Study of M-Polynomials of Chemo Drugs Via Degree Based Topological Indices

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Abstract:

In the field of chemical graph theory Topological indices are also known as connectivity index used to build Quantitative Structure Activity Relationship(QSAR). In this article, using the technique of edge partition of graphs the chemo drugs of and 5-Fluorouracil molecular structure, whereas M-polynomials are very essential tools used to find exact and significant results of a topological indices with the help of certain degree based topological indices such as First k-Banhatti index, Second k-Banhatti index, Third Zagreb index, Redefined third Zagreb index, inverse sum indeg index and Augmented Zagreb index.

Key words: Topological index, M-polynomial, Paclitaxel, KBanhatti index, Augmmented Zagreb index.

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Introduction: Cancer is a genetic disease which starts anywhere in the human body where the cells grow uncontrollably and spread to other parts of the body. Cancer causes cells to divide uncontrollably, some types of cancer causes rapid cell growth, while other causes cells to grow and divide at a slower rate. Cancer cells may appear in one area, then spread through lymph nodes. These are clusters of immune cells located throughout the body, There are 100 types of cancer. For female breast and cervical cancer were considerably high in transitioning versus transitioned countries[1][2]. According to American cancer society there will be approximately 89,500 cancer cases diagnosed and about 9270 cancer deaths in adolescents and young adults aged 15 to 39 years in US. According to American cancer society many different kinds of Chemotherapy (or) Chemo drugs are used to treat cancer either alone (or) in combination with other drugs.

Chemotherapy work with a cell cycle, every time a new cell is formed[3][4]. This process involves a series of phases and is called the cell cycle. In this paper we have considered two types of Chemo drugs such as ,Paclitaxel, 5Fluorouracil[5].

In the area of chemical graph theory topological indices are also known as connectivity index they are used to build Quantitative Structure Activity Relationship(QSARs). Chemical graph theory can be used in different branches like quantum chemistry, computer science, biology, stereochemistry and engineering which is explained by Gutman and Trinajstic(1972)[6] Balbaan(1985)[7], Trinajstiec(1992), Shiriniva et al (2010) and Vergnioryetal(2017). Now a days topological indices are extensively used in the study of QSAR(Quanititative Structure Activity Relationship) let us consider G=(V,E) be a graph having 'n' number of vertices and 'm' number of edges. the symbol *du* is the degree of vertex *u* ∈ *V* (*G*) and is the number of vertices that are adjacent to u. In this article we were using MPolynomials to find the exact and significant results of a topological indices of a graph[8][9].

Review of Literature:

In chemical graph theory M-polynomials are the power full tool to find the topological indices of a graph Deutsch and Klawzar(2015) introduced M-poynomials and is defined as[10]

$$M(G,x,y)(G)x^iy^j$$

where G=(V,E) be a graph with $v \in g$ and dv denotes the degree of v. and $mi.j\ (G)$, $(i, j) \geq 1$, be the number of

$$= \sum_{i \leq j} m_{i,j}$$

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edges e=uv of G such that $dv(G)$, $du(G) = i, j$

First and second k-Banhatti indices were introduced by kulli. The first k-Banhatti index is defined as[11][12]

$$B_1[T(n,m)] = \sum_{(u,v)\in(T(n,m))} [d_u + d_{u,v}]$$

The second k-Banhatti index is defined as

$$B_2[T(n,m)] = \sum_{(u,v)\in(T(n,m))} [d_u * d_{u,v}]$$

In 2013, Ranjini et al, re-defined the Zagreb indices, i.e. the redefined third Zagreb indices is defined as[13]

$$ReZG_3[G(n,m)] = \sum_{(u,v)\in E(T\,n,m\,)} [d_u * d_v][d_u + d_v]$$

Inverse sum indeg index, defined by $ISI(GK)$ which is used to find total surface area for octane isomers and is represented as[14]

$$ISI(G\ \ (n.m)) = \sum_{(u,v)\in E(T(n,m))} \left(\frac{v}{d_u + d_v}\right)$$

Sedlar et al. investigated graph theoretical characteristics of ISI(G) index. Boris Furtula et al recently introduced new topological index called augmented zagreb index(AZI) defined as[15]

$$A(g\ \ (n.m)) = \sum_{(u,v)\in E(T(n,m))} \left(\frac{d_u * d_v}{d_u + d_v - 2}\right)^3$$

from which he predicts that power is better than Atom Bond Connectivity index. Boris Furtula et al proved that AZI is a very important index in the study of the heat of formation in heptanes and octanes and also Ivan Gutman and Jelena Tosovic recently tested that the correlation ability of 20 vertexdegree-based topological indices for the case of standard heats of formation and normal boiling points of octane isomers and they were found that AZI yield the best results. Boris Furtula et al. Havee studied extermal properties of AZI index of trees and Chemical trees they proved that among all trees the star has the minimum AZI value.

