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A STUDY ON DEGREE-BASED TOPOLOGICAL INDICES AND M-POLYNOMIAL USED IN CANCER TREATMENT

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Abstract. Topological indices are utilized in the fields of chemoinformatics, biomedicine, and bioinformatics to predict the physical and chemical properties as well as biological activities of compounds. Cancer ranks as the second most common cause of death in both Europe and America. Significant global efforts are being made to allocate resources towards the development of approaches to prevent, diagnose, and treat cancer. Each year, approximately ten million people are affected by this disease globally. Anticancer drugs, such as alkylating agents, hormones, and antimetabolites, are available in various forms. Hypomethylating medications are employed in the treatment of patients with more severe forms of myelodysplastic syndromes, chronic myelomonocytic leukemia, and acute myeloid leukemia who are not eligible for aggressive treatment methods such as induction chemotherapy. Malignant cells undergo metabolic changes in comparison to healthy cells as a result of both genetic and epigenetic modifications. Various drugs utilized in cancer therapy operate through different mechanisms. This article computes the different indices for drugs like Azacitidine, Dasatinib, Nelarabine, etc., using the $\bar{M}$ polynomial.

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1. Introduction

Chemical graph theory is a field within mathematical chemistry that focuses on the investigation of chemical graphs, which are representations of chemical systems. Its purpose is to analyze and predict various properties of chemical compounds [1]. Chemists use physical characteristics to understand the structure of molecules, and one way to analyze molecular structure is by converting it into a numerical value known as a topological index . Topological indices are important in the analysis of the physical and chemical properties of chemical compounds. There are five types of topological indices: degree,

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distance, eigenvalue, matching, and mixed. In general, a chemical compound can be depicted as a graph, with elements and bonds represented as vertices and edges. In this particular study, the cancer drugs being investigated are also considered as chemical compounds, and topological indices are utilized. Graph theory offers tools such as "QSAR, QSPR, and QSTR", which are used by chemists and pharmacists use these data for further research work [2].

Cancer is a disease characterized by abnormal cell growth, which leads to the development of tumors that can quickly spread to other parts of the body. It can be caused by genetic changes or environmental factors that affect the body's cells [3]. In 2018, there were 18 million reported cases of cancer worldwide, with 9.5 million affecting males and 8.5 million affecting females. Different types of cancer include carcinoma, sarcoma, leukemia, lymphoma, myeloma, and central nervous system cancer. Common examples of cancer include breast, lung, prostate, non-melanoma skin, stomach, and colorectal cancer [4]. Detecting cancer symptoms is crucial for treatment, although a cure is not guaranteed in advanced stages of the disease [5]. Early stages of cancer may not show noticeable symptoms, while later stages often present obvious symptoms that vary depending on the type of cancer. Once cancer is identified, prompt action is necessary, and conventional treatment is typically recommended. Symptoms of cancer include a persistent cough, changes in bowel habits, weight loss, blood in excretions, anemia, nausea, vomiting, fatigue, and pain in the back, stomach, and bones [6]. Laboratory tests such as urine and blood analysis, as well as imaging tests like CT scans, MRIs, nuclear and bone scans, PET scans, ultrasounds, X-rays, and biopsies, can be used to diagnose individuals with cancer symptoms [7].

A new approach to cancer treatment is urgently needed. The concept of using herbal medicine as an alternative to traditional commercial treatment is becoming increasingly popular due to its potential to alleviate financial burdens and health complications associated with modern treatment methods [8,9]. Herbal remedies are more cost-effective, making them more readily available to individuals residing in rural regions [10]. According to the World Health Organization, there have been numerous cases and deaths related to different types of cancer, such as lung cancer, liver cancer, breast cancer, stomach cancer, prostate cancer, skin cancer, and colorectal cancer. Blood cancer, also known as leukemia, is caused by a mutation in the DNA of blood cells, leading to abnormal behavior and potential infections. It can also become chronic and result in bone tumors. Approximately 1.24 million people are affected by blood cancer annually worldwide. Medical professionals and scientists are constantly searching for better ways to care for cancer patients. However, drug development is a challenging and expensive process. Nevertheless, new technologies and innovative medicines have been discovered in recent times to treat cancer. Drug therapy is used to inhibit the growth of cancer cells, eliminate them from the body, and restore healthy cells [11–13].

