

Topological indices of some anticancer drugs

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Abstract

Every sixth death in the world is due to cancer, making it the second leading cause of death. Around one-third of deaths from cancer are due to tobacco use, high body mass index, alcohol use, low fruit and vegetable intake, and lack of physical activity. Anticancer drugs are those which are used to cure malignant disease i.e., cancer. Topological indices are used to model physico-chemical properties and biological activities of chemical compounds. In this paper, we compute *M-polynomial* and *NM-polynomial* of anticancer drugs. Further, we retrieve some degree and neighborhood degree based topological indices of anticancer drugs from their respective *M-polynomial* and *NM-polynomial*. The theoretical results obtained in this article have promising aspects in designing novel drug for the treatment of cancer. This study may assist chemists and pharmaceutical industry workers forecast the features of anticancer drugs without experimenting.

Keywords: M-polynomial; NM-polynomial; degree-based topological indices; neighborhood degree-based topological indices; edge partitions; graph invariant.

2020 AMS subject classifications: 05C07, 05C31. ¹

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1 Introduction

Up to now, cancer remains a global and serious public health challenge. Cancer is the uncontrolled growth of abnormal cells in the body. Cancer develops when the body's normal control mechanism stops working. Old cells do not die and instead grow out of control, forming new, abnormal cells. It is estimated that there are more than 200 different types of cancer, generally named according to the tissue where the cancer was recognized for the first time. Any drug that is effective in the treatment of malignant, or cancerous, disease is called anticancer drug. There are several major classes of anticancer drugs; these include alkylating agents, antimetabolites, natural products, and hormones.

It is always interesting to find some properties of graphs which are invariant. Topological indices and polynomials are foremost among them. Over the last decade there are numerous research papers devoted to topological indices and polynomials. Several topological indices have been defined in the literature. For details of topological indices one can refer to [15, 19]. For different topological indices and their applications one can refer to [2, 3, 10–12]. Some topological indices are already computed in literature on various anticancer drugs to determine physico-chemical properties [9, 13, 24].

Molecular topological indices are important in mathematical chemistry, particularly in the study of quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR). It is an effective technique to eliminate expensive and time-consuming laboratory studies. Information on physicochemical qualities and biological activity of molecular graphs of compounds is required in pharmaceutical drug design. These features may be predicted using the topological index, a well-known method in chemical graph theory.

There are many graph polynomials refer to [5, 28]. The Hosoya polynomial is the most well-known polynomial which plays a vital role in determining distance-based topological indices such as Wiener index [27], hyper Wiener index [5] of graphs. There are various types of algebraic polynomials are found in the literature. Some examples for polynomials in the theory of chemical graphs are PI polynomial [1], Tutte polynomial [7], Theta polynomial [8], Schultz polynomial [17], Hub polynomial [25], Gourava and hyper-Gourava polynomial [4], M-polynomial [6], NM-polynomial [20] etc.

Throughout this paper, by a graph $G = (V, E)$ we mean a simple, undirected, finite graph of order n and size m . Let $V(G)$ and $E(G)$ denote the vertex set and an edge set, respectively. For undefined graph theoretic terminologies and notions, refer to [16, 18, 26].

The M -polynomial [6] is one among other algebraic polynomials which was introduced in 2015 and useful in determining many degree-based topological in-

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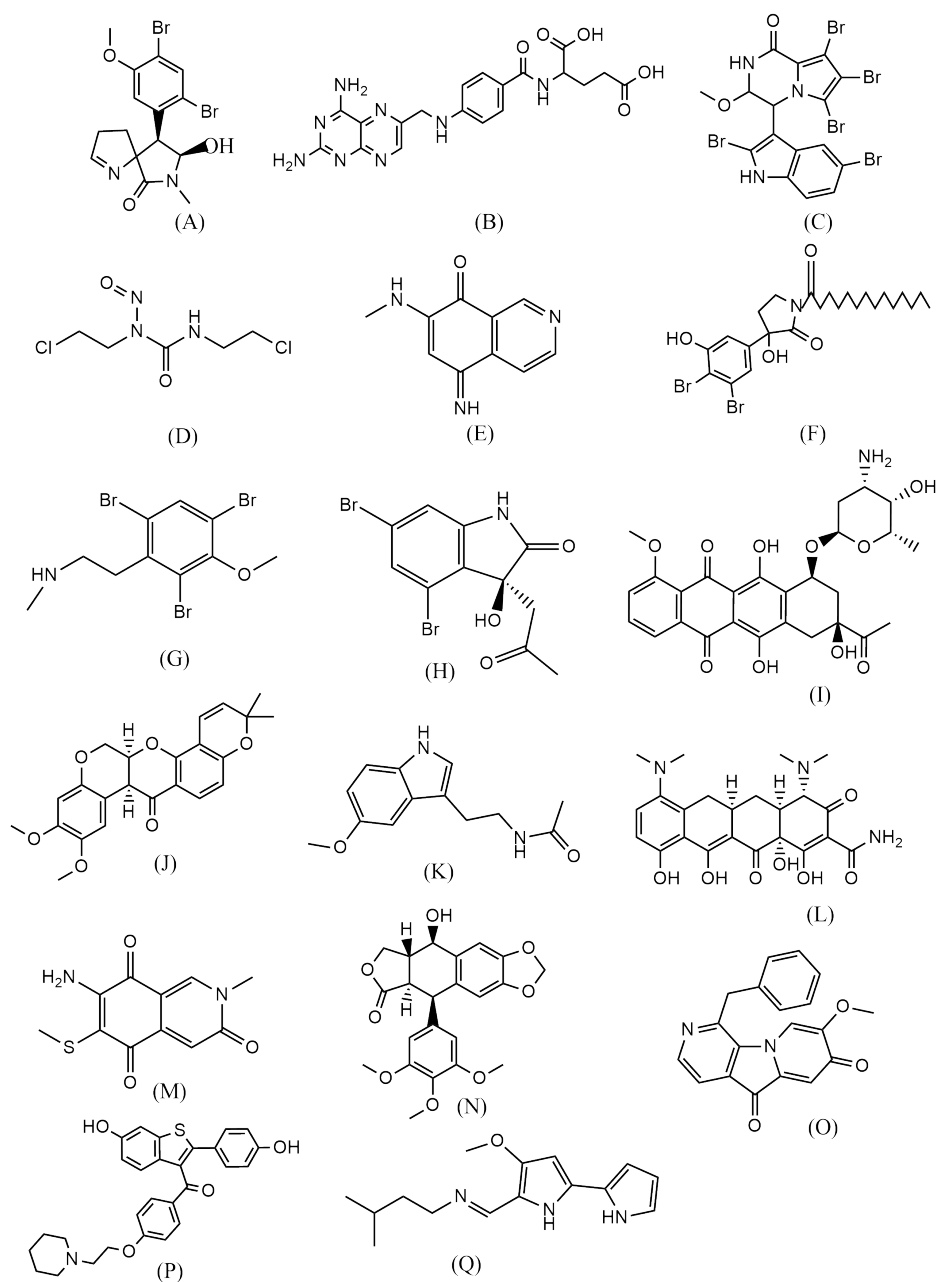


Figure 1: Molecular structure of anticancer drugs (A) Amathaspiramide E; (B) Aminopterin; (C) Aspidostomide E; (D) Carmustine; (E) caulibugulone E; (F) Convolutamide A; (G) Convolutamine F; (H) convolutamydine A; (I) Daunorubicin; (J) Deguelin; (K) Melatonin; (L) Minocycline; (M) Perfragilin A; (N) Podophyllotoxin; (O) Pterocellin; (P) Raloxifene; (Q) Tambjamine K.

dices (listed in Table 2) [15, 19]. Recently, the study of M -polynomial is reported in [21–23]. Let $\psi(u)$ denote the degree of vertex u of a graph G .

Definition 1.1. [6] If G is a graph, then M – polynomial of G is defined as

$$M(G; x, y) = \sum_{i \leq j} m_{ij}(G) x^i y^j, \quad (1)$$

where $m_{ij}, (i, j \geq 1)$, is the number [14] of edges uv in G such that $\psi(u) = i$ and $\psi(v) = j$.

Neighborhood M -polynomial [20] play the similar role for neighborhood degree sum-based indices. Let $\Psi(u)$ denote the degree sum of all vertices of G that are adjacent u . We call $\Psi(u)$ as neighborhood degree sum of u in G .

Definition 1.2. [20] If G is a graph, then NM – polynomial of G is defined as

$$NM(G; x, y) = \sum_{i \leq j} m_{ij}^*(G) x^i y^j, \quad (2)$$

where $m_{ij}^*, (i, j \geq 1)$ is the number of edges uv in G such that $\Psi(u) = i$ and $\Psi(v) = j$.

D	$g(\psi(u), \psi(v))$	ND	$g(\Psi(u), \Psi(v))$
First Zagreb index $M_1(G)$	$\psi(u) + \psi(v)$	Third version Zagreb index $M_1'(G)$	$\Psi(u) + \Psi(v)$
Second Zagreb index $M_2(G)$	$\psi(u)\psi(v)$	Neighborhood second Zagreb index M_2^*	$\Psi(u)\Psi(v)$
Forgotten topological index $F(G)$	$\psi(u)^2 + \psi(v)^2$	Neighborhood Forgotten topological index F_N^*	$\Psi(u)^2 + \Psi(v)^2$
Second modified Zagreb index ${}^m M_2(G)$	$\frac{1}{\psi(u)\psi(v)}$	Neighborhood second modified Zagreb index ${}^{nm} M_2(G)$	$\frac{1}{\Psi(u)\Psi(v)}$
Randić index $R_\alpha(G)$	$(\psi(u)\psi(v))^\alpha$	Neighborhood Randić index $NR_\alpha(G)$	$(\Psi(u)\Psi(v))^\alpha$
Redefined third Zagreb index $ReZG_3(G)$	$(\psi(u) + \psi(v))\psi(u)\psi(v)$	Third NDe index $ND_3(G)$	$(\Psi(u) + \Psi(v))\Psi(u)\Psi(v)$
Symmetric division index $SDD(G)$	$\frac{\psi^2(u) + \psi^2(v)}{\psi(u)\psi(v)}$	Fifth NDe index $ND_5(G)$	$\frac{\Psi^2(u) + \Psi^2(v)}{\Psi(u)\Psi(v)}$
Harmonic index $H(G)$	$\frac{\psi(u) + \psi(v)}{2}$	Neighborhood Harmonic index $NH(G)$	$\frac{\Psi(u) + \Psi(v)}{2}$
Inverse sum indeg index $I(G)$	$\frac{\psi(u)\psi(v)}{(\psi(u) + \psi(v))}$	Neighborhood Inverse sum indeg index $NI(G)$	$\frac{\Psi(u)\Psi(v)}{(\Psi(u) + \Psi(v))}$
Augmented Zagreb index $A(G)$	$\left\{ \frac{\psi(u)\psi(v)}{(\psi(u) + \psi(v))} \right\}^3$	Sanskriti index $S(G)$	$\left\{ \frac{\Psi(u)\Psi(v)}{(\Psi(u) + \Psi(v))} \right\}^3$

Table 1: Description of some topological indices.

Degree based(D) and neighborhood degree sum-based (ND) topological indices defined on edge set $E(G)$ of a graph G can be expressed as

$$D(G) = \sum_{uv \in E(G)} g(\psi(u), \psi(v)), ND(G) = \sum_{uv \in E(G)} g(\Psi(u), \Psi(v)),$$

where the formulation of $g(\psi(u), \psi(v))$ and $g(\Psi(u), \Psi(v))$ are given in Table 1.

