;x,y) = \frac{1}{2}xy^2 + xy^3 + xy^4 + \frac{3}{4}x^2y^2 + \frac{4}{3}x^2y^3 + \frac{3}{8}x^2y^4 + \frac{1}{9}x^3y^3 + \frac{5}{12}x^3y^4 + \frac{1}{8}x^4y^4$$

$$JM(G;x,y) = x^3 + 6x^4 + 12x^5 + 4x^6 + 5x^7 + 2x^8$$

$$S_xJM(G;x,y) = \frac{1}{3}x^3 + \frac{3}{2}x^4 + \frac{12}{5}x^5 + \frac{2}{3}x^6 + \frac{5}{7}x^7 + \frac{1}{4}x^8$$

$$S_xJD_xD_yM(G;x = \frac{2}{3}x^3 + \frac{21}{4}x^4 + \frac{64}{5}x^5 + \frac{11}{2}x^6 + \frac{60}{7}x^7 + 4x^8$$

$$S_x^3Q_{-2}JD_x^3D_y^3\big(M(G;x,y)\big) = 8x + \frac{273}{8}x^2 + \frac{1984}{27}x^3 + \frac{2265}{64}x^4 + \frac{8840}{125}x^5 + \frac{8192}{216}x^6$$

$$D_x^\alpha D_y^\alpha\big(M(G;x,y)\big) = 2^\alpha xy^2 + 3^{\alpha+1}xy^3 + 2^{2\alpha+2}xy^4 + 3\cdot 2^{2\alpha}x^2y^2 + 2^{\alpha+3}\cdot 3^\alpha x^2y^3 + 3\cdot 2^{3\alpha}x^2y^4 + 3^{2\alpha}x^3y^3 + 5\cdot 2^{2\alpha}\cdot 3^\alpha x^3y^4 + 2^{4\alpha+1}x^4y^4$$

$$S_x^\alpha S_y^\alpha\big(M(G;x,y)\big) = \frac{1}{2^\alpha}xy^2 + \frac{1}{3^{\alpha-1}}xy^3 + \frac{1}{2^{2\alpha-2}}xy^4 + \frac{3}{2^{2\alpha}}x^2y^2 + \frac{1}{2^{\alpha-3}\cdot 3^\alpha}x^2y^3 + \frac{3}{2^{3\alpha}}x^2y^4 + \frac{1}{3^{2\alpha}}x^3y^3 + \frac{5}{2^{2\alpha}\cdot 3^\alpha}x^3y^4 + \frac{1}{2^{4\alpha+1}}x^4y^4$$

The topological indices described in table 1 is now obtained by using all the above-mentioned values.

1. First Zagreb Index
$$M_1(G) = (D_x + D_y)\big(M(G;x,y)\big)|_{x=y=1} = 165$$

2. Second Zagreb Index
$$M_2(G) = (D_xD_y)\big(M(G;x,y)\big)|_{x=y=1} = 212$$

3. Modified second Zagreb index
$$mM_2(G) = (S_xS_y)\big(M(G;x,y)\big)|_{x=y=1} = \frac{101}{18}$$

4. Randić index
$$R_\alpha(G) = (D_x^\alpha D_y^\alpha)\big(M(G;x,y)\big)|_{x=y=1} = 2^\alpha + 3^{\alpha+1} + 2^{2\alpha+2} + 3\cdot 2^{2\alpha} + 2^{\alpha+3}\cdot 3^\alpha + 3\cdot 2^{3\alpha} + 3^{2\alpha} + 5\cdot 2^{2\alpha}\cdot 3^\alpha + 2^{4\alpha+1}$$

5. Inverse Randić index
$$RR_\alpha(G) = (S_x^\alpha S_y^\alpha)\big(M(G;x,y)\big)|_{x=y=1} = \frac{1}{2^\alpha} + \frac{1}{3^{\alpha-1}} + \frac{1}{2^{2\alpha-2}} + \frac{3}{2^{2\alpha}} + \frac{1}{2^{\alpha-3}\cdot 3^\alpha} + \frac{3}{2^{3\alpha}} + \frac{1}{3^{2\alpha}} + \frac{5}{2^{2\alpha}\cdot 3^\alpha} + \frac{1}{2^{4\alpha-1}}$$