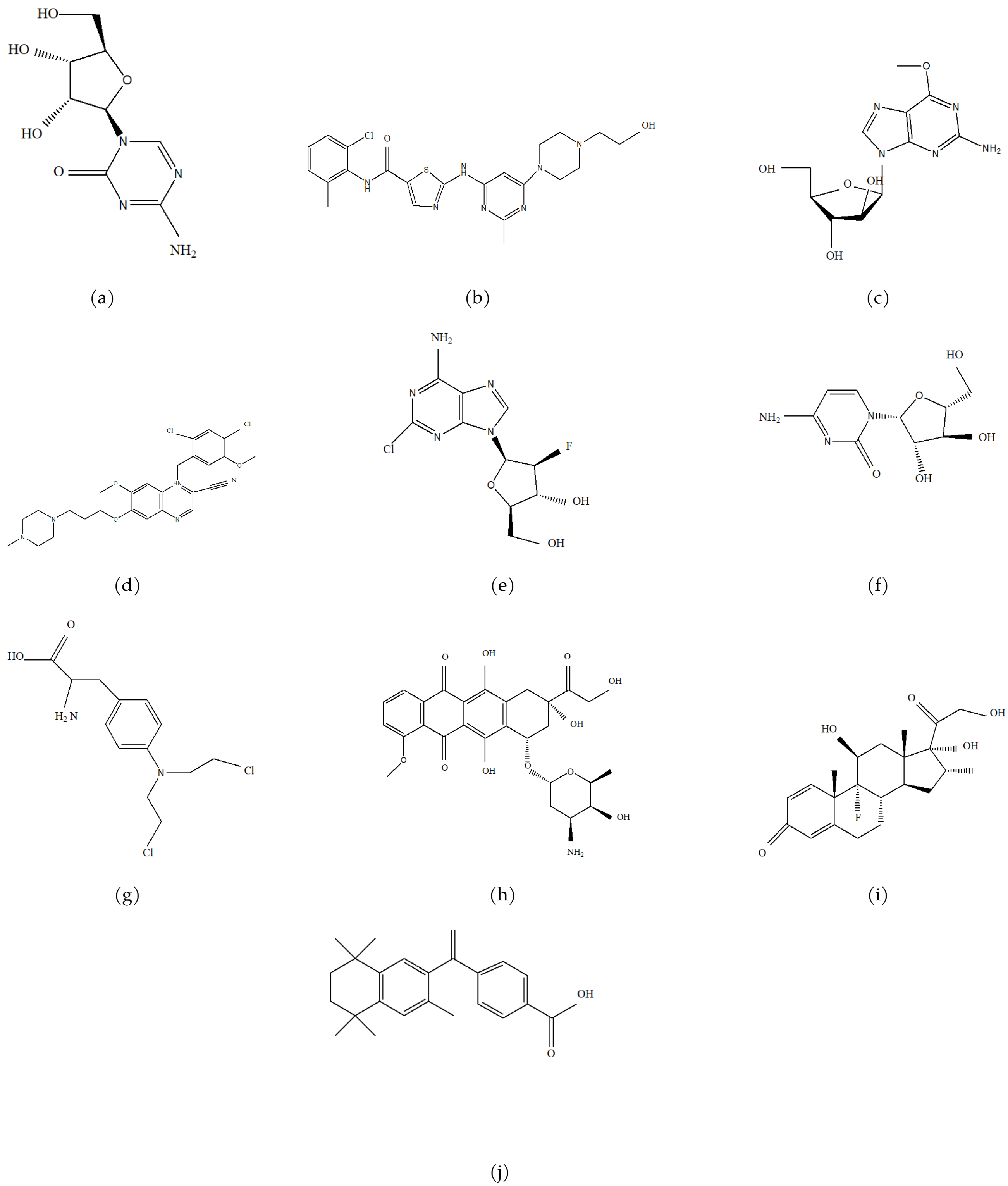

FIGURE 1. (a) Azaticidine, (b) Dasatinib (c) Nelarabine (d) Bosutinib (e) Clofarabine (f) Cytarabine (g) Melphalan (h) Doxorubicine (i) Dexamethasone (j) Bexarotene

Anticancer drugs are employed to eradicate and prevent the growth of cancer cells, and numerous drug trials are conducted to combat this deadly disease. Early detection, screening, and medication are crucial in helping patients manage and control this fatal illness in the future [14]. Cancer is a highly lethal condition characterized by the rapid proliferation of abnormal cells in the body. It was estimated that there would be 18.1 million new cases of cancer and 9.6 million cancer-related deaths in 2018 [15]. Carcinogens, such as tobacco smoke, are substances that can cause cancer and have the potential to spread to other parts of the body. Symptoms of this disease include the presence of a lump, abnormal bleeding, persistent cough, weight loss, and more. The main causes of cancer include tobacco use, obesity, poor diet, sedentary lifestyle, and excessive alcohol consumption. Various treatments, such as surgery, radiation therapy, chemotherapy, hormone therapy, and targeted therapy, can be utilized to cure this dangerous disease [16,17]. Nanotechnology has shown promising results in the diagnosis and treatment of cancer, including drug delivery, gene therapy, detection and diagnosis, drug transport, biomarker mapping, targeted therapy, and molecular mapping [18]. The M-polynomial, proposed by Deutsch and Klavzar [19], is a polynomial based on degrees that can be used to create different indices. It has been widely used in research to generate topological indices, particularly polynomials based on non-adjacent pairings of vertices in chemical compounds [20]. In 2022, Kirmani et al. introduced a new M-polynomial called the $\bar{M}(\mathscr{H})$ polynomial, and their focus on the degree-based topological indices (DBTI) [21].

The empirical formula of Azacitidine is $C_8H_{12}N_4O_5$. Azacitidine is a medication that inhibits the activity of DNA methyltransferase. It is prescribed for individuals with chronic myelomonocytic leukemia (CMML), acute myeloid leukemia (AML), and myelodysplastic syndrome. The empirical formula of Dasatinib is $C_{22}H_{26}ClNO_2$S. It functions by obstructing specific proteins in cancer cells that promote the growth of cancer. This can aid in reducing the size of the cancer or halting its progression. It is used to treat chronic myeloid leukemia (CML) and acute lymphoblastic leukemia (ALL) with Philadelphia chromosome-positive when other treatments are ineffective. The molecular formula of Nelarabine is $C_{11}H_{15}N_5O_5$. It is also known as Atriance. Nelarabine belongs to a group of drugs called antimetabolites. It is used to treat a type of leukemia called T cell acute lymphoblastic leukemia and a type of lymphoma called T cell lymphoblastic lymphoma. The molecular formula of bosutinib is $C_{26}H_{29}Cl_2N_5O_3$. It is used as a treatment for individuals with newly diagnosed chronic myeloid leukemia (CML) that has an abnormal Philadelphia chromosome. The Philadelphia chromosome is a specific chromosome that is associated with a certain type of drug known as a protein tyrosine kinase inhibitor (TKI). These inhibitors target tyrosine kinases, which are proteins that stimulate the growth of cancer cells. Clofarabine, with the empirical formula $C_{10}H_{11}ClFN_5O_5$, is a TKI used to treat acute lymphoblastic leukemia (ALL) in children and young adults aged 1 to 21 who have already undergone at least two other treatments. Its mechanism of action involves killing existing cancer cells and preventing the growth of new ones.