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Table 1: Degree based Topological indices

First K-Banhatti index	$B_1[T(n,m)] = \sum_{(u,v)\in(T(n,m))} [d_u + d_{u,v}]$
Second K-Banhatti index	$B_2[T(n,m)] = \sum_{(u,v)\in(T(n,m))} [d_u * d_{u,v}]$
Third Zagreb index	$ZG_3(G(n,m)) = \sum_{(u,v)\in(T(n,m))} [\lvert d_u - d_u \rvert]$
Redefined third Zagreb index	$ReZG_3[G(n,m)] = \sum_{(u,v)\in E(T(n,m))} [d_u * d_v][d_u + d_v]$
Inverse sum indeg index	$ISI\ (G(n.m)) = \sum_{(u,v)\in E(T(n,m))} \left(\frac{v}{d_u + d_v}\right)\ d_u * d$
Augmented Zagreb index	$A\ (G(n.m)) = \sum_{(u,v)\in E(T(n,m))} \left(\frac{d_u * d_v}{d_u + d_v - 2}\right)^3$

Table 2: Derivatives of some M-Polynomials

Topological Index	Derivations from M(G, x, y)
First K-Banhatti index	$B_1[T(n,m)] = (D_x + D_y + 2D_xQ_{-2}(J))\lvert f(x,y)\rvert_{x=y=1}$
Second K-Banhatti index	$B_2[T(n,m)] = D_xQ_{-2}J(D_x + D_y)f(x,y)\rvert_{x=y=1}$
Third Zagreb index	$ZG_3(G(n,m)) = (D_x - D_y)f(x,y)\rvert_{x=y=1}$
Redefined Third Zagreb index	$ReZG_3(G(n,m)) = (D_x + D_y)(D_x * D_y)f(x,y)\rvert_{x=y=1}$
Inverse sum indeg index	$ISI(G(n,m)) = S_xJD_xD_yf(x,y)\rvert_{x=y=1}$
Augmented Zagreb index	$AZ(G) = S_{x3}Q_2JD_{3x}D_{3y}f(x,y)\rvert_{x=y=1}$

M-polynomial of Paclitaxel

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

$= \sum_{2\le2} m_{2,2}(G)x^2 * y^2 + \sum_{2\le3} m_{2,3}\, x^2 * y^3 + \sum_{3\le3} m_{3,3}\, x^3 * y^3 + \sum_{1\le3} m_{1,3}\, x^1 * y^3 +$

$\sum_{1\le2} m_{1,2}x^1 * y^2 + \sum_{1\le4} m_{1,4}x^1 * y^4 + \sum_{4\le4} m_{4,4}\, x^4 * y^4 + \sum_{3\le4} m_{3,4}x^3 * y^4 + \sum_{2\le4} m_{2,4}x^2 * y^4$

$= 12x^2y^2 + 15x^2y^3 + 10x^3y^3 + 11xy^3 + xy^2 + 3xy^4 + 16x^1y^4 + 4x^4y^4 + 2x^3y^4 + 3x^2y^4$

$D_x = x\left(\frac{\delta f(x,y)}{\delta x}\right)$, $D_x = y\left(\frac{\delta f(x,y)}{\delta y}\right)$, $Jf(x,y) = f(x)|_{x=y=1}$, $S_x = \int_0^x \frac{f(x,y)}{t} dt|_{x=y=1}$, $S_y = \int_0^y \frac{f(x,y)}{t} dt|_{x=y=1}$

D_x=$24x^2y^2 + 30x^2y^3 + 30x^3y^3 + 11xy^3 + xy^2 + 3xy^4 + 16x^1y^4 + 16x^4y^4 + 6x^3y^4 + 6x^2y^4$

D_y=$24x^2y^2 + 45x^2y^3 + 30x^3y^3 + 33xy^3 + 2xy^2 + 12xy^4 + 64x^1y^4 + 16x^4y^4 + 8x^3y^4 + 12x^2y^4$ **Theorem 1:** Fig 1 is a chemical structure of paclitaxel then prove the following indices.