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Topological Index	Derivation from $M(G; x, y)$	Topological Index	Derivation from $NM(G; x, y)$
$M_1(G)$	$(D_x + D_y)(M(G; x, y)) _{x=y=1}$	$M'_1(G)$	$(D_x + D_y)(M(G; x, y)) _{x=y=1}$
$M_2(G)$	$(D_x D_y)(M(G; x, y)) _{x=y=1}$	$M_2^*(G)$	$(D_x D_y)(M(G; x, y)) _{x=y=1}$
$F(G)$	$(D_x^2 + D_y^2)(M(G; x, y)) _{x=y=1}$	F_N^*	$(D_x^2 + D_y^2)(M(G; x, y)) _{x=y=1}$
${}^m M_2(G)$	$(I_x I_y)(M(G; x, y)) _{x=y=1}$	${}^{nm} M_2(G)$	$(I_x I_y)(M(G; x, y)) _{x=y=1}$
$R_\alpha(G)$	$(D_x^\alpha D_y^\alpha)(M(G; x, y)) _{x=y=1}$	$NR_\alpha(G)$	$(D_x^\alpha D_y^\alpha)(M(G; x, y)) _{x=y=1}$
$ReZG_3(G)$	$D_x D_y (D_x + D_y)(M(G; x, y)) _{x=y=1}$	$ND_3(G)$	$D_x D_y (D_x + D_y)(M(G; x, y)) _{x=y=1}$
$SDD(G)$	$(D_x I_y + D_y I_x)(M(G; x, y)) _{x=y=1}$	$ND_5(G)$	$(D_x I_y + D_y I_x)(M(G; x, y)) _{x=y=1}$
$H(G)$	$2I_x J(M(G; x, y)) _{x=1}$	$NH(G)$	$2I_x J(M(G; x, y)) _{x=1}$
$I(G)$	$I_x J D_x D_y (M(G; x, y)) _{x=1}$	$NI(G)$	$I_x J D_x D_y (M(G; x, y)) _{x=1}$
$A(G)$	$I_x^3 Q_{-2} J D_x^2 D_y^3 (M(G; x, y)) _{x=1}$	$S(G)$	$I_x^3 Q_{-2} J D_x^2 D_y^3 (M(G; x, y)) _{x=1}$

Table 2: Operations to derive degree-based topological indices from M -polynomial and NM -polynomial.

Where $D_x = x \frac{\partial f(x,y)}{\partial x}$, $D_y = y \frac{\partial f(x,y)}{\partial y}$, $I_x = \int_0^x \frac{f(t,y)}{t} dt$, $I_y = \int_0^y \frac{f(x,t)}{t} dt$, $J(f(x, y)) = f(x, x)$ and $Q_\alpha(f(x, y)) = x^\alpha f(x, y)$ are the operators.

Molecular topological indices are important in mathematical chemistry, particularly in the study of quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR). It is an effective technique to eliminate expensive and time-consuming laboratory studies. Information on physicochemical qualities and biological activity of molecular graphs of compounds is required in pharmaceutical drug design. These features may be predicted using the topological index, a well-known method in chemical graph theory. This motivates us to study M and NM polynomials from which we retrieve topological indices.

2 Main Results

In this section, we obtain the expression for M and NM -polynomials of molecular graphs of some anticancer drugs using edge partition technique, degree and neighborhood counting method.

Theorem 2.1. *Let G be the molecular graph of amathaspiramide E. Then,*

$$(i) \quad M(G; x, y) = xy^2 + 5xy^3 + 3x^2y^2 + 5x^2y^3 + 2x^2y^4 + 6x^3y^3 + 2x^3y^4,$$

$$(ii) \quad NM(G; x, y) = x^2y^4 + x^3y^5 + x^3y^6 + 2x^3y^7 + x^3y^8 + x^4y^4 + 2x^4y^6 + x^4y^7 + x^5y^6 + x^5y^8 + x^6y^6 + 2x^6y^7 + x^6y^8 + 2x^6y^{10} + x^7y^7 + x^7y^8 + x^7y^{10} + 2x^8y^{10} + x^{10}y^{10}.$$

Proof. Let G be the molecular graph of amathaspiramide E (Figure 1). It has 24 number of edges. Let $M_{(i,j)}$ be the set of all edges with degree of end vertices i, j ,

i. e., $M_{(i,j)} = \{uv \in E(G) : \psi(u) = i, \psi(v) = j\}$. Let $m_{(i,j)}$ be the number of edges in $M_{(i,j)}$. From Figure 1, it is clear that $m_{(1,2)} = 1, m_{(1,3)} = 5, m_{(2,2)} = 3, m_{(2,3)} = 5, m_{(3,3)} = 6, m_{(3,4)} = 2$ and $m_{(2,4)} = 2$.

Thus, the M – polynomial of G is

$$\begin{aligned} M(G; x, y) &= \sum_{i \leq j} m_{(i,j)} x^i y^j \\ &= m_{(1,2)} x^1 y^2 + m_{(1,3)} x^1 y^3 + m_{(2,2)} x^2 y^2 + m_{(2,3)} x^2 y^3 \\ &\quad + m_{(2,4)} x^2 y^4 + m_{(3,3)} x^3 y^3 + m_{(3,4)} x^3 y^4 \\ &= xy^2 + 5xy^3 + 3x^2y^2 + 5x^2y^3 + 2x^2y^4 + 6x^3y^3 + 2x^3y^4. \end{aligned}$$

Let $M_{(i,j)}^*$ be the set of all edges with neighborhood degree sum of end vertices i, j , i. e., $M_{(i,j)}^* = \{uv \in E(G) : \Psi(u) = i, \Psi(v) = j\}$. Let $m_{(i,j)}^*$ be the number of edges in $M_{(i,j)}^*$. From Figure 1, it is clear that $m_{(2,4)}^* = 1, m_{(3,5)}^* = 1, m_{(3,6)}^* = 1, m_{(3,7)}^* = 2, m_{(3,8)}^* = 1, m_{(4,4)}^* = 1, m_{(2,4)}^* = 6, m_{(4,7)}^* = 1, m_{(5,6)}^* = 1, m_{(5,8)}^* = 1, m_{(6,6)}^* = 1, m_{(6,7)}^* = 2, m_{(6,8)}^* = 1, m_{(6,10)}^* = 2, m_{(7,7)}^* = 1, m_{(7,8)}^* = 1, m_{(7,10)}^* = 1, m_{(8,10)}^* = 2$ and $m_{(10,10)}^* = 1$.

Thus, the NM – polynomial of G is

$$\begin{aligned} NM(G; x, y) &= \sum_{i \leq j} m_{(i,j)}^* x^i y^j \\ &= m_{(2,4)}^* x^2 y^4 + m_{(3,5)}^* x^3 y^5 + m_{(3,6)}^* x^3 y^6 + m_{(3,7)}^* x^3 y^7 + m_{(3,8)}^* x^3 y^8 \\ &\quad + m_{(4,4)}^* x^4 y^4 + m_{(4,6)}^* x^4 y^6 + m_{(4,7)}^* x^4 y^7 + m_{(5,6)}^* x^5 y^6 + m_{(5,8)}^* x^5 y^8 \\ &\quad + m_{(6,6)}^* x^6 y^6 + m_{(6,7)}^* x^6 y^7 + m_{(6,8)}^* x^6 y^8 + m_{(6,10)}^* x^6 y^{10} \\ &\quad + m_{(7,7)}^* x^7 y^7 + m_{(7,8)}^* x^7 y^8 + m_{(7,10)}^* x^7 y^{10} + m_{(8,10)}^* x^8 y^{10} + m_{(10,10)}^* x^{10} y^{10} \\ &= x^2 y^4 + x^3 y^5 + x^3 y^6 + 2x^3 y^7 + x^3 y^8 + x^4 y^4 + 2x^4 y^6 + x^4 y^7 + x^5 y^6 + x^5 y^8 \\ &\quad + x^6 y^6 + 2x^6 y^7 + x^6 y^8 + 2x^6 y^{10} + x^7 y^7 + x^7 y^8 + x^7 y^{10} + 2x^8 y^{10} + x^{10} y^{10}. \end{aligned}$$

□

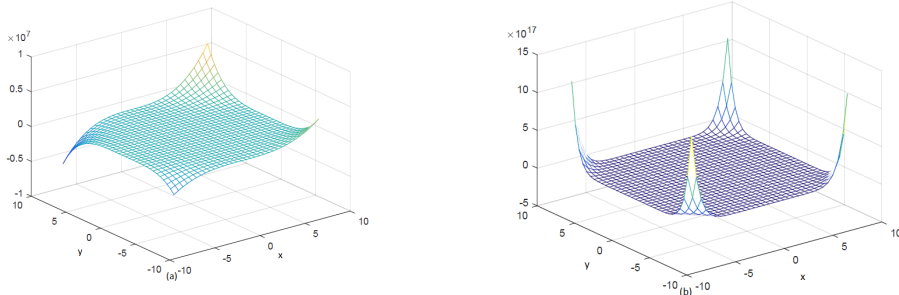


Figure 2: Plotting of (a) M-polynomial and (b) NM-polynomial of amathaspiramide E.

Corollary 2.1. *Let G be the molecular graph of amathaspiramide E. Then*

- (i) $M_1(G) = 122, M_1'(G) = 303,$
- (ii) $M_2(G) = 153, M_2^*(G) = 992,$
- (iii) $F(G) = 342, F_N^*(G) = 2141,$
- (iv) ${}^m M_2(G) = 4.833, {}^{nm} M_2(G) = 0.832,$
- (v) $R_\alpha(G) = 2^\alpha + 5(3)^\alpha + 3(4)^\alpha + 5(6)^\alpha + 2(8)^\alpha + 6(9)^\alpha + 2(12)^\alpha, NR_\alpha(G) = (8)^\alpha + (15)^\alpha + (18)^\alpha + 2(21)^\alpha + (24)^\alpha + (16)^\alpha + 2(24)^\alpha + (28)^\alpha + (30)^\alpha + (40)^\alpha + (36)^\alpha + 2(42)^\alpha + (48)^\alpha + 2(60)^\alpha + (49)^\alpha + (56)^\alpha + (70)^\alpha + 2(80)^\alpha + (100)^\alpha,$
- (vi) $ReZG_3(G) = 852, ND_3(G) = 14492,$
- (vii) $SDD(G) = 57.166, ND_5(G) = 53.65,$
- (viii) $H(G) = 9.904, NH(G) = 4.13,$
- (ix) $I(G) = 28.511, NI(G) = 72.36,$
- (x) $A(G) = 2572.2, S(G) = 852.94.$

Proof. Let $M(G) = f(x, y) = xy^2 + 5xy^3 + 3x^2y^2 + 5x^2y^3 + 2x^2y^4 + 6x^3y^3 + 2x^3y^4$. Then, we have

$$\begin{aligned} (D_x + D_y)(f(x, y)) &= 3xy^2 + 20xy^3 + 12x^2y^2 + 25x^2y^3 + 12x^2y^4 + 36x^3y^3 + 14x^3y^4, \\ D_x D_y(f(x, y)) &= 2xy^2 + 15xy^3 + 12x^2y^2 + 30x^2y^3 + 16x^2y^4 + 54x^3y^3 + 24x^3y^4, \\ (D_x^2 + D_y^2)(f(x, y)) &= 5xy^2 + 50xy^3 + 24x^2y^2 + 65x^2y^3 + 40x^2y^4 + 108x^3y^3 + 50x^3y^4, \\ I_x I_y(f(x, y)) &= \frac{1}{2}xy^2 + \frac{5}{3}xy^3 + \frac{3}{4}x^2y^2 + \frac{5}{6}x^2y^3 + \frac{1}{4}x^2y^4 + \frac{2}{3}x^3y^3 + \frac{1}{6}x^3y^4, \\ D_x^\alpha D_y^\alpha(f(x, y)) &= 2^\alpha xy^2 + 5(3)^\alpha xy^3 + 3(4)^\alpha x^2y^2 + 5(6)^\alpha x^2y^3 + 2(8)^\alpha x^2y^4 + 6(9)^\alpha x^3y^3 \\ &\quad + 2(12)^\alpha x^3y^4, \\ D_x D_y(D_x + D_y)(f(x, y)) &= 6xy^2 + 60xy^3 + 48x^2y^2 + 150x^2y^3 + 96x^2y^4 + 324x^3y^3 \\ &\quad + 168x^3y^4, \\ (D_x I_y + I_x D_y)(f(x, y)) &= \frac{5}{2}xy^2 + \frac{50}{3}xy^3 + 6x^2y^2 + \frac{65}{6}x^2y^3 + \frac{5}{x}x^2y^4 + 12x^3y^3 + \frac{25}{6}x^3y^4, \\ I_x J(f(x, y)) &= \frac{2}{3}x^3 + 4x^4 + 2x^5 + \frac{8}{3}x^6 + \frac{4}{7}x^7, \\ I_x J D_x D_y(f(x, y)) &= \frac{2}{3}x^3 + \frac{27}{4}x^4 + 6x^5 + \frac{35}{3}x^6 + \frac{24}{7}x^7, \\ I_x^3 Q_{-2} J D_x^3 D_y^3(f(x, y)) &= 8x + \frac{327}{2}x^2 + 360x^3 + \frac{5398}{4}x^4 + \frac{3456}{5}x^5 \end{aligned}$$