6. Symmetric index
$$SSD(G) = (D_xS_y + S_xD_y)\big(M(G;x,y)\big)|_{x=y=1} = \frac{307}{4}$$

7. Harmonic index
$$H(G) = (2S_xJ)\big(M(G;x,y)\big)|_{x=1} = \frac{821}{70}$$

8. Inverse sum index
$$I(G) = (S_xJD_xD_y)\big(M(G;x,y)\big)|_{x=1} = \frac{15451}{420}$$

9. Augumented Zagreb index
$$A(G) = S_x^\alpha Q_{-2}JD_x^3D_y^3\big(M(G;x,y)\big)|_{x=1} = \frac{11216579}{43200}$$

IV. MAIN RESULTS

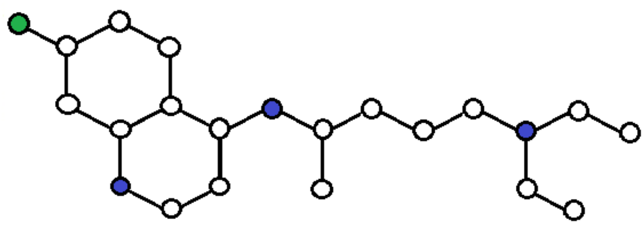

Fig. 2. Chloroquine 2D molecular graph

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Number of edges	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
Frequency	2	2	5	12	2

Theorem 2: *The M-polynomial of Chloroquine graph G is*

$$M(G;x,y) = 2xy^2 + 2xy^3 + 5x^2y^2 + 12x^2y^3 + 2x^3y^3$$

Proof: From Fig. 1, we can see that edge set of Dexamethasone has nine edge partitions,

$E_{\{1,2\}} = \{e = uv \in E(G) | d_u = 1, d_v = 2\}$

$E_{\{1,3\}} = \{e = uv \in E(G) | d_u = 1, d_v = 3\}$

$E_{\{2,2\}} = \{e = uv \in E(G) | d_u = 2, d_v = 2\}$

$E_{\{2,3\}} = \{e = uv \in E(G) | d_u = 2, d_v = 3\}$

$E_{\{3,3\}} = \{e = uv \in E(G) | d_u = 3, d_v = 3\}$

Such that

$|E_{\{1,2\}}| = 2$, $|E_{\{1,3\}}| = 2$,
$|E_{\{2,2\}}| = 5$, $|E_{\{2,3\}}| = 12$,
$|E_{\{3,3\}}| = 2$

Now

$$M(G;x,y) = \sum_{(i\le j)} m_{ij}\, x^i y^j$$

$$M(G;x,y) = \sum_{(1\le 2)} m_{12}\, xy^2 + \sum_{(1\le 3)} m_{13}\, xy^3 + \sum_{(2\le 2)} m_{22}\, x^2y^2 + \sum_{(2\le 3)} m_{23}\, x^2y^3 + \sum_{(3\le 3)} m_{33}\, x^3y^3$$

$$M(G;x,y) = |E_{\{1,2\}}| xy^2 + |E_{\{1,3\}}| xy^3 + |E_{\{2,2\}}| x^2y^2 + |E_{\{2,3\}}| x^2y^3 + |E_{\{3,3\}}| x^3y^3$$

$$M(G;x,y) = 2xy^2 + 2xy^3 + 5x^2y^2 + 12x^2y^3 + 2x^3y^3$$

Proposition: Let G be graph of Chloroquine, we then have following connectivity dependent topological indices.

10. $M_1(G) = 106$
11. $M_2(G) = 120$
12. $mM_2(G) = \frac{185}{36}$
13. $R_\alpha(G) = 2^{\alpha+1} + 2\cdot 3^\alpha + 5\cdot 2^{2\alpha} + 2^{\alpha+2}\cdot 3^{\alpha+1} + 2\cdot 3^{2\alpha}$
14. $RR_\alpha(G) = \frac{1}{2^{\alpha-1}} + \frac{2}{3^\alpha} + \frac{5}{2^{2\alpha}} + \frac{1}{2^{\alpha-2}.3^{\alpha-1}} + \frac{2}{3^{2\alpha}}$
15. $SSD(G) = \frac{155}{3}$
16. $H(G) = \frac{103}{10}$
17. $I(G) = \frac{757}{30}$
18. $A(G) = \frac{5809}{32}$

Proof: Now the following calculations are available by using the above formulas.