1. $B_1[T(n,m)] = 650$
2. $B_2[T9n,m)] = 976$
3. $ZG_3(G(n,m)) = 44$
4. $ReZG_3(G(n,m))$ =3504
5. $ISI(G(n,m)) = 70.8285$ 6. $A(G(n.m)) = 511.542$

Proof: From the figure 1 we have E(2,2)=12, E(2,3)=15, E(3,3)=10, E(3,1)=11, E(2,1)=1, E(4,1)=3, E(4,4)=3, E(3,4)=2, E(4,2)=3

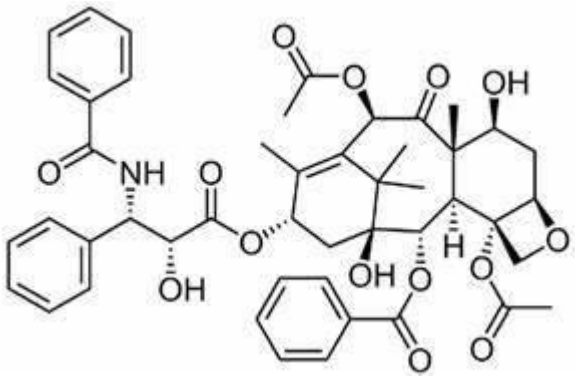

Fig 1: Chemical structure of Paclitaxel

(1) First K-Banhatti index

$$B_1[T(n,m)] = \sum_{(u,v)\in(T(n,m))} [d_u + d_{u,v}]$$

$$B_1[T(n,m)] = (D_x + D_y + 2D_xQ_{-2}(J))|f(x,y)|_{x=y=1}$$

f(x, y) = $12x^2y^2 + 15x^2y^3 + 10x^3y^3 + 11xy^3 + xy^2 + 3xy^4 + 16x^1y^4 + 4x^4y^4 + 2x^3y^4 + 3x^2y^4$

$(D_x + D_y)$f(x, y) = $48x^2y^2 + 75x^2y^3 + 60x^3y^3 + 36xy^3 + 3xy^2 + 15xy^4 + 32x^4y^4 + 14x^3y^4 + 18x^2y^4$

=298

$$2D_xQ_{-2}(J)f(x,y) = 48x^2 + 90x^3 + 80x^4 + 24x + 18x^3 + 48x^6 + 20x^5 + 24x^4$$

=356
$B_1[T(n,m)]$ =650

(2) **Second K-Banhatti index**:

$$B_2[T(n,m)] = \sum_{(u,v)\in(T(n,m))} [d_u * d_{u,v}]$$

$$B_2[T(n,m)] = D_xQ_{-2}J(D_x + D_y)f(x,y)|_{x=1}$$

$D_xQ_{-2}J(D_x + D_y)f(x,y)$=96x^2 + 225x^3 + 240x^4 + 36x + 45x^3 + 192x^6 + 70x^5 + 72x^4

$D_xQ_{-2}J(D_x + D_y)f(x,y)|_{x=1}$=976

(3) . **Third Zagreb index**

$$ZG_3(G(n,m)) = \sum_{(u,v)\in(T(n,m))} [|d_u - d_u|]$$

$$ZG_3(G(n,m)) = |(D_x - D_y)|f(x,y))|_{x=y=1}$$

$$|(D_x - D_y)| = |15xy^3 - 12xy^2 - 9xy^4 - 2x^3y^4 - 6x^2y^4|$$

$|(D_x - D_y)|f(x,y))|_{x=y=1}$=44

(4) **Redefined Third Zagreb Index:**

$$ReZG_3[G(n,m)] = \sum_{(u,v)\in E(T(n,m))} [d_u * d_v][d_u + d_v]$$

$$ReZG_3(G(n,m)) = (D_x + D_y)(D_x * D_y)f(G,x,y)|_{x=y=1}$$

($D_x + D_y$) f(x, y) = $48x^2y^2 + 75x^2y^3 + 60x^3y^3 + 36xy^3 + 3xy^2 + 15xy^4 + 32x^4y^4 +$
$14x^3y^4 + 18x^2y$
4