Using Table 2, we have

$$\begin{aligned} M_1(G) &= 3xy^2 + 20xy^3 + 12x^2y^2 + 25x^2y^3 + 12x^2y^4 + 36x^3y^3 + 14x^3y^4|_{x=y=1} = 122, \\ M_2(G) &= 2xy^2 + 15xy^3 + 12x^2y^2 + 30x^2y^3 + 16x^2y^4 + 54x^3y^3 + 24x^3y^4|_{x=y=1} = 153, \end{aligned}$$

$$F(G) = 5xy^2 + 50xy^3 + 24x^2y^2 + 65x^2y^3 + 40x^2y^4 + 108x^3y^3 + 50x^3y^4|_{x=y=1} = 342,$$

$${}^mM_2(G) = \frac{1}{2}xy^2 + \frac{5}{3}xy^3 + \frac{3}{4}x^2y^2 + \frac{5}{6}x^2y^3 + \frac{1}{4}x^2y^4 + \frac{2}{3}x^3y^3 + \frac{1}{6}x^3y^4|_{x=y=1} = 4.833,$$

$$R_\alpha = 2^\alpha xy^2 + 5(3)^\alpha xy^3 + 3(4)^\alpha x^2y^2 + 5(6)^\alpha x^2y^3 + 2(8)^\alpha x^2y^4 + 6(9)^\alpha x^3y^3 \\ + 2(12)^\alpha x^3y^4|_{x=y=1} = 2^\alpha + 5(3)^\alpha + 3(4)^\alpha + 5(6)^\alpha + 2(8)^\alpha + 6(9)^\alpha \\ + 2(12)^\alpha,$$

$$ReZG_3(G) = 6xy^2 + 60xy^3 + 48x^2y^2 + 150x^2y^3 + 96x^2y^4 + 324x^3y^3 \\ + 168x^3y^4|_{x=y=1} = 852,$$

$$SDD(G) = \frac{5}{2}xy^2 + \frac{50}{3}xy^3 + 6x^2y^2 + \frac{65}{6}x^2y^3 + \frac{5}{x}y^4 + 12x^3y^3 + \frac{25}{6}x^3y^4|_{x=y=1} = 57.166,$$

$$H(G) = \frac{2}{3}x^3 + 4x^4 + 2x^5 + \frac{8}{3}x^6 + \frac{4}{7}x^7|_{x=1} = 9.904,$$

$$I(G) = \frac{2}{3}x^3 + \frac{27}{4}x^4 + 6x^5 + \frac{35}{3}x^6 + \frac{24}{7}x^7|_{x=1} = 28.511,$$

$$A(G) = 8x + \frac{327}{2}x^2 + 360x^3 + \frac{5398}{4}x^4 + \frac{3456}{5}x^5|_{x=1} = 2572.2.$$

For neighborhood degree sum-based indices, we consider $g(x, y) = NM(G) = x^2y^4 + x^3y^5 + x^3y^6 + 2x^3y^7 + x^3y^8 + x^4y^4 + 2x^4y^6 + x^4y^7 + x^5y^6 + x^5y^8 + x^6y^6 + 2x^6y^7 + x^6y^8 + 2x^6y^{10} + x^7y^7 + x^7y^8 + x^7y^{10} + x^8y^{10} + x^{10}y^{10}$. Then, applying the above operations and Table 2, we can easily obtain the neighborhood degree sum-based indices. This completes the proof. \square

Theorem 2.2. *Let G be the molecular graph of aminopterin. Then,*

$$(i) M(G; x, y) = 7xy^3 + 5x^2y^2 + 18x^2y^3 + 4x^3y^3,$$

$$(ii) NM(G; x, y) = 3x^3y^4 + 2x^3y^5 + 2x^3y^6 + x^4y^5 + 2x^4y^6 + 5x^5y^5 \\ + 5x^5y^6 + 5x^5y^7 + 3x^6y^6 + 3x^6y^7 + 2x^6y^8 + x^7y^8.$$

Proof. Let G be the molecular graph of aminopterin (Figure 1). It has 34 edges. Let $M_{(i,j)}$ be the set of all edges with degree of end vertices i, j , i. e., $M_{(i,j)} = \{uv \in E(G) : \psi(u) = i, \psi(v) = j\}$. Let $m_{(i,j)}$ be the number of edges in $M_{(i,j)}$. From Figure 1, it is clear that $m_{(1,3)} = 7$, $m_{(2,2)} = 5$, $m_{(2,3)} = 18$ and $m_{(3,3)} = 4$. Let $M_{(i,j)}^*$ be the set of all edges with neighbourhood degree sum of end vertices i, j , i. e., $M_{(i,j)}^* = \{uv \in E(G) : \Psi(u) = i, \Psi(v) = j\}$. Let $m_{(i,j)}^*$ be the number of edges in $M_{(i,j)}^*$. From Figure 1, it is clear that $m_{(3,4)}^* = 3$, $m_{(3,5)}^* = 2$, $m_{(3,6)}^* = 2$, $m_{(4,5)}^* = 1$, $m_{(4,6)}^* = 2$, $m_{(5,5)}^* = 5$, $m_{(5,6)}^* = 5$, $m_{(5,7)}^* = 5$, $m_{(6,6)}^* = 3$, $m_{(6,7)}^* = 3$, $m_{(6,8)}^* = 2$ and $m_{(7,8)}^* = 1$. The proof is similar as that of Theorem 2.1. \square

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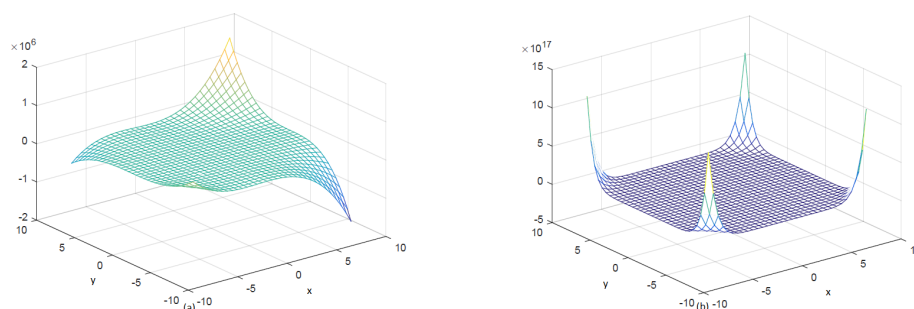


Figure 3: Plotting of (a) M-polynomial and (b) NM-polynomial of aminopterin.

Corollary 2.2. *Let G be the molecular graph of aminopterin. Then*

- (i) $M_1(G) = 162, M_1'(G) = 367,$
- (ii) $M_2(G) = 185, M_2^*(G) = 1006,$
- (iii) $F(G) = 416, F_N^*(G) = 2087,$
- (iv) ${}^m M_2(G) = 7.027, {}^{nm} M_2(G) = 1.35,$
- (v) $R_\alpha(G) = 7(3)^\alpha + 5(4)^\alpha + 18(6)^\alpha + 4(9)^\alpha, NR_\alpha(G) = 3(12)^\alpha + 2(15)^\alpha + 2(18)^\alpha + (20)^\alpha + 2(24)^\alpha + 5(25)^\alpha + 5(30)^\alpha + 5(35)^\alpha + 3(36)^\alpha + 3(42)^\alpha + 2(48)^\alpha + (56)^\alpha,$
- (vi) $ReZG_3(G) = 920, ND_3(G) = 11594,$
- (vii) $SDD(G) = 80.333, ND_5(G) = 71.16,$
- (viii) $H(G) = 7.266, NH(G) = 6.54,$
- (ix) $I(G) = 37.85, NI(G) = 89.91,$
- (x) $A(G) = 253.187, S(G) = 701.33.$

Theorem 2.3. *Let G be the molecular graph of aspidostomide E. Then,*

- (i) $M(G; x, y) = xy^2 + 6xy^3 + x^2y^2 + 9x^2y^3 + 12x^3y^3,$
- (ii) $NM(G; x, y) = x^2y^4 + x^3y^5 + 2x^3y^6 + 3x^3y^7 + x^4y^7 + 2x^5y^5 + x^5y^6 + x^5y^7 + 2x^6y^6 + 2x^6y^7 + x^6y^8 + 2x^6y^9 + 2x^7y^7 + x^7y^8 + 3x^7y^9 + x^8y^9 + 3x^9y^9.$

Proof. Let G be the molecular graph of aspidostomide E (Figure 1). It has 29 edges. Let $M_{(i,j)}$ be the set of all edges with degree of end vertices i, j , i. e., $M_{(i,j)} = \{uv \in E(G) : \psi(u) = i, \psi(v) = j\}$. Let $m_{(i,j)}$ be the number of edges in $M_{(i,j)}$. From Figure 1, it is clear that $m_{(1,2)} = 1, m_{(1,3)} = 6, m_{(2,2)} = 1, m_{(2,3)} = 9$ and $m_{(3,3)} = 12$. Let $M_{(i,j)}^*$ be the set of all edges with neighbourhood degree sum of end vertices i, j , i. e., $M_{(i,j)}^* = \{uv \in E(G) : \Psi(u) = i, \Psi(v) = j\}$. Let $m_{(i,j)}^*$ be the number of edges in $M_{(i,j)}^*$. From Figure 1, it is clear that $m_{(2,4)}^* = 1, m_{(3,5)}^* = 1, m_{(3,6)}^* = 2, m_{(3,7)}^* = 3, m_{(4,7)}^* = 1, m_{(5,5)}^* = 2, m_{(5,6)}^* = 1, m_{(5,7)}^* = 1, m_{(6,6)}^* = 2, m_{(6,7)}^* = 2, m_{(6,8)}^* = 1, m_{(6,9)}^* = 2, m_{(7,7)}^* = 1, m_{(7,8)}^* = 1, m_{(7,9)}^* = 3, m_{(8,9)}^* = 1$ and $m_{(9,9)}^* = 3$. Using the edge partition of G , the M and NM polynomials can be obtained easily. \square

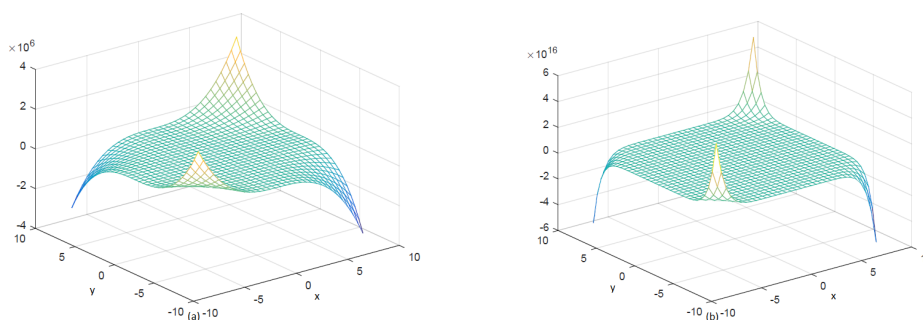


Figure 4: Plotting of (a) M-polynomial and (b) NM-polynomial of aspidostomide E.