Let

$$M(G;x,y) = 2xy^2 + 2xy^3 + 5x^2y^2 + 12x^2y^3 + 2x^3y^3$$

$$D_xM(G;x,y) = 2xy^2 + 2xy^3 + 10x^2y^2 + 24x^2y^3 + 6x^3y^3$$

$$D_yM(G;x,y) = 4xy^2 + 6xy^3 + 10x^2y^2 + 36x^2y^3 + 6x^3y^3$$

$$D_xD_yM(G;x,y) = 4xy^2 + 6xy^3 + 20x^2y^2 + 72x^2y^3 + 18x^3y^3$$

$$S_xD_yM(G;x,y) = 4xy^2 + 6xy^3 + 5x^2y^2 + 18x^2y^3 + 2x^3y^3$$

$$S_yM(G;x,y) = xy^2 + \frac{2}{3}xy^3 + \frac{5}{2}x^2y^2 + 4x^2y^3 + \frac{2}{3}x^3y^3$$

$$D_xS_yM(G;x,y) = xy^2 + \frac{2}{3}xy^3 + 5x^2y^2 + 8x^2y^3 + 2x^3y^3$$

$$S_xS_yM(G;x,y) = xy^2 + \frac{2}{3}xy^3 + \frac{5}{4}x^2y^2 + 2x^2y^3 + \frac{2}{9}x^3y^3$$

$$JM(G;x,y) = 2x^3 + 7x^4 + 12x^5 + 2x^6$$

$$S_xJM(G;x,y) = \frac{2}{3}x^3 + \frac{7}{4}x^4 + \frac{12}{5}x^5 + \frac{1}{3}x^6$$

$$S_xJD_xD_yM(G;x = \frac{4}{3}x^3 + \frac{13}{2}x^4 + \frac{72}{5}x^5 + 3x^6$$

$$S_x^3Q_{-2}JD_x^3D_y^3(M(G;x,y)) = 16x + \frac{374}{8}x^2 + \frac{2592}{7}x^3 + \frac{1458}{64}x^4$$

$$D_x^\alpha D_y^\alpha(M(G;x,y)) = 2^{\alpha+1}xy^2 + 2\cdot 3^\alpha xy^3 + 5\cdot 2^{2\alpha}x^2y^2 + 2^{\alpha+2}\cdot 3^{\alpha+1}x^2y^3 + 2\cdot 3^{2\alpha}x^3y^3$$

$$S_x^\alpha S_y^\alpha(M(G;x,y)) = \frac{1}{2^{\alpha-1}}xy^2 + \frac{2}{3^\alpha}xy^3 + \frac{5}{2^{2\alpha}}x^2y^2 + \frac{1}{2^{\alpha-2}\cdot 3^{\alpha-1}}x^2y^3 + \frac{2}{3^{2\alpha}}x^3y^3$$

The topological indices described in table 1 is now obtained by using all the above-mentioned values.

1. First Zagreb Index

$$M_1(G) = (D_x + D_y)(M(G;x,y))|_{x=y=1} = 106$$

2. Second Zagreb Index

$$M_2(G) = (D_xD_y)(M(G;x,y))|_{x=y=1} = 120$$

3. Modified second Zagreb index

$$mM_2(G) = (S_xS_y)(M(G;x,y))|_{x=y=1} = \frac{185}{36}$$

4. Randić index

$$R_\alpha(G) = (D_x^\alpha D_y^\alpha)(M(G;x,y))|_{x=y=1} = 2^{\alpha+1} + 2\cdot 3^\alpha + 5\cdot 2^{2\alpha} + 2^{\alpha+2}\cdot 3^{\alpha+1} + 2\cdot 3^{2\alpha}$$