The molecular formula for cytarabine is $C_9H_{13}N_3O_5$. It is a chemotherapy drug used to treat acute leukemia and some lymphomas. It is also known as Ara C. Its mechanism of action involves inhibiting the production and repair of DNA in cancer cells, thus preventing their growth and multiplication. Melphalan, with an empirical formula of $C_{13}H_{18}Cl_2N_2O_2$, is another chemotherapy treatment used for various types of cancer. It may be administered prior to a stem cell or bone marrow transplant. Doxorubicin, also known as Adriamycin, is a chemotherapy drug used to treat multiple types of cancer. The way it operates is by inhibiting the activity of an enzyme known as topo isomerase 2, which is crucial for the proliferation and development of cancer cells. Its empirical formula is $C_{27}H_{29}NO_{11}$. Carboplatin, with a molecular formula of $C_6H_{12}N_2O_2Pt$, belongs to a group of chemotherapy drugs called alkylating agents. It is administered through a long plastic tube inserted into a large vein in the chest and remains in place throughout the treatment. Bexarotene, also known as Targetin, is a retinoid cancer drug used to treat advanced skin lymphomas, specifically cutaneous T cell lymphomas such as mycosis fungoides and Sezary syndrome. The molecular formula for flutamide is $C_6H_{28}O_2$. Flutamide is an antiandrogen hormone drug that inhibits the action of testosterone on cancer cells, potentially slowing down cancer growth and causing shrinkage. The molecular formula for flutamide is $C_{11}H_{11}F_3N_2O_3$. Pemigatinib, also known as Pemazyre, is a drug used to treat bile duct cancer, also known as Cholangiocarcinoma. Its molecular formula is $C_{24}H_{27}F_2N_5O_4$. Pemigatinib is a targeted cancer drug, also known as Nerlynax, used to treat early stage breast cancer that is hormone receptor positive and human epidermal growth factor receptor 2 positive (HER2 +ve). Its molecular formula is $C_{30}H_{29}ClN_6O_3$.

Deutsch and Klavzar introduced the M-Polynomial, a polynomial based on the degree of vertices, which has been used in various studies to create different topological indices[10]. Its flexibility has made it a popular choice in this field. In order to calculate additional types of graph coindices, a polynomial that considers nonadjacent pairings of vertices in chemical compounds was developed. In 2022, Kirmani et al. proposed a new version of the M-Polynomial called the $\bar{M}$ polynomial, which aims to generalize the original M-Polynomial.

2. Results

Let G be a simple, connected graph with vertex set V and edge set E. The degree of a vertex u, is the number of edges incident to u, denoted by d_u. The notation$|V_i|$ is the number of vertices in V_i and $|E(\mathscr{H})|$ is the number of edges in a graph $\mathscr{H}$ or the size of a graph. Define

$\sigma_i = |V_i|$, where $V_i = \{u \epsilon V(\mathscr{H}) | d_u = i\}$

$\omega_{ij} = |E_{ij}|$, where $E_{ij} = \{uv \epsilon V(\mathscr{H}) | d_u = i, d_v = j\}$

$\bar{\omega}_{ij} = |E_{ij}|$, where $E_{ij} = \{uv \epsilon V(\bar{\mathscr{H}}) | d_u = i, d_v = j\}$

The M-polynomial for a non-adjacent pair of vertices is denoted as $\bar{M}(\mathscr{H}, u, v)$ and is defined as the sum of $\bar{M}$ polynomial as follows

$\bar{M}(\mathscr{H}, u, v) = \sum_{i \leq j} \bar{\tau}_{ij}(\mathscr{H}) u^i v^j$

where $\bar{\tau}_{ij}$ is the number of edges $uv \notin E(\mathscr{H})$ such that $\{d(u), d(v)\} = \{ij\}$

On the edge set E(G) of a graph $\mathscr{H}$, the DBTI can be defined as

$$DBTI(\mathscr{H}) = \sum_{uv \notin E(\mathscr{H})} z(u, v)$$

The DBTI (Degree-Based Topological indices) of a graph $\mathscr{H}$, denoted as DBTI($\mathscr{H}$), is defined as the sum of $z(u, v)$ for all uv not in E($\mathscr{H}$). Certain indices can be formulated from the $\bar{M}$ polynomial, and Table 1 lists a few DBTI along with their connections to the $\bar{M}$ polynomial of graph $\mathscr{H}$.