Corolary 2.3. Let G be the molecular graph of aspidostomide E. Then

- (i) $M_1(G) = 148, M_1'(G) = 372,$
- (ii) $M_2(G) = 186, M_2^*(G) = 1235,$
- (iii) $F(G) = 406, F_N^*(G) = 2596,$
- (iv) ${}^m M_2(G) = 5.583, {}^{nm} M_2(G) = 0.94,$
- (v) $R_\alpha(G) = 2^\alpha + 6(3)^\alpha + 4^\alpha + 9(6)^\alpha + 12(9)^\alpha, NR_\alpha(G) = (8)^\alpha + (15)^\alpha + 2(18)^\alpha + 3(21)^\alpha + (28)^\alpha + 2(25)^\alpha + (30)^\alpha + (35)^\alpha + 2(36)^\alpha + 2(42)^\alpha + (48)^\alpha + 2(54)^\alpha + (56)^\alpha + 3(63)^\alpha + 2(49)^\alpha + (72)^\alpha + 3(81)^\alpha,$
- (vi) $ReZG_3(G) = 1012, ND_3(G) = 17762,$
- (vii) $SDD(G) = 68, ND_5(G) = 63.20,$
- (viii) $H(G) = 5.883, NH(G) = 4.85,$

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(ix) $I(G) = 34.966, NI(G) = 90.06,$

(x) $A(G) = 244.937, S(G) = 1070.91.$

Theorem 2.4. *Let G be the molecular graph of carmustine. Then*

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

(ii) $NM(G; x, y) = 2x^2y^3 + x^2y^4 + x^3y^4 + x^3y^5 + x^3y^6 + x^4y^5 + x^4y^7$
 $+ x^5y^6 + x^5y^7 + x^6y^7.$

Proof. Let G be the molecular graph of carmustine (Figure 1). It has 11 edges. Let $M_{(i,j)}$ be the set of all edges with degree of end vertices i, j , i. e., $M_{(i,j)} = \{uv \in E(G) : \psi(u) = i, \psi(v) = j\}$. Let $m_{(i,j)}$ be the number of edges in $M_{(i,j)}$. From Figure 1, it is clear that $m_{(1,2)} = 3, m_{(1,3)} = 1, m_{(2,2)} = 3, m_{(2,3)} = 3$ and $m_{(3,3)} = 1$. Let $M_{(i,j)}^*$ be the set of all edges with neighbourhood degree sum of end vertices i, j , i. e., $M_{(i,j)}^* = \{uv \in E(G) : \Psi(u) = i, \Psi(v) = j\}$. Let $m_{(i,j)}^*$ be the number of edges in $M_{(i,j)}^*$. From Figure 1, it is clear that $m_{(2,3)}^* = 2, m_{(2,4)}^* = 1, m_{(3,4)}^* = 1, m_{(3,5)}^* = 1, m_{(3,6)}^* = 1, m_{(4,5)}^* = 1, m_{(4,7)}^* = 1, m_{(5,6)}^* = 1, m_{(5,7)}^* = 1$ and $m_{(6,7)}^* = 1$. The M and NM polynomials can be obtained by using the edge partition of G . □

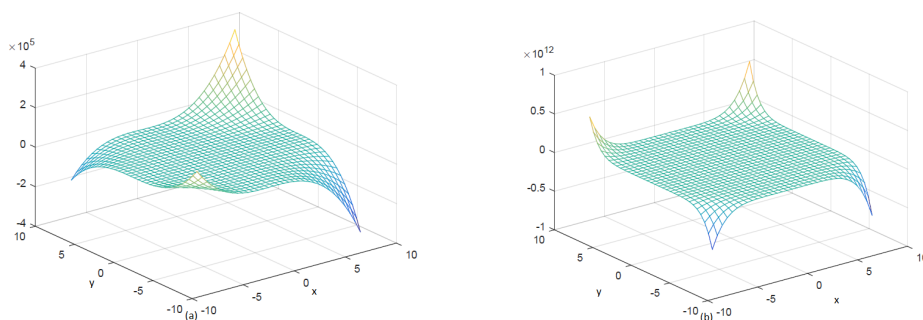


Figure 5: Plotting of (a) M-polynomial and (b) NM-polynomial of carmustine.

Corollary 2.4. *Let G be the molecular graph of carmustine. Then*

(i) $M_1(G) = 46, M_1'(G) = 96,$

(ii) $M_2(G) = 48, M_2^*(G) = 220,$

(iii) $F(G) = 106, F_N^*(G) = 476,$

(iv) ${}^m M_2(G) = 3.194, {}^{nm} M_2(G) = 0.835,$

- (v) $R_\alpha(G) = 3(2)^\alpha + (3)^\alpha + 3(4)^\alpha + 3(6)^\alpha + (9)^\alpha$, $NR_\alpha(G) = 2(6)^\alpha + (8)^\alpha + (12)^\alpha + (18)^\alpha + (15)^\alpha + (20)^\alpha + (28)^\alpha + (30)^\alpha + (35)^\alpha + (42)^\alpha$,
- (vi) $ReZG_3(G) = 222$, $ND_3(G) = 2258$,
- (vii) $SDD(G) = 25.33$, $ND_5(G) = 24.22$,
- (viii) $H(G) = 5.53$, $NH(G) = 2.79$,
- (ix) $I(G) = 10.85$, $NI(G) = 22.96$,
- (x) $A(G) = 12.86$, $S(G) = 131.74$.

Theorem 2.5. *Let G be the molecular graph of caulibugulone E. Then*

- (i) $M(G; x, y) = xy^2 + 2xy^3 + 3x^2y^2 + 5x^2y^3 + 4x^3y^3$,
- (ii) $NM(G; x, y) = x^2y^4 + x^3y^6 + x^3y^7 + x^4y^4 + 2x^4y^5 + x^4y^7 + 2x^5y^8 + x^6y^6 + x^6y^7 + x^7y^7 + x^7y^8 + x^8y^6 + x^8y^8$.

Proof. Let G be the molecular graph of caulibugulone E (Figure 1). It has 15 edges. Let $M_{(i,j)}$ be the set of all edges with degree of end vertices i, j , i. e., $M_{(i,j)} = \{uv \in E(G) : \psi(u) = i, \psi(v) = j\}$. Let $m_{(i,j)}$ be the number of edges in $M_{(i,j)}$. From Figure 1, it is clear that $m_{(1,2)} = 1$, $m_{(1,3)} = 2$, $m_{(2,2)} = 3$, $m_{(2,3)} = 5$ and $m_{(3,3)} = 4$. Let $M_{(i,j)}^*$ be the set of all edges with neighbourhood degree sum of end vertices i, j , i. e., $M_{(i,j)}^* = \{uv \in E(G) : \Psi(u) = i, \Psi(v) = j\}$. Let $m_{(i,j)}^*$ be the number of edges in $M_{(i,j)}^*$. From Figure 1, it is clear that $m_{(2,4)}^* = 1$, $m_{(3,6)}^* = 1$, $m_{(3,7)}^* = 1$, $m_{(4,4)}^* = 1$, $m_{(4,5)}^* = 2$, $m_{(4,7)}^* = 1$, $m_{(5,8)}^* = 2$, $m_{(6,6)}^* = 1$, $m_{(6,7)}^* = 1$, $m_{(6,8)}^* = 1$, $m_{(7,7)}^* = 1$, $m_{(7,8)}^* = 1$, $m_{(8,6)}^* = 1$ and $m_{(8,8)}^* = 1$. By making use of the edge partition of G , the M and NM polynomials can be computed. \square

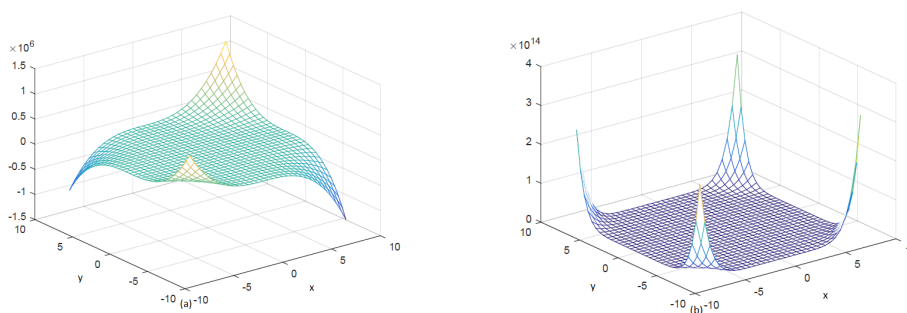


Figure 6: Plotting of (a) M-polynomial and (b) NM-polynomial of caulibugulone E.

Corollary 2.5. Let G be the molecular graph of caulibugulone E. Then

- (i) $M_1(G) = 72, M'_1(G) = 172,$
- (ii) $M_2(G) = 86, M_2^*(G) = 506,$
- (iii) $F(G) = 186, F_N^*(G) = 1076,$
- (iv) ${}^m M_2(G) = 3.194, {}^{nm} M_2(G) = 0.60,$
- (v) $R_\alpha(G) = (2)^\alpha + 2(3)^\alpha + 3(4)^\alpha + 5(6)^\alpha + 4(9)^\alpha, NR_\alpha(G) = (8)^\alpha + (18)^\alpha + (21)^\alpha + (16)^\alpha + 2(20)^\alpha + (28)^\alpha + 2(40)^\alpha + (36)^\alpha + (42)^\alpha + (48)^\alpha + (49)^\alpha + (56)^\alpha + (64)^\alpha,$
- (vi) $ReZG_3(G) = 444, ND_3(G) = 1072,$
- (vii) $SDD(G) = 34, ND_5(G) = 32.75,$
- (viii) $H(G) = 6.5, NH(G) = 2.80,$
- (ix) $I(G) = 17.16, NI(G) = 41.46,$
- (x) $A(G) = 26.28, S(G) = 384.26.$

Theorem 2.6. Let G be the molecular graph of convolutamide A. Then

- (i) $M(G; x, y) = xy^2 + 5xy^3 + xy^4 + 12x^2y^2 + 6x^2y^3 + x^2y^4 + 4x^3y^3 + 2x^3y^4,$
- (ii) $NM(G; x, y) = x^2y^3 + x^3y^4 + 3x^3y^6 + 2x^3y^7 + 9x^4y^4 + x^4y^5 + x^4y^9 + 2x^5y^6 + x^5y^8 + 2x^6y^6 + 2x^6y^7 + 3x^6y^8 + x^6y^9 + x^7y^8 + x^7y^9 + x^8y^9.$

Proof. Let G be the molecular graph of convolutamide A (Figure 1). It has 32 edges. Let $M_{(i,j)}$ be the set of all edges with degree of end vertices i, j , i. e., $M_{(i,j)} = \{uv \in E(G) : \psi(u) = i, \psi(v) = j\}$. Let $m_{(i,j)}$ be the number of edges in $M_{(i,j)}$. From Figure 1, it is clear that $m_{(1,2)} = 1, m_{(1,3)} = 5, m_{(1,4)} = 1, m_{(2,2)} = 12, m_{(2,3)} = 6, m_{(2,4)} = 1, m_{(3,3)} = 4$ and $m_{(3,4)} = 2$. Let $M_{(i,j)}^*$ be the set of all edges with neighbourhood degree sum of end vertices i, j , i. e., $M_{(i,j)}^* = \{uv \in E(G) : \Psi(u) = i, \Psi(v) = j\}$. Let $m_{(i,j)}^*$ be the number of edges in $M_{(i,j)}^*$. From Figure 1, it is clear that $m_{(2,3)}^* = 1, m_{(3,4)}^* = 1, m_{(3,6)}^* = 3, m_{(3,7)}^* = 2, m_{(4,4)}^* = 9, m_{(4,5)}^* = 1, m_{(4,9)}^* = 1, m_{(5,6)}^* = 2, m_{(5,8)}^* = 1, m_{(6,6)}^* = 2, m_{(6,7)}^* = 2, m_{(6,8)}^* = 3, m_{(6,9)}^* = 1, m_{(7,8)}^* = 1, m_{(7,9)}^* = 1$ and $m_{(8,9)}^* = 1$. Using the edge partition of G , the M and NM polynomials can be obtained easily. \square

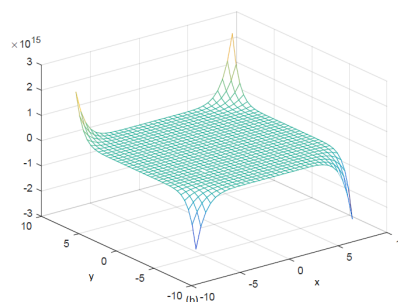


Figure 7: Plotting of (a) M-polynomial and (b) NM-polynomial of convolutamide A.