5. Inverse Randić index

$$RR_\alpha(G) = (S_x^\alpha S_y^\alpha)(M(G;x,y))|_{x=y=1} = \frac{1}{2^{\alpha-1}} + \frac{2}{3^\alpha} + \frac{5}{2^{2\alpha}} + \frac{1}{2^{\alpha-2}.3^{\alpha-1}} + \frac{2}{3^{2\alpha}}$$

6. Symmetric index

$$SSD(G) = (D_xS_y + S_xD_y)(M(G;x,y))|_{x=y=1} = \frac{155}{3}$$

7. Harmonic index

$$H(G) = (2S_xJ)(M(G;x,y))|_{x=1} = \frac{103}{10}$$

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8. Inverse sum index

$$I(G) = \left(S_x J D_x D_y\right)\left(M(G;x,y)\right)|_{x=1} = \frac{757}{30}$$

9. Augumented Zagreb index

$$A(G) = S_x^{\alpha} Q_{-2} J D_x^3 D_y^3\left(M(G;x,y)\right)|_{x=1} = \frac{5809}{32}$$

V. MAIN RESULTS

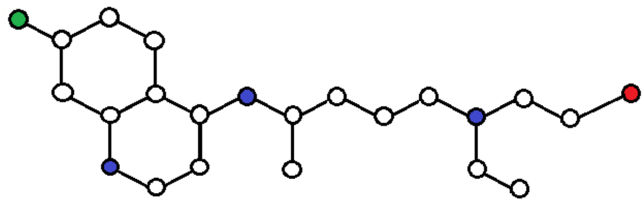

Fig. 3. Hydroxychloroquine 2D molecular graph

Number of edges	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
Frequency	2	2	6	12	2

Theorem 3: *The M-polynomial of Chloroquine graph G is*

$$M(G;x,y) = 2xy^2 + 2xy^3 + 6x^2y^2 + 12x^2y^3 + 2x^3y^3$$

Proof: From Fig. 1, we can see that edge set of Dexamethasone has nine edge partitions,

$E_{\{1,2\}} = \{e = uv \in E(G) | d_u = 1, d_v = 2\}$

$E_{\{1,3\}} = \{e = uv \in E(G) | d_u = 1, d_v = 3\}$

$E_{\{2,2\}} = \{e = uv \in E(G) | d_u = 2, d_v = 2\}$

$E_{\{2,3\}} = \{e = uv \in E(G) | d_u = 2, d_v = 3\}$

$E_{\{3,3\}} = \{e = uv \in E(G) | d_u = 3, d_v = 3\}$

Such that

$|E_{\{1,2\}}| = 2$,

$|E_{\{1,3\}}| = 2$,

$|E_{\{2,2\}}| = 6$,

$|E_{\{2,3\}}| = 12$,

$|E_{\{3,3\}}| = 2$

Now

$$M(G;x,y) = \sum_{(i\le j)} m_{ij}\, x^i y^j$$

$$M(G;x,y) = \sum_{(1\le 2)} m_{12}\, xy^2 + \sum_{(1\le 3)} m_{13}\, xy^3 + \sum_{(2\le 2)} m_{22}\, x^2y^2 + \sum_{(2\le 3)} m_{23}\, x^2y^3 + \sum_{(3\le 3)} m_{33}\, x^3y^3$$

$$M(G;x,y) = |E_{\{1,2\}}|xy^2 + |E_{\{1,3\}}|xy^3 + |E_{\{2,2\}}|x^2y^2 + |E_{\{2,3\}}|x^2y^3 + |E_{\{3,3\}}|x^3y^3$$

$$M(G;x,y) = 2xy^2 + 2xy^3 + 6x^2y^2 + 12x^2y^3 + 2x^3y^3$$

Proposition: Let G be graph of Hydroxychloroquine, we then have following connectivity dependent topological indices.