DBTI	$Z(d_u, d_v)$	Derivation from $\bar{M}(\mathscr{H}, u, v)$
First Zagreb index [22]	$d_u + d_v$	$(\phi_u + \phi_v)\ \bar{M}(\mathscr{H})$ at $u = v = 1$
Second Zagreb index [22]	$d_u.d_v$	$(\phi_u.\phi_v)\ \bar{M}(\mathscr{H})$ at $u = v = 1$
Redefined Zagreb index [23]	$(d_u.d_v)(d_u + d_v)$	$\phi_u.\phi_v(\phi_u + \phi_v)\ \bar{M}(\mathscr{H})$ at $u = v = 1$
Second Modified Zagreb index [24]	$\frac{1}{d_u.d_v}$	$S_u S_v\ \bar{M}(\mathscr{H})$ at $u = v = 1$
Forgotten topological index [25]	$(d_u^2 + d_v^2)$	$(\phi_u^2 + \phi_v^2)\ \bar{M}(\mathscr{H})$ at $u = v = 1$
Inverse Sum index [26]	$\frac{d_u.d_v}{d_u + d_v}$	$S_u J \phi_u \phi_v\ \bar{M}(\mathscr{H})$ at $u = v = 1$
Harmonic index [27]	$\frac{2}{d_u + d_v}$	$2 S_u J\ \bar{M}(\mathscr{H})$ at $u = v = 1$

where

$$\phi_u f(u, v) = u \frac{\partial z(u, v)}{\partial u}$$
$$\phi_v f(u, v) = v \frac{\partial z(u, v)}{\partial v}$$
$$S_u Z(u, v) = \int_0^u \frac{z(t, v)}{t}\, dt$$
$$S_v Z(u, v) = \int_0^v \frac{z(u, t)}{t}\, dt$$
$$J(Z(u, v)) = Z(u, u)$$
$$Q_u Z(u, v) = u^{\alpha} Z(u, v)$$

The credit for proving the following observation goes to (36). We have the following statement for a connected graph $\mathscr{H}$ with n vertices [20].

1. If $i = j$ then $\bar{M}_{ij} = |\bar{E}_{ij}| = \frac{\sigma_i(\sigma_i - 1)}{2}$ - ω_{ii}
2. If $i \leq j$ then $\bar{M}_{ij} = |\bar{E}_{ij}| = \sigma_i \sigma_j$ - ω_{ij}

Theorem 2.1. *If we consider the molecular graph of Azacitidine as $\mathscr{H}$, then $\bar{M}$ polynomial can be expressed as* $\bar{M}(\mathscr{H}, u, v)$=$24uv^2$+$31uv^3$+$9u^2v^2$+$28u^2v^3$+$16u^3v^3$.

Proof. To determine the edge partition of the molecular graph of azacitidine , there are 17 vertices and 18 edges. We can divide the edge set of the graph into five divisions based on the degree of the vertices. Specifically, $\omega_{12} = |E_{12}| = 1, \omega_{13} = |E_{13}| = 4, \omega_{22} = |E_{22}| = 1, \omega_{23} = |E_{23}| = 7, \omega_{33} = |E_{33}| = 5.$ Additionally the partition of vertices based on their degree is $\sigma_1 = |V_1| = 5, \sigma_2 = |V_2| = 5, \sigma_3 = |V_3| = 7$ By observing these values, we can obtain the desired edge partition.

$$\overline{\omega_{12}} = \sigma_1\sigma_2 \text{ - } \omega_{12} = 5(5) - 1 = 24$$
$$\overline{\omega_{13}} = \sigma_1\sigma_3 \text{ - } \omega_{13} = 5(7) - 4 = 31$$
$$\overline{\omega_{22}} = \frac{\sigma_2(\sigma_2 - 1)}{2} \text{ - } \omega_{22} = \frac{5(4)}{2} \text{ - } 1 = 9$$
$$\overline{\omega_{23}} = \sigma_2\sigma_3 \text{ - } \omega_{23} = 5(7) - 7 = 28$$
$$\overline{\omega_{33}} = \frac{\sigma_3(\sigma_3 - 1)}{2} \text{ - } \omega_{33} = \frac{7(6)}{2} \text{ - } 5 = 16$$

By the definition of polynomial, we have

$$\begin{aligned}
\bar{M}(\mathscr{H}, u, v) &= \sum_{i \leq j} \bar{\omega}_{ij}(\mathscr{H}) u^i v^j \\
&= \sum_{1 \leq 2} \bar{\omega}_{12}(\mathscr{H}) uv^2 + \sum_{1 \leq 3} \bar{\omega}_{13}(\mathscr{H}) uv^3 + \sum_{2 \leq 2} \bar{\omega}_{22}(\mathscr{H}) u^2v^2 \\
&+ \sum_{2 \leq 3} \bar{\omega}_{23}(\mathscr{H}) u^2v^3 + \sum_{3 \leq 3} \bar{\omega}_{33}(\mathscr{H}) u^3v^3 \\
\bar{M}(\mathscr{H}, u, v) &= 24uv^2 + 31uv^3 + 9u^2v^2 + 28u^2v^3 + 16u^3v^3.
\end{aligned}$$