=298

$(D_x * D_y)$f(x, y) = $(24 * 24)x^2y^2 + (30 * 45)x^2y^3 + (30 * 30)x^3y^3 + (11 * 24)xy^3 +$
$(1 * 2)xy^2 + (3 * 12)xy^4 + (16 * 16)x^4y^4 + (8 * 6)x^3y^4 + (6 * 12)x^2y^4$

$(D_x * D_y)f(x,y)|_{x=y=1}$ =3504

(5) **Inverse Sum indeg index:**

$$ISI(G \quad (n.m)) = \sum_{(u,v)\in E(T(n,m))} \left(\frac{v}{d_u + d_v}\right) \quad d_u * d$$

$$ISI(G(n,m)) = S_x JD_x D_y M(G,x,y)|_{x=y=1}$$

$$S_x JD_x D_y M(G,x,y)|_{x=y=243} x3 + 484\, x4 + 1025\, x5 + 1146\, x6 + 247\, x7 + 8x8$$

$$S_x JD_x D_y M(G,x,y)|_{x=y=1}=70.8285$$

(6) **. Augmented Zagreb Index:** 223

$$A(G \quad (n.m)) = \sum_{(u,v)\in E(T(n,m))} \left(\frac{d_u * d_v}{d_u + d_v - 2}\right)^3$$

$$A(G(n,m)) = S_{x3} Q_2 JD_{3x} D_{3y} f(x,y)|_{x=y=1}$$

$$S_{x3} Q_2 JD_{3x} D_{3y} f(x,y)=\frac{768}{8}\, x2 + 324027\, x3 + 729064\, x4 + 96x + 1928\, x2 + 16384216\, x6 + 153664\, x4$$

$$S_{x3} Q_2 JD_{3x} D_{3y} f(x,y)|_{x=y=1}=511.542.$$

M-Polynomials of the drug 5- Flourouracil

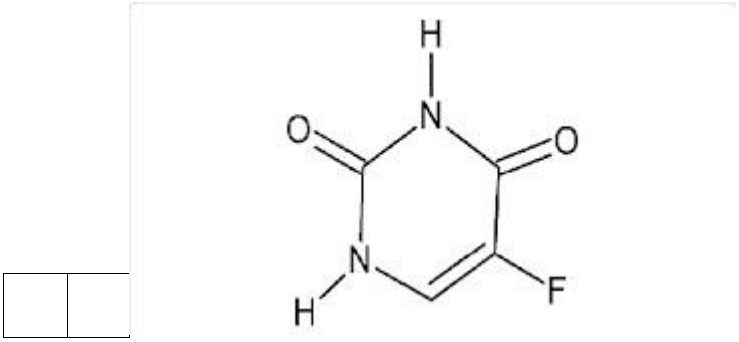

Fig 2. Chemical structure of 5- Fluorouracil

Theorem 2: Fig 2 is a molecular graph of Fluorouracil fpr this graph prove the following indices

1.$B_1[T(n,m)] = 650$

2.$B_2[T9n,m)] = 976$

3. $ZG_3(G(n,m)) = 44$

4. $ReZG_3(G(n,m)) = 313$

5. $ISI(G(n,m)) = 70.8285$ 6. $AG(G(n.m)) = 511.542$

Proof: The graph is having 10 edges of E(2,2)=1, E(1, 3)=4, E(3,3)=3, E(2, 3)=2

$$M(G,x,y) = \sum m_{i,j}(G) x^i y^j$$

$$i \leq j$$

$$= \sum_{2\leq 2} m_{2,2}(G)x^2 * y^2 + \sum_{1\leq 3} m_{1,3}\, x^1 * y^3 + \sum_{3\leq 3} m_{3,3}\, x^3 * y^3 + \sum_{2\leq 3} m_{2,3}\, x^2 * y^3 +$$

$$= 1x^2y^2 + 4x^1y^3 + 3x^3y^3 + 2x^2y^3$$

$$\mathbf{D_x = 2x^2y^2 + 4x^1y^3 + 9x^3y^3 + 4x^2y^3}$$

$$D_y = 2x^2y^2 + 12x^1y^3 + 9x^3y^3 + 6x^2y^3$$

$$S_x = \frac{x2y2}{2} + \frac{4x1y3}{1} + \frac{3x3y3}{3} + \frac{2x2y3}{2}$$

$$S_y = \frac{x2y2}{2} + \frac{4x1y3}{3} + \frac{3x3y3}{3} + \frac{2x2y3}{3}$$

1). **First K-Banhatti index** [224]