Corolary 2.6. Let G be the molecular graph of convolutamide A. Then

- (i) $M_1(G) = 150, M_1^*(G) = 343,$
- (ii) $M_2(G) = 173, M_2^*(G) = 959,$
- (iii) $F(G) = 388, F_N^*(G) = 2045,$
- (iv) ${}^m M_2(G) = 7.15, {}^{nm} M_2(G) = 1.47,$
- (v) $R_\alpha(G) = (2)^\alpha + 5(3)^\alpha + 13(4)^\alpha + 6(6)^\alpha + (8)^\alpha + 4(9)^\alpha + 2(12)^\alpha, NR_\alpha(G) = (6)^\alpha + (12)^\alpha + 3(18)^\alpha + 2(21)^\alpha + 9(16)^\alpha + (20)^\alpha + (36)^\alpha + 2(30)^\alpha + 2(36)^\alpha + 2(42)^\alpha + 3(48)^\alpha + (54)^\alpha + (56)^\alpha + (63)^\alpha + (72)^\alpha + (40)^\alpha,$
- (vi) $ReZG_3(G) = 890, ND_3(G) = 11854,$
- (vii) $SDD(G) = 75.07, ND_5(G) = 68.86,$
- (viii) $H(G) = 14.20, NH(G) = 6.47,$
- (ix) $I(G) = 35.17, NI(G) = 82.89,$
- (x) $A(G) = 51.23, S(G) = 701.26.$

Theorem 2.7. Let G be the molecular graph of convolutamine F. Then

- (i) $M(G; x, y) = 2xy^2 + 3xy^3 + 2x^2y^2 + 4x^2y^3 + 4x^3y^3,$
- (ii) $NM(G; x, y) = x^2y^3 + x^2y^4 + x^3y^4 + 2x^3y^6 + x^3y^7 + x^4y^5 + x^4y^8 + x^5y^8 + 2x^6y^6 + 2x^6y^8 + 2x^7y^8.$

Proof. Let G be the molecular graph of convolutamine F (Figure 1). It has 15 edges. Let $M_{(i,j)}$ be the set of all edges with degree of end vertices i, j , i. e., $M_{(i,j)} = \{uv \in E(G) : \psi(u) = i, \psi(v) = j\}$. Let $m_{(i,j)}$ be the number of edges in

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$M_{(i,j)}$. From Figure 1, it is clear that $m_{(1,2)} = 2, m_{(1,3)} = 3, m_{(2,2)} = 2, m_{(2,3)} = 4$ and $m_{(3,3)} = 4$. Let $M_{(i,j)}^*$ be the set of all edges with neighbourhood degree sum of end vertices i, j , i. e., $M_{(i,j)}^* = \{uv \in E(G) : \Psi(u) = i, \Psi(v) = j\}$. Let $m_{(i,j)}^*$ be the number of edges in $M_{(i,j)}^*$. From Figure 1, it is clear that $m_{(2,3)}^* = 1, m_{(2,4)}^* = 1, m_{(3,4)}^* = 1, m_{(3,6)}^* = 2, m_{(3,7)}^* = 1, m_{(4,5)}^* = 1, m_{(4,8)}^* = 1, m_{(5,8)}^* = 1, m_{(6,6)}^* = 2, m_{(6,8)}^* = 2$ and $m_{(7,8)}^* = 2$. The M and NM polynomials are obtained by using the edge partition of G . \square

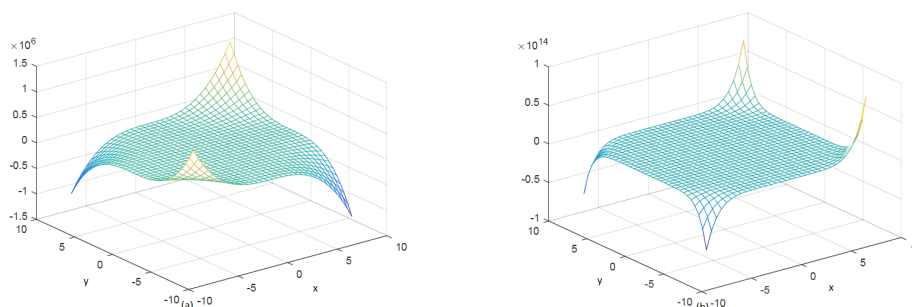


Figure 8: Plotting of (a) M-polynomial and (b) NM-polynomial of convolutamine F.

Corollary 2.7. *Let G be the molecular graph of convolutamine F. Then*

- (i) $M_1(G) = 70, M'_1(G) = 162,$
- (ii) $M_2(G) = 81, M_2^*(G) = 455,$
- (iii) $F(G) = 180, F_N^*(G) = 986,$
- (iv) ${}^m M_2(G) = 3.44, {}^{nm} M_2(G) = 0.77,$
- (v) $R_\alpha(G) = 2(2)^\alpha + 3(3)^\alpha + 2(4)^\alpha + 4(6)^\alpha + 4(9)^\alpha, NR_\alpha(G) = (6)^\alpha + (8)^\alpha + (12)^\alpha + 2(18)^\alpha + (21)^\alpha + (20)^\alpha + (32)^\alpha + (40)^\alpha + 2(36)^\alpha + 2(48)^\alpha + 2(56)^\alpha,$
- (vi) $ReZG_3(G) = 416, ND_3(G) = 5668,$
- (vii) $SDD(G) = 35.66, ND_5(G) = 33.48,$
- (viii) $H(G) = 6.76, NH(G) = 3.09,$
- (ix) $I(G) = 16.38, NI(G) = 38.63,$
- (x) $A(G) = 24.27, S(G) = 332.14.$

Theorem 2.8. *Let G be the molecular graph of convolutamydine A. Then*

- (i) $M(G; x, y) = 5xy^3 + xy^4 + 7x^2y^3 + x^2y^4 + 2x^3y^3 + 2x^3y^4,$
- (ii) $NM(G; x, y) = 2x^3y^4 + x^3y^5 + x^3y^6 + x^3y^7 + x^4y^7 + x^4y^9 + 2x^5y^6$
 $+ x^6y^6 + 3x^6y^7 + x^6y^{10} + 2x^7y^9 + x^7y^{10} + x^9y^{10}.$

Proof. Let G be the molecular graph of convolutamydine A (Figure 1). It has 18 edges. Let $M_{(i,j)}$ be the set of all edges with degree of end vertices i, j , i. e., $M_{(i,j)} = \{uv \in E(G) : \psi(u) = i, \psi(v) = j\}$. Let $m_{(i,j)}$ be the number of edges in $M_{(i,j)}$. From Figure 1, it is clear that $m_{(1,3)} = 5, m_{(1,4)} = 1, m_{(2,3)} = 7, m_{(2,4)} = 1, m_{(3,3)} = 2$ and $m_{(3,4)} = 2$. Let $M_{(i,j)}^*$ be the set of all edges with neighbourhood degree sum of end vertices i, j , i. e., $M_{(i,j)}^* = \{uv \in E(G) : \Psi(u) = i, \Psi(v) = j\}$. Let $m_{(i,j)}^*$ be the number of edges in $M_{(i,j)}^*$. From Figure 1, it is clear that $m_{(3,4)}^* = 2, m_{(3,5)}^* = 1, m_{(3,6)}^* = 1, m_{(3,7)}^* = 1, m_{(4,7)}^* = 1, m_{(4,9)}^* = 1, m_{(5,6)}^* = 2, m_{(6,6)}^* = 1, m_{(6,7)}^* = 3, m_{(6,10)}^* = 1, m_{(7,9)}^* = 2, m_{(9,10)}^* = 1$ and $m_{(7,10)}^* = 1$. The proof is similar as that of Theorem 2.1. \square

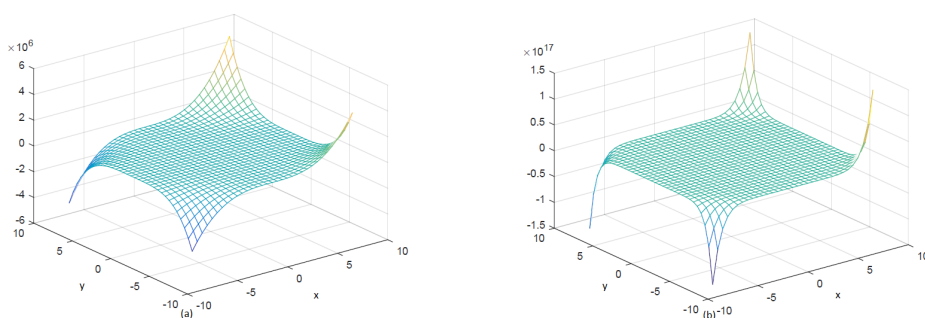


Figure 9: Plotting of (a) M-polynomial and (b) NM-polynomial of convolutamydine A.

Corolary 2.8. Let G be the molecular graph of convolutamydine A. Then

- (i) $M_1(G) = 82, M_1'(G) = 222,$
- (ii) $M_2(G) = 111, M_2^*(G) = 710,$
- (iii) $F(G) = 264, F_N^*(G) = 1524,$
- (iv) ${}^m M_2(G) = 3.59, {}^{nm} M_2(G) = 0.63,$
- (v) $R_\alpha(G) = 5(3)^\alpha + (4)^\alpha + (6)^\alpha + 2(9)^\alpha + 2(12)^\alpha, NR_\alpha(G) = 2(12)^\alpha + (15)^\alpha + (18)^\alpha + (21)^\alpha + (28)^\alpha + (36)^\alpha + 2(30)^\alpha + (36)^\alpha + 3(42)^\alpha + (60)^\alpha + 2(63)^\alpha + (70)^\alpha + (90)^\alpha,$
- (vi) $ReZG_3(G) = 614, ND_3(G) = 10042,$

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(vii) $SDD(G) = 42.58, ND_5(G) = 39.38,$

(viii) $H(G) = 4.27, NH(G) = 3.16,$

(ix) $I(G) = 20.71, NI(G) = 53.34,$

(x) $A(G) = 33.91, S(G) = 591.32.$

Theorem 2.9. *Let G be the molecular graph of Daunorubicin. Then*

(i) $M(G; x, y) = xy^2 + 9xy^3 + xy^4 + 2x^2y^2 + 10x^2y^3 + 2x^2y^4 + 16x^3y^3 + x^3y^4,$

(ii) $NM(G; x, y) = x^2y^4 + 4x^3y^6 + 5x^3y^7 + 2x^4y^5 + x^4y^7 + x^4y^8 + x^5y^7 + x^5y^8 + 5x^6y^6 + 3x^6y^7 + x^6y^8 + x^7y^7 + 5x^7y^8 + 8x^7y^9 + 2x^8y^9 + x^9y^9.$

Proof. Let G be the molecular graph of Daunorubicin (Figure 1). It has 42 edges. Let $M_{(i,j)}$ be the set of all edges with degree of end vertices i, j , i. e., $M_{(i,j)} = \{uv \in E(G) : \psi(u) = i, \psi(v) = j\}$. Let $m_{(i,j)}$ be the number of edges in $M_{(i,j)}$. From Figure 1, it is clear that $m_{(1,2)} = 1, m_{(1,3)} = 9, m_{(1,4)} = 1, m_{(2,2)} = 2, m_{(2,3)} = 10, m_{(2,4)} = 2, m_{(3,3)} = 16$ and $m_{(3,4)} = 1$. Let $M_{(i,j)}^*$ be the set of all edges with neighbourhood degree sum of end vertices i, j , i. e., $M_{(i,j)}^* = \{uv \in E(G) : \Psi(u) = i, \Psi(v) = j\}$. Let $m_{(i,j)}^*$ be the number of edges in $M_{(i,j)}^*$. From Figure 1, it is clear that $m_{(2,4)}^* = 1, m_{(3,6)}^* = 4, m_{(3,7)}^* = 5, m_{(4,5)}^* = 2, m_{(4,7)}^* = 1, m_{(4,8)}^* = 1, m_{(5,7)}^* = 1, m_{(5,8)}^* = 1, m_{(6,6)}^* = 5, m_{(6,7)}^* = 3, m_{(6,8)}^* = 1, m_{(7,7)}^* = 1, m_{(7,8)}^* = 5, m_{(7,9)}^* = 8, m_{(8,9)}^* = 2$ and $m_{(9,9)}^* = 1$. Now by making use of the edge partition of G , the M and NM polynomials are obtained. \square

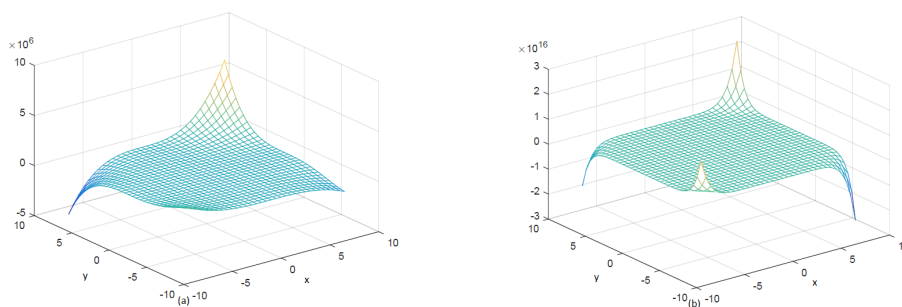


Figure 10: Plotting of (a) M-polynomial and (b) NM-polynomial of Daunorubicin.