□

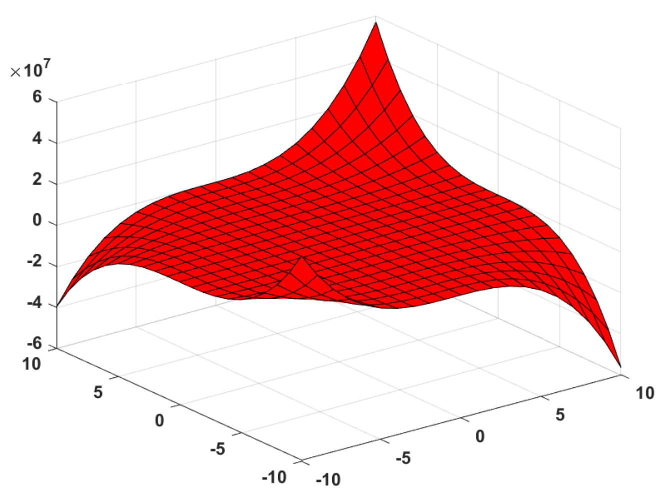

FIGURE 2. M-polynomial of Azacitidine

Theorem 2.2. *Let $\mathscr{H}$ be the molecular graph of Azacitidine, then*
(1) $\overline{M_1}(\mathscr{H}) = 468$ (2) $\overline{M_2}(\mathscr{H}) = 413$ (3) $\overline{ReZ}(\mathscr{H}) = 2364$ (4) $\overline{^{m}M_2}(G\mathscr{H}) = 39.25$ (5) $\overline{F}(\mathscr{H}) = 894$ (6)$\overline{ISI}(\mathscr{H}) = 291$ (7) $\overline{F}(G\mathscr{H}) = 157.67$

Proof. For determing the DBTI, we consider $\bar{M}(G\mathscr{H}, u, v)$= $24uv^2 + 31uv^3 + 9u^2v^2 + 28u^2v^3 + 16u^3v^3$

$\phi_u\ f(u,v) = 24uv^2 + 31uv^3 + 18u^2v^2 + 56u^2v^3 + 48u^3v^3$

$\phi_v\ f(u,v) = 48uv^2 + 93uv^3 + 18u^2v^2 + 84u^2v^3 + 48u^3v^3$

$\phi_u + \phi_v\ f(u,v)$ =$72uv^2 + 124uv^3 + 36u^2v^2 + 140u^2v^3 + 96u^3v^3$

$(\phi_u\phi_v)(\phi_u + \phi_v)\ f(u,v) = 144uv^2 + 372uv^3 + 144u^2v^2 + 840u^2v^3 + 864u^3v^3$

$(S_uS_v)\ f(u,v) = 12uv^2 + \dfrac{31}{3}uv^3 + \dfrac{9}{4}u^2v^2 + \dfrac{28}{6}u^2v^3 + \dfrac{16}{9}u^3v^3$

$(\phi_u^2 + \phi_v^2)\ f(u,v) = 120uv^2 + 310uv^3 + 72u^2v^2 + 364u^2v^3 + 288u^3v^3$

$(S_uJ\phi_u\phi_v)\ f(u,v) = 48u^3 + 93u^4 + 18u^4 + 84u^5 + 48u^6$

$(2S_uJ)\ f(u,v) = 48u^3 + 62v^4 + 9u^4 + 28u^5 + \dfrac{32}{3}u^6$

The data presented in Table 1 immediately produce the aforementioned results.

$\overline{M_1}(\mathscr{H}) = (\phi_u + \phi_v)f(u,v)|_{u=v=1} = 468$

$\overline{M_2}(\mathscr{H})$=$(\phi_u.\phi_v)f(u,v)|_{u=v=1} = 413$

$\overline{ReZ}(\mathscr{H}) = (\phi_u\phi_v)(\phi_u + \phi_v)f(u,v)|_{u=v=1} = 2364$

$\overline{^mM_2}(\mathscr{H})$= $(S_uS_v)f(u,v)|_{u=v=1} = 39.25$

$\overline{F}(\mathscr{H})$= $(\phi_u^2 + \phi_v^2)f(u,v)|_{u=v=1} = 894$

$\overline{ISI}(\mathscr{H}) = (S_uJ\phi_u\phi_v)f(u,v)|_{u=v=1} = 291$

$\overline{H}(\mathscr{H}) = (2S_uJ)f(u,v)|_{u=v=1} = 157.67$

Hence the proof. □

Theorem 2.3. *Let $\mathscr{H}$ be the molecular graph of Dasatinib . The $\overline{M}$ polynomial for $\mathscr{H}$ is* $\overline{M}(\mathscr{H}, u, v)$=$143uv^2$+$124uv^3$+$30u^2v^2$+$51u^2v^3$+$24u^3v^3$.

Proof. Consider the graph $\mathscr{H}$ of dasatinib which contains 33 vertices and 36 edges. We have five division of edge set of $\mathscr{H}$ based on the degree of vertices. Here $\omega_{12} = |E_{12}| = 1$, $\omega_{13} = |E_{13}| = 4$, $\omega_{22} = |E_{22}| = 6$, $\omega_{23} = |E_{23}| = 21$, $\omega_{33} = |E_{33}| = 4$. And the partition of vertices that depend on their degrees are given as $\sigma_1 = |V_1| = 16$, $\sigma_2 = |V_2| = 9$, $\sigma_3 = |V_3| = 8$, we obtain

$$\overline{\omega_{12}} = \sigma_1\sigma_2 \text{ - } \omega_{12} = 16(9) - 1 = 143$$
$$\overline{\omega_{13}} = \sigma_1\sigma_3 \text{ - } \omega_{13} = 16(8) - 4 = 124$$
$$\overline{\omega_{22}} = \frac{\sigma_2(\sigma_2 - 1)}{2} \text{ - } \omega_{22} = \frac{9(8)}{2} \text{ - } 6 = 30$$
$$\overline{\omega_{23}} = \sigma_2\sigma_3 \text{ - } \omega_{23} = 9(8) - 21 = 51$$
$$\overline{\omega_{33}} = \frac{\sigma_3(\sigma_3 - 1)}{2} \text{ - } \omega_{33} = \frac{8(7)}{2} \text{ - } 4 = 24$$

we have

$$\begin{aligned}
\overline{M}(\mathscr{H},u,v) &= \sum_{i\leq j}\bar{\omega}_{ij}(\mathscr{H})u^i v^j \\
&= \sum_{1\leq 2}\bar{\omega}_{12}(\mathscr{H})uv^2 + \sum_{1\leq 3}\bar{\omega}_{13}(\mathscr{H})uv^3 + \sum_{2\leq 2}\bar{\omega}_{22}(\mathscr{H})u^2v^2 \\
&+ \sum_{2\leq 3}\bar{\omega}_{23}(\mathscr{H})u^2v^3 + \sum_{3\leq 3}\bar{\omega}_{33}(\mathscr{H})u^3v^3 \\
\overline{M}(\mathscr{H},u,v) &= 143uv^2 + 124uv^3 + 30u^2v^2 + 51u^2v^3 + 24u^3v^3.
\end{aligned}$$