19. $M_1(G) = 110$
20. $M_2(G) = 124$
21. $mM_2(G) = \frac{97}{18}$
22. $R_\alpha(G) = 2^{\alpha+1} + 2\cdot 3^{\alpha} + 3\cdot 2^{2\alpha+1} + 2^{\alpha+2}\cdot 3^{\alpha+1} + 2\cdot 3^{2\alpha}$
23. $RR_\alpha(G) = \frac{1}{2^{\alpha-1}} + \frac{2}{3^{\alpha}} + \frac{3}{2^{2\alpha-1}} + \frac{1}{2^{\alpha-2}.3^{\alpha-1}} + \frac{2}{3^{2\alpha}}$
24. $SSD(G) = \frac{161}{3}$
25. $H(G) = \frac{162}{15}$
26. $I(G) = \frac{787}{30}$
27. $A(G) = \frac{6065}{32}$

Proof: Now the following calculations are available by using the above formulas.

Let

$$M(G;x,y) = 2xy^2 + 2xy^3 + 6x^2y^2 + 12x^2y^3 + 2x^3y^3$$

$$D_xM(G;x,y) = 2xy^2 + 2xy^3 + 12x^2y^2 + 24x^2y^3 + 6x^3y^3$$

$$D_yM(G;x,y) = 4xy^2 + 6xy^3 + 12x^2y^2 + 36x^2y^3 + 6x^3y^3$$

$$D_xD_yM(G;x,y) = 4xy^2 + 6xy^3 + 24x^2y^2 + 72x^2y^3 + 18x^3y^3$$

$$S_xD_yM(G;x,y) = 4xy^2 + 6xy^3 + 6x^2y^2 + 18x^2y^3 + 2x^3y^3$$

$$S_yM(G;x,y) = xy^2 + \frac{2}{3}xy^3 + 3x^2y^2 + 4x^2y^3 + \frac{2}{3}x^3y^3$$

$$D_xS_yM(G;x,y) = xy^2 + \frac{2}{3}xy^3 + 6x^2y^2 + 8x^2y^3 + 2x^3y^3$$

$$S_xS_yM(G;x,y) = xy^2 + \frac{2}{3}xy^3 + \frac{3}{2}x^2y^2 + 2x^2y^3 + \frac{2}{9}x^3y^3$$

$$JM(G;x,y) = 2x^3 + 8x^4 + 12x^5 + 2x^6$$

$$S_xJM(G;x,y) = \frac{2}{3}x^3 + 2x^4 + \frac{12}{5}x^5 + \frac{1}{3}x^6$$

$$S_xJD_xD_yM(G;x = \frac{4}{3}x^3 + \frac{15}{2}x^4 + \frac{72}{5}x^5 + 3x^6$$

$$S_x^3Q_{-2}JD_x^3D_y^3\left(M(G;x,y)\right) = 16x + \frac{219}{4}x^2 + 96x^3 + \frac{729}{32}x^4$$

$$D_x^{\alpha}D_y^{\alpha}\left(M(G;x,y)\right) = 2^{\alpha+1}xy^2 + 2\cdot 3^{\alpha}xy^3 + 3\cdot 2^{2\alpha+1}x^2y^2 + 2^{\alpha+2}\cdot 3^{\alpha+1}x^2y^3 + 2\cdot 3^{2\alpha}x^3y^3$$

$$S_x^{\alpha}S_y^{\alpha}\left(M(G;x,y)\right) = \frac{1}{2^{\alpha-1}}xy^2 + \frac{2}{3^{\alpha}}xy^3 + \frac{3}{2^{2\alpha-1}}x^2y^2 + \frac{1}{2^{\alpha-2}\cdot 3^{\alpha-1}}x^2y^3 + \frac{2}{3^{2\alpha}}x^3y^3$$

The topological indices described in table 1 is now obtained by using all the above-mentioned values.