Corollary 2.9. *Let G be the molecular graph of Daunorubicin. Then*

(i) $M_1(G) = 217, M_1'(G) = 540,$

(ii) $M_2(G) = 273, M_2^*(G) = 1772,$

(iii) $F(G) = 611, F_N^*(G) = 3750,$

(iv) ${}^m M_2(G) = 8.02, {}^{nm} M_2(G) = 1.31,$

(v) $R_\alpha(G) = (2)^\alpha + 9(3)^\alpha + (4)^\alpha + 2(4)^\alpha + 10(6)^\alpha + 2(8)^\alpha + 16(9)^\alpha + (12)^\alpha,$
 $NR_\alpha(G) = (8)^\alpha + 4(18)^\alpha + 5(21)^\alpha + 2(20)^\alpha + (28)^\alpha + (32)^\alpha + (35)^\alpha +$
 $(40)^\alpha + 5(36)^\alpha + 3(42)^\alpha + (48)^\alpha + (49)^\alpha + 5(56)^\alpha + 8(63)^\alpha + 2(72)^\alpha + (81)^\alpha,$

(vi) $ReZG_3(G) = 1510, ND_3(G) = 25064,$

(vii) $SDD(G) = 101.5, ND_5(G) = 92.35,$

(viii) $H(G) = 16.85, NH(G) = 6.92,$

(ix) $I(G) = 50.59, NI(G) = 130.24,$

(x) $A(G) = 87.66, S(G) = 1502.98.$

Theorem 2.10. *Let G be the molecular graph of Deguelin. Then*

(i) $M(G; x, y) = 2xy^2 + xy^3 + 2xy^4 + 3x^2y^2 + 14x^2y^3 + 2x^2y^4 + 9x^3y^3,$

(ii) $NM(G; x, y) = 2x^2y^4 + x^3y^7 + 2x^4y^6 + 2x^4y^7 + 2x^5y^5 + x^5y^6$
 $+ 3x^5y^7 + 2x^5y^8 + x^6y^6 + 5x^6y^7 + 2x^6y^8 + 2x^7y^7$
 $+ 3x^7y^8 + 2x^7y^9 + 2x^8y^8 + x^8y^9.$

Proof. Let G be the molecular graph of Deguelin (Figure 1). It has 33 edges. Let $M_{(i,j)}$ be the set of all edges with degree of end vertices i, j , i. e., $M_{(i,j)} = \{uv \in E(G) : \psi(u) = i, \psi(v) = j\}$. Let $m_{(i,j)}$ be the number of edges in $M_{(i,j)}$. From Figure 1, it is clear that $m_{(1,2)} = 2, m_{(1,3)} = 1, m_{(1,4)} = 2, m_{(2,2)} = 3, m_{(2,3)} = 14, m_{(2,4)} = 2$ and $m_{(3,3)} = 9$. Let $M_{(i,j)}^*$ be the set of all edges with neighbourhood degree sum of end vertices i, j , i. e., $M_{(i,j)}^* = \{uv \in E(G) : \Psi(u) = i, \Psi(v) = j\}$. Let $m_{(i,j)}^*$ be the number of edges in $M_{(i,j)}^*$. From Figure 1, it is clear that $m_{(2,4)}^* = 2, m_{(3,7)}^* = 1, m_{(4,6)}^* = 2, m_{(4,7)}^* = 2, m_{(5,5)}^* = 2, m_{(5,6)}^* = 1, m_{(5,7)}^* = 3, m_{(5,8)}^* = 2, m_{(6,6)}^* = 1, m_{(6,7)}^* = 5, m_{(6,8)}^* = 2, m_{(7,7)}^* = 2, m_{(7,8)}^* = 3, m_{(7,9)}^* = 2, m_{(8,8)}^* = 2$ and $m_{(8,9)}^* = 1$. With the help of edge partition of G , the M and NM polynomials can be computed. \square

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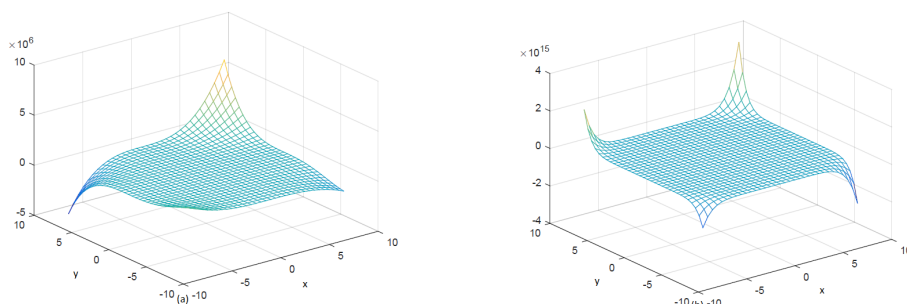


Figure 11: Plotting of (a) M-polynomial and (b) NM-polynomial of Deguelin.

Corollary 2.10. *Let G be the molecular graph of Deguelin. Then*

- (i) $M_1(G) = 158, M_1'(G) = 416,$
- (ii) $M_2(G) = 208, M_2^*(G) = 1340,$
- (iii) $F(G) = 462, F_N^*(G) = 2786,$
- (iv) ${}^m M_2(G) = 6.16, {}^{nm} M_2(G) = 1.06,$
- (v) $R_\alpha(G) = (2)^\alpha + (3)^\alpha + 2(4)^\alpha + 3(4)^\alpha + 14(6)^\alpha + 2(8)^\alpha + 9(9)^\alpha, NR_\alpha(G) = 2(8)^\alpha + (21)^\alpha + 2(24)^\alpha + 2(28)^\alpha + 2(25)^\alpha + (30)^\alpha + 3(35)^\alpha + 2(40)^\alpha + (36)^\alpha + 5(442)^\alpha + 2(48)^\alpha + 2(49)^\alpha + 3(56)^\alpha + 2(63)^\alpha + 2(64)^\alpha + (72)^\alpha,$
- (vi) $ReZG_3(G) = 1114, ND_3(G) = 18218,$
- (vii) $SDD(G) = 57.20, ND_5(G) = 70.04,$
- (viii) $H(G) = 13.4, NH(G) = 5.54,$
- (ix) $I(G) = 39.65, NI(G) = 101.61,$
- (x) $A(G) = 64.34, S(G) = 1103.$

Theorem 2.11. *Let G be the molecular graph of Melatonin. Then*

- (i) $M(G; x, y) = xy^2 + 2xy^3 + 4x^2y^2 + 9x^2y^3 + 2x^3y^3,$
- (ii) $NM(G; x, y) = x^2y^4 + 2x^3y^4 + 3x^4y^5 + x^4y^6 + 2x^5y^5 + x^5y^6 + 4x^5y^7 + x^6y^6 + x^6y^8 + 2x^7y^8.$

Proof. Let G be the molecular graph of Melatonin (Figure 1). It has 18 edges. Let $M_{(i,j)}$ be the set of all edges with degree of end vertices i, j , i. e., $M_{(i,j)} = \{uv \in E(G) : \psi(u) = i, \psi(v) = j\}$. Let $m_{(i,j)}$ be the number of edges in $M_{(i,j)}$. From Figure 1, it is clear that $m_{(1,2)} = 1, m_{(1,3)} = 2, m_{(2,2)} = 4, m_{(2,3)} = 9$

and $m_{(3,3)} = 2$. Let $M_{(i,j)}^*$ be the set of all edges with neighbourhood degree sum of end vertices i, j , i. e., $M_{(i,j)}^* = \{uv \in E(G) : \Psi(u) = i, \Psi(v) = j\}$. Let $m_{(i,j)}^*$ be the number of edges in $M_{(i,j)}^*$. From Figure 1, it is clear that $m_{(2,4)}^* = 1$, $m_{(3,4)}^* = 2$, $m_{(4,5)}^* = 3$, $m_{(4,6)}^* = 1$, $m_{(5,5)}^* = 2$, $m_{(5,6)}^* = 1$, $m_{(5,7)}^* = 4$, $m_{(6,6)}^* = 1$, $m_{(6,8)}^* = 1$ and $m_{(7,8)}^* = 2$. The proof is similar as that of Theorem 2.1. \square

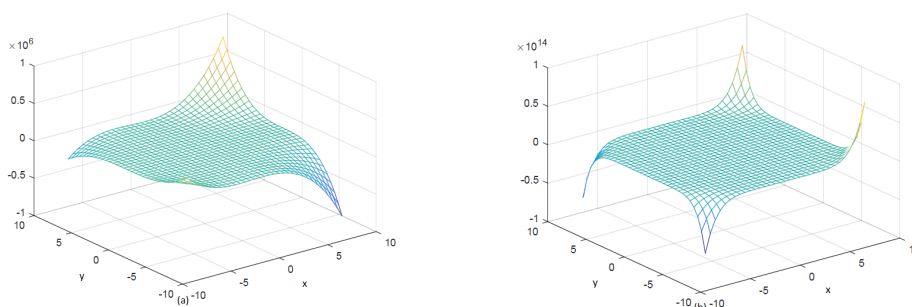


Figure 12: Plotting of (a) M-polynomial and (b) NM-polynomial of Melatonin.

Corolary 2.11. Let G be the molecular graph of Melatonin. Then

- (i) $M_1(G) = 84$, $M_1'(G) = 192$,
- (ii) $M_2(G) = 96$, $M_2^*(G) = 532$,
- (iii) $F(G) = 210$, $F_N^*(G) = 1100$,
- (iv) ${}^m M_2(G) = 3.88$, ${}^{nm} M_2(G) = 0.79$,
- (v) $R_\alpha(G) = (2)^\alpha + 2(3)^\alpha + 4(4)^\alpha + 9(6)^\alpha + 2(9)^\alpha$, $NR_\alpha(G) = (8)^\alpha + 2(12)^\alpha + 3(20)^\alpha + (24)^\alpha + 2(25)^\alpha + (30)^\alpha + 4(35)^\alpha + (36)^\alpha + (48)^\alpha + 2(56)^\alpha$,
- (vi) $ReZG_3(G) = 472$, $ND_3(G) = 6290$,
- (vii) $SDD(G) = 40.66$, $ND_5(G) = 37.59$,
- (viii) $H(G) = 7.93$, $NH(G) = 3.59$,
- (ix) $I(G) = 19.96$, $NI(G) = 47.11$,
- (x) $A(G) = 27.43$, $S(G) = 381.34$.

Theorem 2.12. Let G be the molecular graph of Minocycline. Then

- (i) $M(G; x, y) = 11xy^3 + xy^4 + x^2y^2 + 6x^2y^3 + 14x^3y^3 + 3x^3y^4$,

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$$(ii) \quad NM(G; x, y) = 6x^3y^5 + x^3y^6 + 2x^3y^7 + 2x^3y^8 + x^4y^{10} + x^5y^5 + x^5y^6 \\ + 2x^5y^8 + 2x^5y^9 + 2x^6y^7 + x^6y^8 + 2x^6y^9 + 5x^7y^9 \\ + x^8y^8 + 3x^8y^9 + 2x^8y^{10} + x^9y^9 + x^9y^{10}.$$

Proof. Let G be the molecular graph of Minocycline (Figure 1). It has 36 edges. Let $M_{(i,j)}$ be the set of all edges with degree of end vertices i, j , i. e., $M_{(i,j)} = \{uv \in E(G) : \psi(u) = i, \psi(v) = j\}$. Let $m_{(i,j)}$ be the number of edges in $M_{(i,j)}$. From Figure 1, it is clear that $m_{(1,3)} = 11$, $m_{(1,4)} = 1$, $m_{(2,2)} = 1$, $m_{(2,3)} = 6$, $m_{(3,3)} = 14$ and $m_{(3,4)} = 3$. Let $M_{(i,j)}^*$ be the set of all edges with neighbourhood degree sum of end vertices i, j , i. e., $M_{(i,j)}^* = \{uv \in E(G) : \Psi(u) = i, \Psi(v) = j\}$. Let $m_{(i,j)}^*$ be the number of edges in $M_{(i,j)}^*$. From Figure 1, it is clear that $m_{(3,5)}^* = 6$, $m_{(3,6)}^* = 1$, $m_{(3,7)}^* = 2$, $m_{(3,8)}^* = 2$, $m_{(4,10)}^* = 1$, $m_{(5,5)}^* = 1$, $m_{(5,6)}^* = 1$, $m_{(5,8)}^* = 2$, $m_{(5,9)}^* = 2$, $m_{(6,7)}^* = 2$, $m_{(6,8)}^* = 1$, $m_{(6,9)}^* = 2$, $m_{(7,9)}^* = 5$, $m_{(8,8)}^* = 1$, $m_{(8,9)}^* = 3$, $m_{(8,10)}^* = 2$, $m_{(9,9)}^* = 1$ and $m_{(9,10)}^* = 1$. With the help of edge partition of G , the M and NM polynomials can be computed. \square

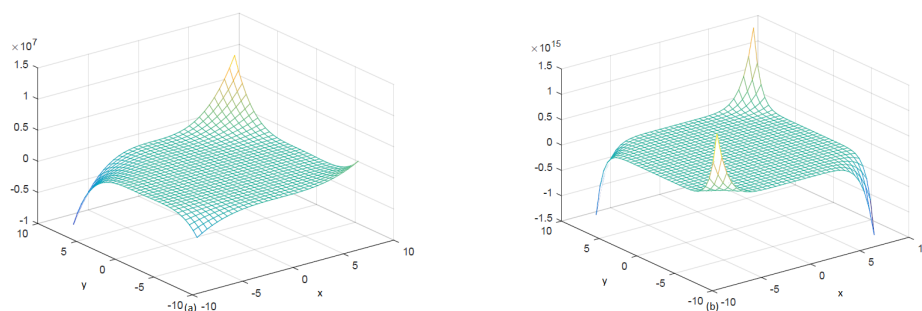


Figure 13: Plotting of (a) M-polynomial and (b) NM-polynomial of Minocycline.