□

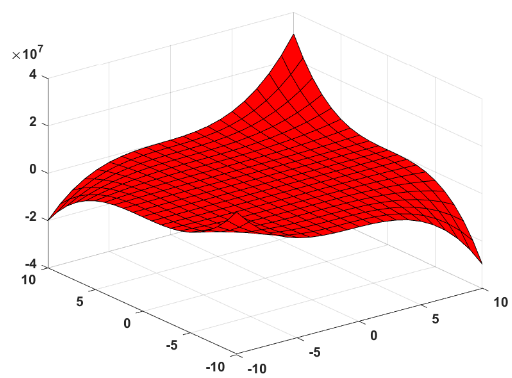

FIGURE 3. M-polynomial of Dasatinib

Theorem 2.4. *Let $\mathscr{H}$ be the molecular graph of dasatinib, then*
(1) $\overline{M_1}(\mathscr{H}) = 1444$ (2) $\overline{M_2}(\mathscr{H}) = 1300$ (3) $\overline{ReZ}(\mathscr{H}) = 5652$ (4) $\overline{^mM_2}(\mathscr{H}) = 128.67$ (5) $\overline{F}(\mathscr{H}) = 3290$
(6)$\overline{ISI}(\mathscr{H}) = 943$ (7) $\overline{H}(\mathscr{H}) = 631$

Proof. For determing the DBTI, we consider $\bar{M}(\mathscr{H},u,v)$= $143uv^2 + 124uv^3 + 30u^2v^2 + 51u^2v^3 + 24u^3v^3$.
$\phi_u\ f(u,v) = 143uv^2 + 124uv^3 + 60u^2v^2 + 102u^2v^3 + 72u^3v^3$
$\phi_v\ f(u,v) = 286uv^2 + 372uv^3 + 60u^2v^2 + 153u^2v^3 + 72u^3v^3$
$\phi_u + \phi_v\ f(u,v)$ =$429uv^2 + 496uv^3 + 120u^2v^2 + 255u^2v^3 + 144u^3v^3$
$(\phi_u\phi_v)(\phi_u + \phi_v)\ f(u,v) = 858uv^2 + 1488uv^3 + 480u^2v^2 + 1530u^2v^3 + 1296u^3v^3$
$(S_uS_v)\ f(u,v) = \dfrac{143}{2}uv^2 + \dfrac{124}{3}uv^3 + \dfrac{15}{2}u^2v^2 + \dfrac{17}{3}u^2v^3 + \dfrac{8}{3}u^3v^3$
$(\phi_u^2 + \phi_v^2)\ f(u,v) = 715uv^2 + 1240uv^3 + 360u^2v^2 + 663u^2v^3 + 432u^3v^3$
$(S_uJ\phi_u\phi_v)\ f(u,v) = 858u^3 + 1488u^4 + 240u^4 + 765u^5 + 432u^6$
$(2S_uJ)\ f(u,v) = 286u^3 + 248u^4 + 30u^4 + 51u^5 + 16u^6$

Now these data in Table.1 immediately yied the aforementioned.
$\overline{M_1}(\mathscr{H})$= $(\phi_u + \phi_v)f(u,v)|_{u=v=1} = 1444$

$\overline{M_2}(\mathscr{H})$ =$(\phi_u.\phi_v)f(u,v)|_{u=v=1}$ = 1300

$\overline{ReZ}(\mathscr{H})$ = $(\phi_u\phi_v)(\phi_u+\phi_v)f(u,v)|_{u=v=1}$ = 5652

$^{m}\overline{M_2}(\mathscr{H})$= $(S_uS_v)f(u,v)|_{u=v=1}$ = 128.67

$\overline{F}(\mathscr{H})$ = $(\phi_u^2+\phi_v^2)f(u,v)|_{u=v=1}$ = 3290

$\overline{ISI}(\mathscr{H})$ = $(S_uJ\phi_u\phi_v)f(u,v)|_{u=v=1}$ = 943

$\overline{H}(\mathscr{H})$ = $(2S_uJ)f(u,v)|_{u=v=1}$ = 631

Hence the proof. □

Theorem 2.5. *Let $\mathscr{H}$ be the molecular graph of Nelarabine . The $\bar{M}$ polynomial for $\mathscr{H}$ is* $\overline{M}(\mathscr{H},u,v)$=$22uv^2$+$69uv^3$+$15u^2v^3$+$30u^3v^3$.