1. First Zagreb Index

$$M_1(G) = \left(D_x + D_y\right)\left(M(G;x,y)\right)|_{x=y=1} = 110$$

2. Second Zagreb Index

$$M_2(G) = \left(D_xD_y\right)\left(M(G;x,y)\right)|_{x=y=1} = 124$$

3. Modified second Zagreb index

$$mM_2(G) = \left(S_xS_y\right)\left(M(G;x,y)\right)|_{x=y=1} = \frac{97}{18}$$

4. Randić index

$$R_\alpha(G) = \left(D_x^\alpha D_y^\alpha\right)\left(M(G;x,y)\right)|_{x=y=1} = 2^{\alpha+1} + 2\cdot 3^\alpha + 3\cdot 2^{2\alpha+1} + 2^{\alpha+2}\cdot 3^{\alpha+1} + 2\cdot 3^{2\alpha}$$

5. Inverse Randić index

$$RR_\alpha(G) = \left(S_x^\alpha S_y^\alpha\right)\left(M(G;x,y)\right)|_{x=y=1} = \frac{1}{2^{\alpha-1}} + \frac{2}{3^\alpha} + \frac{3}{2^{2\alpha-1}} + \frac{1}{2^{\alpha-2}\cdot 3^{\alpha-1}} + \frac{2}{3^{2\alpha}}$$

6. Symmetric index

$$SSD(G) = \left(D_xS_y + S_xD_y\right)\left(M(G;x,y)\right)|_{x=y=1} = \frac{161}{3}$$

7. Harmonic index

$$H(G) = (2S_xJ)\left(M(G;x,y)\right)|_{x=1} = \frac{162}{15}$$

8. Inverse sum index

$$I(G) = \left(S_xJD_xD_y\right)\left(M(G;x,y)\right)|_{x=1} = \frac{787}{30}$$

9. Augumented Zagreb index

$$A(G) = S_x^\alpha Q_{-2}JD_x^3D_y^3\left(M(G;x,y)\right)|_{x=1} = \frac{6065}{32}$$

VI. Conclusion

In the article, we have first find M-polynomial and then calculated degree dependent topological indices of Dexamethasone, chloroquine and Hydroxychloroquine. For drug design, molecular structural properties are useful. In this respect, these topological indices will help to design new drug for treating and preventing from complication in coronavirus disease COVID-19.

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References

[1] E. Cahan. Drug recently shown to reduce coronavirus death risk could run out, experts warn. https://www.sciencemag.org/news/2020/06/corticosteroid-drug-recentlyshown-reduce-coronavirus-death-risk-could-run-out-experts, 2020. Jun. 21, 2020.

[2] E. Deutsch and S. Klavžar. "M-polynomial and degree-based topological indices", *Iranian Journal of Mathematical Chemistry*, 6(2):93–102, 2015.

[3] C. Gupta, V. Lokesha, S. B. Shwetha, and P. Ranjini. "On the symmetric division deg index of graph". *Southeast Asian Bulletin of Mathematics*, 40(1), 2016.

[4] I. Gutman and K. C. Das. "The first zagreb index 30 years after". *MATCH Commun. Math. Comput. Chem*, 50(1):83–92, 2004.

[5] I. Gutman and O. E. Polansky. "Topological indices. In *Mathematical Concepts in Organic Chemistry"*, pages 123–134. Springer, 1986.

[6] I. Gutman and N. Trinajstić. "Graph theory and molecular orbitals. total ϕ-electron energy of alternant hydrocarbons". *Chemical Physics Letters*, 17(4):535–538, 1972.

[7] Y. Huang, B. Liu, and L. Gan. "Augmented zagreb index of connected graphs. *Match-Communications in Mathematical and Computer Chemistry"*, 67(2):483, 2012.

[8] V. Kulli. "Revan polynomials of chloroquine, hydroxychloroquine, remdesivir": Research for the treatment of covid-19.

[9] V. Lokesha and T. Deepika. "Symmetric division deg index of tricyclic and tetracyclic graphs". *Sci. Eng. Res*, 7(5):53–55, 2016.

[10] M. Randić. "Characterization of molecular branching". *Journal of the American Chemical Society*, 97(23):6609–6615, 1975.

[11] N. Trinajstić, S. Nikolić, A. Miličević, and I. Gutman. "About the zagreb indices". *Kemija u industriji: Casopis kemi˘cara i kemijskih in˘zenjera˘ Hrvatske*, 59(12):577–589, 2010.

[12] H. Wiener. "Structural determination of paraffin boiling points". *Journal of the American Chemical Society*, 69(1):17–20, 1947.

[13] L. Zhong. "The harmonic index for graphs". *Applied Mathematics Letters*, 25(3):561–566, 2012.