Corollary 2.12. *Let G be the molecular graph of Minocycline. Then, we have*

- (i) $M_1(G) = 188$, $M_1'(G) = 478$,
- (ii) $M_2(G) = 239$, $M_2^*(G) = 1629$,
- (iii) $F(G) = 544$, $F_N^*(G) = 3516$,
- (iv) ${}^m M_2(G) = 6.97$, ${}^{nm} M_2(G) = 1.117$,
- (v) $R_\alpha(G) = 11(3)^\alpha + 2(4)^\alpha + 6(6)^\alpha + 14(9)^\alpha + 3(12)^\alpha$, $NR_\alpha(G) = 6(15)^\alpha + (18)^\alpha + 2(21)^\alpha + 2(24)^\alpha + (40)^\alpha + (25)^\alpha + (30)^\alpha + 2(40)^\alpha + 2(45)^\alpha + 2(42)^\alpha + (48)^\alpha + 2(54)^\alpha + 5(63)^\alpha + (64)^\alpha + 3(72)^\alpha + 2(80)^\alpha + (81)^\alpha + (90)^\alpha$,
- (vi) $ReZG_3(G) = 1356$, $ND_3(G) = 24438$,

(vii) $SDD(G) = 90.16, ND_5(G) = 80.73,$

(viii) $H(G) = 14.32, NH(G) = 5.86,$

(ix) $I(G) = 43.39, NI(G) = 114.08,$

(x) $A(G) = 78.87, S(G) = 1441.95.$

Theorem 2.13. *Let G be the molecular graph of Perfragilin A. Then*

(i) $M(G; x, y) = xy^2 + 5xy^3 + 5x^2y^3 + 7x^3y^3,$

(ii) $NM(G; x, y) = x^2y^4 + 2x^3y^6 + 3x^3y^7 + x^4y^8 + 3x^6y^6 + 2x^6y^8 + x^7y^7 + 4x^7y^8 + x^8y^8.$

Proof. Let G be the molecular graph of Perfragilin A (Figure 1). It has 18 number of edges. Let $M_{(i,j)}$ be the set of all edges with degree of end vertices i, j , i. e., $M_{(i,j)} = \{uv \in E(G) : \psi(u) = i, \psi(v) = j\}$. Let $m_{(i,j)}$ be the number of edges in $M_{(i,j)}$. From Figure 1, it is clear that $m_{(1,2)} = 1, m_{(1,3)} = 5, m_{(2,3)} = 5$ and $m_{(3,3)} = 7$. Let $M_{(i,j)}^*$ be the set of all edges with neighborhood degree sum of end vertices i, j , i. e., $M_{(i,j)}^* = \{uv \in E(G) : \Psi(u) = i, \Psi(v) = j\}$. Let $m_{(i,j)}^*$ be the number of edges in $M_{(i,j)}^*$. From Figure 1, it is clear that $m_{(2,4)}^* = 1, m_{(3,6)}^* = 2, m_{(3,7)}^* = 3, m_{(4,8)}^* = 1, m_{(6,6)}^* = 3, m_{(6,8)}^* = 2, m_{(7,7)}^* = 1, m_{(7,8)}^* = 4$ and $m_{(8,8)}^* = 1$. Now by making use of the edge partition of G , the M and NM -polynomials are obtained. □

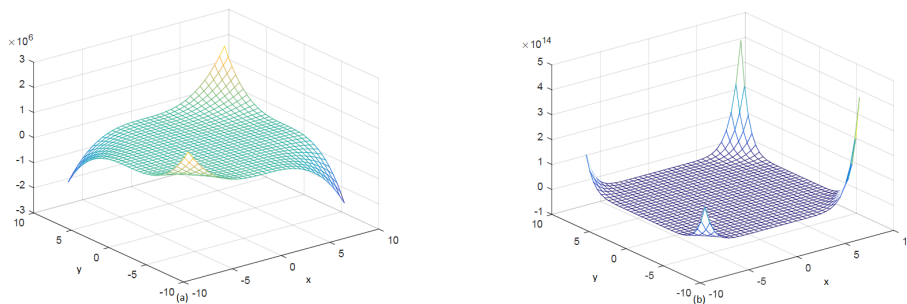


Figure 14: Plotting of (a) M-polynomial and (b) NM-polynomial of Perfragilin A.

Corolary 2.13. *Let G be the molecular graph of Perfragilin A. Then*

(i) $M_1(G) = 90, M_1'(G) = 220,$

(ii) $M_2(G) = 110, M_2^*(G) = 680,$

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(iii) $F(G) = 246, F_N^*(G) = 1458,$

(iv) ${}^m M_2(G) = 3.77, {}^{nm} M_2(G) = 0.64,$

(v) $R_\alpha(G) = (2)^\alpha + 5(3)^\alpha + 5(6)^\alpha + 7(9)^\alpha, NR_\alpha(G) = (8)^\alpha + 2(18)^\alpha + 3(21)^\alpha + (32)^\alpha + 3(36)^\alpha + 2(48)^\alpha + (49)^\alpha + 4(56)^\alpha + (64)^\alpha,$

(vi) $ReZG_3(G) = 594, ND_3(G) = 9096,$

(vii) $SDD(G) = 42, ND_5(G) = 40.52,$

(viii) $H(G) = 7.5, NH(G) = 3.13,$

(ix) $I(G) = 20.91, NI(G) = 52.59,$

(x) $A(G) = 34.65, S(G) = 541.73.$

Theorem 2.14. *Let G be the molecular graph of Podophyllotoxin. Then*

(i) $M(G; x, y) = 3xy^2 + 2xy^3 + 3x^2y^2 + 15x^2y^3 + 11x^3y^3,$

(ii) $NM(G; x, y) = 3x^2y^4 + x^3y^6 + x^3y^7 + 2x^4y^5 + 2x^4y^7 + x^4y^8 + x^5y^5 + x^5y^6 + 2x^5y^7 + x^5y^8 + 6x^6y^7 + 2x^6y^8 + x^6y^9 + x^7y^7 + 4x^7y^8 + x^7y^9 + x^8y^8 + 2x^8y^9 + x^9y^9.$

Proof. Let G be the molecular graph of Podophyllotoxin (Figure 1). It has 34 number of edges. Let $M_{(i,j)}$ be the set of all edges with degree of end vertices i, j , i. e., $M_{(i,j)} = \{uv \in E(G) : \psi(u) = i, \psi(v) = j\}$. Let $m_{(i,j)}$ be the number of edges in $M_{(i,j)}$. From Figure 1, it is clear that $m_{(1,2)} = 3, m_{(1,3)} = 2, m_{(2,2)} = 3, m_{(2,3)} = 15$ and $m_{(3,3)} = 11$. Let $M_{(i,j)}^*$ be the set of all edges with neighborhood degree sum of end vertices i, j , i. e., $M_{(i,j)}^* = \{uv \in E(G) : \Psi(u) = i, \Psi(v) = j\}$. Let $m_{(i,j)}^*$ be the number of edges in $M_{(i,j)}^*$. From Figure 1, it is clear that $m_{(2,4)}^* = 3, m_{(3,6)}^* = 1, m_{(3,7)}^* = 1, m_{(4,5)}^* = 2, m_{(4,7)}^* = 2, m_{(4,8)}^* = 1, m_{(5,5)}^* = 1, m_{(5,6)}^* = 1, m_{(5,7)}^* = 2, m_{(5,8)}^* = 1, m_{(6,7)}^* = 6, m_{(6,8)}^* = 2, m_{(6,9)}^* = 1, m_{(7,7)}^* = 1, m_{(7,8)}^* = 4, m_{(7,9)}^* = 1, m_{(8,8)}^* = 1, m_{(8,9)}^* = 2$ and $m_{(9,9)}^* = 1$. Now by making use of the edge partition of G , the M and NM -polynomials can be computed. \square

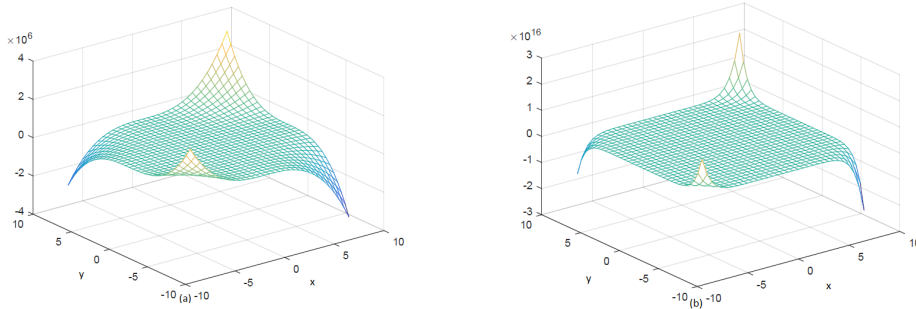


Figure 15: Plotting of (a) M-polynomial and (b) NM-polynomial of Podophyllo toxin.

Corolary 2.14. Let G be the molecular graph of Podophyllo toxin. Then

- (i) $M_1(G) = 170, M'_1(G) = 426,$
- (ii) $M_2(G) = 213, M_2^*(G) = 1383,$
- (iii) $F(G) = 452, F_N^*(G) = 2890,$
- (iv) ${}^m M_2(G) = 6.63, {}^{nm} M_2(G) = 1.2,$
- (v) $R_\alpha(G) = 3(2)^\alpha + 2(3)^\alpha + 3(4)^\alpha + 15(6)^\alpha + 11(9)^\alpha, NR_\alpha(G) = 3(8)^\alpha + (18)^\alpha + (21)^\alpha + 2(20)^\alpha + (25)^\alpha + 2(28)^\alpha + (32)^\alpha + 2(35)^\alpha + (30)^\alpha + (40)^\alpha + 6(42)^\alpha + 4(56)^\alpha + (49)^\alpha + (64)^\alpha + 2(48)^\alpha + 2(72)^\alpha + 2(72)^\alpha + (63)^\alpha + (81)^\alpha + (54)^\alpha,$
- (vi) $ReZG_3(G) = 1134, ND_3(G) = 19230,$
- (vii) $SDD(G) = 74.66, ND_5(G) = 73.13,$
- (viii) $H(G) = 14.16, NH(G) = 5.88,$
- (ix) $I(G) = 41, NI(G) = 103.62,$
- (x) $A(G) = 67.76, S(G) = 1161.65.$

Theorem 2.15. Let G be the molecular graph of Pterocellin. Then

- (i) $M(G; x, y) = xy^2 + 2xy^3 + 5x^2y^2 + 13x^2y^3 + 6x^3y^3,$
- (ii) $NM(G; x, y) = x^2y^4 + x^3y^6 + x^3y^7 + 2x^4y^4 + 2x^4y^5 + x^4y^7 + x^5y^5 + 3x^5y^6 + x^5y^8 + 4x^6y^6 + 2x^6y^7 + 3x^6y^8 + 2x^7y^8 + 3x^8y^8.$

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Proof. Let G be the molecular graph of Pterocellin (Figure 1). It has 27 number of edges. Let $M_{(i,j)}$ be the set of all edges with degree of end vertices i, j , i. e., $M_{(i,j)} = \{uv \in E(G) : \psi(u) = i, \psi(v) = j\}$. Let $m_{(i,j)}$ be the number of edges in $M_{(i,j)}$. From Figure 1, it is clear that $m_{(1,2)} = 1, m_{(1,3)} = 2, m_{(2,2)} = 5, m_{(2,3)} = 13$ and $m_{(3,3)} = 6$. Let $M_{(i,j)}^*$ be the set of all edges with neighborhood degree sum of end vertices i, j , i. e., $M_{(i,j)}^* = \{uv \in E(G) : \Psi(u) = i, \Psi(v) = j\}$. Let $m_{(i,j)}^*$ be the number of edges in $M_{(i,j)}^*$. From Figure 1, it is clear that $m_{(2,4)}^* = 1, m_{(3,6)}^* = 1, m_{(3,7)}^* = 1, m_{(4,4)}^* = 2, m_{(4,5)}^* = 2, m_{(4,7)}^* = 1, m_{(5,5)}^* = 1, m_{(5,6)}^* = 3, m_{(5,8)}^* = 1, m_{(6,6)}^* = 4, m_{(6,7)}^* = 2, m_{(6,8)}^* = 3, m_{(7,8)}^* = 2, m_{(8,8)}^* = 3$. With the help of edge partition of G , the M and NM -polynomials can be computed. \square

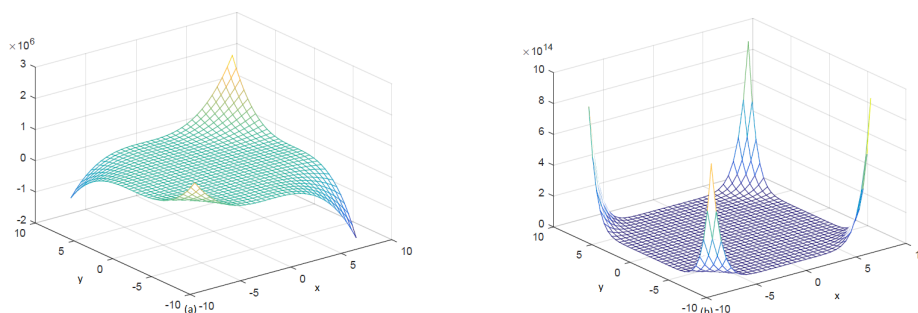


Figure 16: Plotting of (a) M-polynomial and (b) NM-polynomial of Pterocellin.