Proof. Consider the graph $\mathscr{H}$ of nelarabine which contains 21 vertices and 23 edges. We categorize the edge set of G into five divisions based on the vertex degrees. Here ω_{12} = $|E_{12}|$ = 2, ω_{13} = $|E_{13}|$ = 3, ω_{23} = $|E_{23}|$ = 12, ω_{33} = $|E_{33}|$ = 6. And the partition of vertices that depend on their degrees are given as σ_1 = $|V_1|$ = 8, σ_2 = $|V_2|$ = 9, σ_3 = $|V_3|$ = 3, we obtain

$$\overline{\omega_{12}} = \sigma_1\sigma_2 \text{ - } \omega_{12} = 8(3)-2 = 22$$
$$\overline{\omega_{13}} = \sigma_1\sigma_3 \text{ - } \omega_{13} = 8(9)-3 = 69$$
$$\overline{\omega_{23}} = \sigma_2\sigma_3 \text{ - } \omega_{23} = 3(9)-12 = 15$$
$$\overline{\omega_{33}} = \frac{\sigma_3(\sigma_3-1)}{2} \text{ - } \omega_{33} = \frac{9(8)}{2} \text{ - } 6 = 30$$

By the definition of polynomial, we have

$$\begin{aligned}\overline{M}(\mathscr{H},u,v) &= \sum_{i\leq j}\bar{\omega}_{ij}(\mathscr{H})u^iv^j\\ &= \sum_{1\leq 2}\bar{\omega}_{12}(\mathscr{H})uv^2+\sum_{1\leq 3}\bar{\omega}_{13}(\mathscr{H})uv^3+\sum_{2\leq 3}\bar{\omega}_{23}(\mathscr{H})u^2v^3+\sum_{3\leq 3}\bar{\omega}_{33}(\mathscr{H})u^3v^3\\ \overline{M}(\mathscr{H},u,v) &= 22uv^2+69uv^3+15u^2v^3+30u^3v^3.\end{aligned}$$

□

Theorem 2.6. *Let $\mathscr{H}$ be the molecular graph of Nelarabine, then*
(1) $\overline{M_1}(\mathscr{H})$ = 597 (2) $\overline{M_2}(\mathscr{H})$ = 611 (3) $\overline{ReZ}(G\mathscr{H})$ = 3030 (4) $^{m}\overline{M_2}(\mathscr{H})$ = 39.84 (5) $\overline{F}(G\mathscr{H})$ = 1535 (6)$\overline{ISI}(\mathscr{H})$ = 386 (7) $\overline{H}(\mathscr{H})$ = 217

Proof. For determing the DBTI, we consider
$\bar{M}(\mathscr{H},u,v)$=$22uv^2$+$69uv^3$+$15u^2v^3$+$30u^3v^3$. $\phi_u\ f(u,v) = 22uv^2+69uv^3+30u^2v^3+90u^3v^3$

$\phi_v\ f(u,v) = 44uv^2+207uv^3+45u^2v^3+90u^3v^3$

$(\phi_u+\phi_v)\ f(u,v)$ =$66uv^2+276uv^3+75u^2v^3+180u^3v^3$

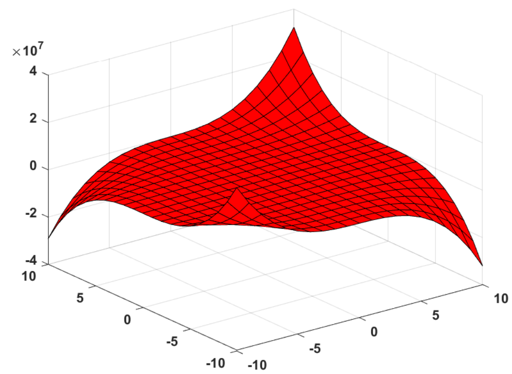

FIGURE 4. M-polynomial of Nelarabine

$(\phi_u.\phi_v)\ f(u,v) = 44uv^2 + 207uv^3 + 90u^2v^3 + 270u^3v^3$

$(\phi_u\phi_v)(\phi_u + \phi_v)\ f(u,v) = 132uv^2 + 828uv^3 + 450u^2u^3 + 1620u^3v^3$

$(S_uS_v)\ f(u,v) = 11uv^2 + 23uv^3 + \dfrac{15}{6}u^2v^3 + \dfrac{10}{3}u^3v^3$

$(\phi_u^2 + \phi_v^2)\ f(u,v) = 110uv^2 + 690uv^3 + 600u^2v^3 + 2700u^3v^3$

$(S_uJ\phi_u\phi_v)\ f(u,v) = 44u^3 + 207u^4 + 45u^5 + 90u^6$

$(2S_uJ)\ f(u,v) = 44u^3 + 138v^4 + 15u^5 + 20v^6$

Now these data in Table.1 immediately yied the aforementioned.

$\overline{M_1}(\mathscr{H}) = (\phi_u + \phi_v)f(u,v)|_{u=v=1} = 597$

$\overline{M_2}(\mathscr{H}) = (\phi_u.\phi_v)f(u,v)|_{u=v=1} = 611$

$\overline{ReZ}(\mathscr{H}) = (\phi_u\phi_v)(\phi_u + \phi_v)f(u,v)|_{u=v=1} = 3030$

$\overline{{}^mM_2}(\mathscr{H}) = (S_uS_v)f(u,v)|_{u=v=1} = 39.84$

$\overline{F}(\mathscr{H}) = (\phi_u^2 + \phi_v^2)f(u,v)|_{u=v=1} = 1535$

$\overline{ISI}(\mathscr{H}) = (S_uJ\phi_u\phi_v)f(u,v)|_{u=v=1} = 386$

$\overline{H}(\mathscr{H}) = (2S_uJ)f(u,v)|_{u=v=1} = 217$

Hence the proof. □

Theorem 2.7. *Let $\mathscr{H}$ be the molecular graph of Bosutinib . The $\bar{M}$ polynomial for $\mathscr{H}$ is*
$\bar{M}(\mathscr{H}, u, v)$=$154uv^2$+$126uv^3$+$60u^2v^2$+$101u^2v^3$+$39u^3v^3$.