$$B_1[T(n,m)] = \sum_{(u,v)\in(T(n,m))} [d_u + d_{u,v}]$$

$$B_1[T(n,m)] = (D_x + D_y + 2D_xQ_{-2}(J))|f(x,y)|_{x=y=1}$$

$(D_x + D_y)\mathrm{f(x, y)} = 4x^2y^2 + 16y^3 + 18x^3y^3 + 10x^2y^3$

$(D_x + D_y)\mathrm{f(x, y)}|_{x=y=1} = 48$

$(D_x + D_y + 2D_xQ_{-2}(J))|_{x=y=1} = 4x^2 + 16x^2 + 24x^4 + 12x^3$

$B_1[T(n,m)] = 103$

2). **Second K-Banhatti index:**

$$B_2[T(n,m)] = \sum_{(u,v)\in(T(n,m))} [d_u * d_{u,v}]$$

$$B_2[T(n,m)] = D_xQ_{-2}J(D_x + D_y)f(x,y)|_{x=1}$$

$D_xQ_{-2}J(D_x + D_y)f(x,y) = 8\mathrm{x}^2 + 32\mathrm{x}^2 + 32\mathrm{x}^4 + 30\mathrm{x}^3$

$D_xQ_{-2}J(D_x + D_y)f(x,y)|_{x=1} = 102$

3. Third Zagreb Index:

$$ZG_3(G(n,m)) = \sum_{(u,v)\in(T(n,m))} [|d_u - d_u|]$$

$$ZG_3(G(n,m)) = |(D_x - D_y)|f(x,y))|_{x=y=1}$$

$$|(D_x - D_y)| = |8xy^3 + 2x^2y^3|$$

$$|(D_x - D_y)|f(x,y))|_{x=y=1}=10$$

4. Redefined Third Zagreb Index:

$$ReZG_3[G(n,m)] = \sum_{(u,v)\in E(T(n,m))} [d_u * d_v][d_u + d_v]$$

$$ReZG_3(G(n,m)) = (D_x + D_y)(D_x * D_y)f(G,x,y)|_{x=y=1}\ (D_x +$$

D_y)f(x,y) $=4x^2y^2 + 16y^3 + 18x^3y^3 + 10x^2y^3$

$(D_x + D_y)$f(x, y)$|_{x=y=1}$ =48

$(D_x * D_y)$f(x, y) $= (2*2)x^2y^2 + (12*12)x^1y^3 + (9*9)x^3y^3 + (6*6)x^2y^3$

$(D_x * D_y)f(x,y)|_{x=y=1}$ =265

$ReZG_3[G(n,m)]$ =313

5. Inverse Sum indeg index:

$$ISI(G(n.m)) = \sum_{(u,v)\in E(T(n,m))} \left(\frac{v}{d_u + d_v}\right)$$

$$ISI(G(n,m)) = S_xJD_xD_yM(G,x,y)|_{x=y=1}$$

$S_xJD_xD_yM(G,x,y)|_{x=y}$=x4 + 3x4 + 276$\overline{x}$6 + 125 $\overline{x}$5 + 1146 $\overline{x}$5

$S_xJD_xD_yM(G,x,y)|_{x=y=1}$=10.9

6. Augmented Zagreb Index:

$$A(G(n.m)) = \sum_{(u,v)\in E(T(n,m))} \left(\frac{d_u * d_v}{d_u + d_v - 2}\right)^3$$

$$A(G(n,m)) = S_{x3}Q_2JD_{3x}D_{3y}f(x,y)|_{x=y=1}$$

$S_{x3}Q_2JD_{3x}D_{3y}f(x,y)$=8x3 $\frac{27}{2}$ +$x2$ + 218764 $\overline{x4}$ + 43227 $x3$

$S_{x3}Q_2JD_{3x}D_{3y}f(x,y)|_{x=y=1}$=71.65625

Conclusion: In this paper we mainly focused on calculating numerical expression using edge partition of a graph by using first and second K-Banhatti index, Third Zagreb index, Redefined

third Zagreb index, Inverse sum indeg index and Augmented Zagreb index. Researchers can try for other drugs with different topological indices.

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