Corollary 2.15. Let G be the molecular graph of Pterocellin. Then

- (i) $M_1(G) = 132, M_1'(G) = 320,$
- (ii) $M_2(G) = 142, M_2^*(G) = 978,$
- (iii) $F(G) = 342, F_N^*(G) = 2024,$
- (iv) ${}^m M_2(G) = 5.25, {}^{nm} M_2(G) = 0.95,$
- (v) $R_\alpha(G) = (2)^\alpha + 2(3)^\alpha + 5(4)^\alpha + 13(6)^\alpha + 6(9)^\alpha, NR_\alpha(G) = (8)^\alpha + (18)^\alpha + (21)^\alpha + 2(16)^\alpha + 2(20)^\alpha + (28)^\alpha + (25)^\alpha + 3(30)^\alpha + 4(36)^\alpha + 2(42)^\alpha + 3(48)^\alpha + 2(56)^\alpha + 3(64)^\alpha + (40)^\alpha,$
- (vi) $ReZG_3(G) = 824, ND_3(G) = 12692,$
- (vii) $SDD(G) = 59.33, ND_5(G) = 56.84,$
- (viii) $H(G) = 11.36, NH(G) = 4.82,$
- (ix) $I(G) = 31.76, NI(G) = 78.39,$

(x) $A(G) = 48.84, S(G) = 772.10.$

Theorem 2.16. *Let G be the molecular graph of Raloxifene. Then*

(i) $M(G; x, y) = 3xy^3 + 11x^2y^2 + 18x^2y^3 + 6x^3y^3,$

(ii) $NM(G; x, y) = 2x^3y^5 + x^3y^7 + 2x^4y^4 + 4x^4y^5 + 8x^5y^5 + 7x^5y^6 + 4x^5y^7 + x^5y^8 + 2x^6y^7 + x^6y^8 + x^7y^7 + 2x^7y^8 + x^7y^9 + 2x^8y^9.$

Proof. Let G be the molecular graph of Raloxifene (Figure 1). It has 38 number of edges. Let $M_{(i,j)}$ be the set of all edges with degree of end vertices i, j , i. e., $M_{(i,j)} = \{uv \in E(G) : \psi(u) = i, \psi(v) = j\}$. Let $m_{(i,j)}$ be the number of edges in $M_{(i,j)}$. From Figure 1, it is clear that $m_{(1,3)} = 3, m_{(2,2)} = 11, m_{(2,3)} = 18$ and $m_{(3,3)} = 6$. Let $M_{(i,j)}^*$ be the set of all edges with neighborhood degree sum of end vertices i, j , i. e., $M_{(i,j)}^* = \{uv \in E(G) : \Psi(u) = i, \Psi(v) = j\}$. Let $m_{(i,j)}^*$ be the number of edges in $M_{(i,j)}^*$. From Figure 1, it is clear that $m_{(3,5)}^* = 2, m_{(3,7)}^* = 1, m_{(4,4)}^* = 2, m_{(4,5)}^* = 4, m_{(5,5)}^* = 8, m_{(5,6)}^* = 7, m_{(5,7)}^* = 4, m_{(5,8)}^* = 1, m_{(6,7)}^* = 2, m_{(6,8)}^* = 1, m_{(7,7)}^* = 1, m_{(7,8)}^* = 2, m_{(7,9)}^* = 1, m_{(8,9)}^* = 2$. Now using the edge partition of G , the M and NM -polynomials can be evaluated. \square

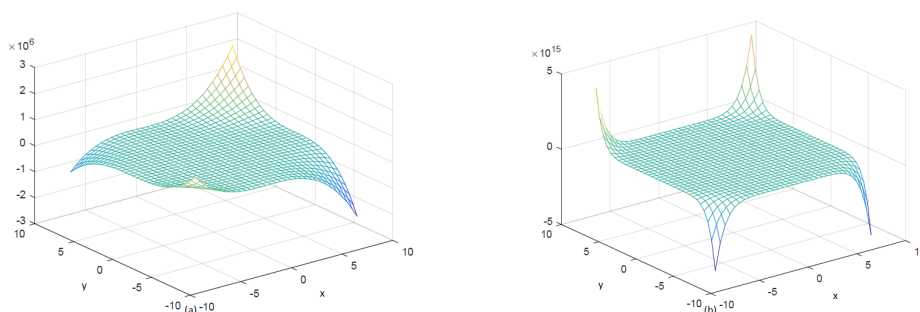


Figure 17: Plotting of (a) M-polynomial and (b) NM-polynomial of Raloxifene.

Corolary 2.16. *Let G be the molecular graph of Raloxifene. Then*

(i) $M_1(G) = 182, M_1'(G) = 430,$

(ii) $M_2(G) = 215, M_2^*(G) = 1253,$

(iii) $F(G) = 460, F_N^*(G) = 2580,$

(iv) ${}^m M_2(G) = 7.41, {}^{nm} M_2(G) = 1.36,$

(v) $R_\alpha(G) = 3(3)^\alpha + 11(4)^\alpha + 18(6)^\alpha + 6(9)^\alpha, NR_\alpha(G) = 2(15)^\alpha + (21)^\alpha + 2(16)^\alpha + 4(20)^\alpha + 8(25)^\alpha + 7(30)^\alpha + 4(35)^\alpha + (40)^\alpha + 2(42)^\alpha + (48)^\alpha + (49)^\alpha + 2(56)^\alpha + (63)^\alpha + 2(72)^\alpha,$

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(vi) $ReZG_3(G) = 1076, ND_3(G) = 15522,$

(vii) $SDD(G) = 83, ND_5(G) = 78.66,$

(viii) $H(G) = 16.2, NH(G) = 7.002,$

(ix) $I(G) = 43.85, NI(G) = 105.83,$

(x) $A(G) = 63.61, S(G) = 945.39.$

Theorem 2.17. *Let G be the molecular graph of Tambjamine K. Then*

(i) $M(G; x, y) = xy^2 + 2xy^3 + 6x^2y^2 + 9x^2y^3 + 2x^3y^3,$

(ii) $NM(G; x, y) = x^2y^4 + 2x^3y^4 + 2x^4y^4 + 5x^4y^5 + x^4y^7 + 3x^5y^7 + 4x^6y^7 + 2x^7y^7.$

Proof. Let G be the molecular graph of Tambjamine K (Figure 1). It has 20 number of edges. Let $M_{(i,j)}$ be the set of all edges with degree of end vertices i, j , i. e., $M_{(i,j)} = \{uv \in E(G) : \psi(u) = i, \psi(v) = j\}$. Let $m_{(i,j)}$ be the number of edges in $M_{(i,j)}$. From Figure 1, it is clear that $m_{(1,2)} = 1, m_{(1,3)} = 2, m_{(2,2)} = 5, m_{(2,3)} = 13$ and $m_{(3,3)} = 6$. Let $M_{(i,j)}^*$ be the set of all edges with neighborhood degree sum of end vertices i, j , i. e., $M_{(i,j)}^* = \{uv \in E(G) : \Psi(u) = i, \Psi(v) = j\}$. Let $m_{(i,j)}^*$ be the number of edges in $M_{(i,j)}^*$. From Figure 1, it is clear that $m_{(2,4)}^* = 1, m_{(3,4)}^* = 2, m_{(4,4)}^* = 2, m_{(4,5)}^* = 5, m_{(4,7)}^* = 1, m_{(5,7)}^* = 3, m_{(6,7)}^* = 4$ and $m_{(7,7)}^* = 2$. Using the edge partition of G , the M and NM -polynomials can be obtained easily. □

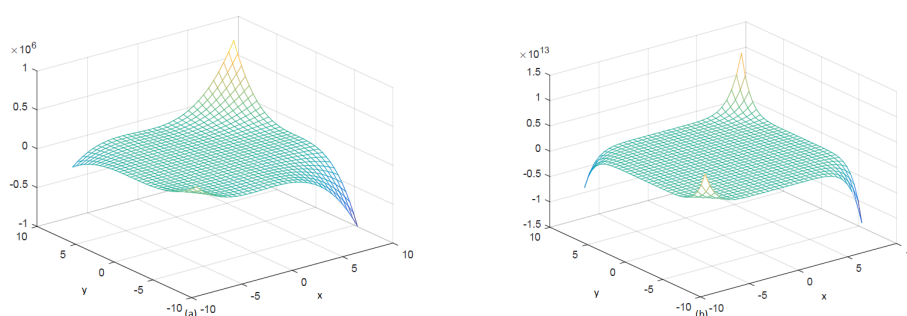


Figure 18: Plotting of (a) M-polynomial and (b) NM-polynomial of Tambjamine K.

Corollary 2.17. *Let G be the molecular graph of Tambjamine K. Then*

(i) $M_1(G) = 92, M_1'(G) = 208,$

- (ii) $M_2(G) = 104, M_2^*(G) = 563,$
- (iii) $F(G) = 226, F_N^*(G) = 1162,$
- (iv) ${}^m M_2(G) = 4.38, {}^{nm} M_2(G) = 0.92,$
- (v) $R_\alpha(G) = (2)^\alpha + 2(3)^\alpha + 6(4)^\alpha + 9(6)^\alpha + 2(9)^\alpha, NR_\alpha(G) = (8)^\alpha + 2(12)^\alpha + 2(16)^\alpha + 5(20)^\alpha + (28)^\alpha + 3(35)^\alpha + 4(42)^\alpha + 2(49)^\alpha,$
- (vi) $ReZG_3(G) = 504, ND_3(G) = 6496,$
- (vii) $SDD(G) = 44.66, ND_5(G) = 41.67,$
- (viii) $H(G) = 8.93, NH(G) = 4.09,$
- (ix) $I(G) = 21.96, NI(G) = 51.09,$
- (x) $A(G) = 29.43, S(G) = 394.88.$



Figure 19: Plotting of R_α and NR_α for aminopterin, amathaspiramide E and carmustine.

M polynomial and NM polynomial give an extensive details on degree based and neighborhood degree based indices, respectively. We hope that a more in-depth analysis of the properties of M polynomial and NM polynomial will open up new general perspectives in the study of topological indices. To visualize the polynomials, their surface plots were performed by Matlab. The expressions of the M and NM polynomials for some anticancer drugs are shown in Figures 2 to 18, respectively. The graphs reveals that the polynomial displays different behaviors corresponding to different parameters. We can control the topology and therefore different properties and operations by tuning the M and NM polynomials via these parameters. Plotting of R_α and NR_α for aminopterin, amathaspiramide E and carmustine are shown in Figure 19. In the horizontal axis, $\alpha = 2, 4, 6, 8, 10$ are taken. In the vertical axis, the logarithmic values of the indices are considered to clearly represent the comparison.

3 Conclusion

In this paper, we have obtained M -polynomial and NM -polynomial of some anticancer drugs with graphical representations. The advantage of M -polynomial and NM -polynomial is from one expression we can obtain several degree-based and neighborhood degree topological indices. It is very challenging to bring all the degree-based and neighborhood degree based topological indices under M -polynomial and NM -polynomial, respectively. As considered topological indices are able to predict different physico-chemical properties. These results can be useful in designing new drug for the treatment of cancer. A research may be conducted for various chemical structures, and a conclusion can be drawn based on their topological indices range.

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