Proof. Consider the graph $\mathscr{H}$ of bosutinib which contains 35 vertices and 37 edges. The edge sets are given $\omega_{12} = |E_{12}| = 2$, $\omega_{13} = |E_{13}| = 4$, $\omega_{22} = |E_{22}| = 6$, $\omega_{23} = |E_{23}| = 19$, $\omega_{33} = |E_{33}| = 6$. And the partition of vertices that depend on their degrees are given as $\sigma_1 = |V_1| = 13$, $\sigma_2 = |V_2| = 12$, $\sigma_3 = |V_3| = 10$, we get

$$\overline{\omega_{12}} = \sigma_1\sigma_2 \text{ - } \omega_{12} = 12(13) - 2 = 154$$

$$\overline{\omega_{13}} = \sigma_1\sigma_3 \text{ - } \omega_{13} = 13(10) - 4 = 126$$

$$\overline{\omega_{22}} = \frac{\sigma_2(\sigma_2-1)}{2} \text{ - } \omega_{22} = \frac{12(11)}{2} \text{ - } 6 = 60$$
$$\overline{\omega_{23}} = \sigma_2\sigma_3 \text{ - } \omega_{23} = 12(10) - 19 = 101$$
$$\overline{\omega_{33}} = \frac{\sigma_3(\sigma_3-1)}{2} \text{ - } \omega_{33} = \frac{10(9)}{2} \text{ - } 6 = 39$$

By the definition of polynomial, we have

$$\begin{aligned}\overline{M}(\mathscr{H},u,v) &= \sum_{i\leq j}\bar{\omega}_{ij}(\mathscr{H})u^iv^j\\ &= \sum_{1\leq 2}\bar{\omega}_{12}(\mathscr{H})uv^2 + \sum_{1\leq 3}\bar{\omega}_{13}(\mathscr{H})uv^3 + \sum_{2\leq 2}\bar{\omega}_{22}(\mathscr{H})u^2v^2\\ &+ \sum_{2\leq 3}\bar{\omega}_{23}(\mathscr{H})u^2v^3 + \sum_{3\leq 3}\bar{\omega}_{33}(\mathscr{H})u^3v^3\\ \overline{M}(\mathscr{H},u,v) &= 154uv^2 + 126uv^3 + 60u^2v^2 + 101u^2v^3 + 39u^3v^3.\end{aligned}$$

□

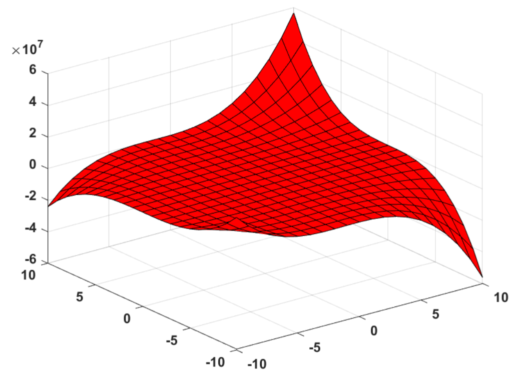

Figure 5. M-Polynomial of Boustinib

Theorem 2.8. *Let $\mathscr{H}$ be the molecular graph of bosutinib, then*

(1) $\overline{M_1}(\mathscr{H}) = 1945$ (2) $\overline{M_2}(\mathscr{H}) = 1883$ (3) $\overline{ReZ}(\mathscr{H}) = 8532$ (4) $\overline{{}^mM_2}(\mathscr{H}) = 155.17$ (5) $\overline{F}(\mathscr{H}) = 4525$ (6)$\overline{ISI}(\mathscr{H}) = 1226$ (7) $\overline{H}(\mathscr{H}) = 747$

Proof. For determing the DBTI, we consider

$\bar{M}(\mathscr{H},u,v)$=$154uv^2$+$126uv^3$+$60u^2v^2$+$101u^2v^3$+$39u^3v^3$.

$\phi_u\ f(u,v) = 154uv^2 + 126uv^3 + 120u^2v^2 + 202u^2v^3 + 117u^3v^3$

$\phi_v\ f(u,v) = 308uv^2 + 378uv^3 + 120u^2v^2 + 1818u^2v^3 + 117u^3v^3$

$\phi_u + \phi_v\ f(u,v)$ =$462uv^2 + 504uv^3 + 240u^2v^2 + 2020u^2v^3 + 234u^3v^3$

$\phi_u.\phi_v\ f(u,v)$ =$308uv^2 + 378uv^3 + 480u^2v^2 + 1212u^2v^3 + 1053u^3v^3$

$(\phi_u\phi_v)(\phi_u+\phi_v)\ f(u,v) = 924uv^2 + 1512uv^3 + 960u^2v^2 + 12120u^2v^3 + 2106u^3v^3$

$(S_uS_v)\ f(u,v) = 77uv^2 + 42uv^3 + 15u^2v^2 + \dfrac{101}{6}u^2v^3 + \dfrac{13}{3}u^3v^3$

$(\phi_u^2 + \phi_v^2)\ f(u,v) = 616uv^2 + 1134uv^3 + 240u^2v^2 + 909u^2v^3 + 351u^3v^3$

$(S_uJ\phi_u\phi_v)\ f(u,v) = 308u^3 + 378u^4 + 240u^4 + 606u^5 + 351u^6$

$(2S_uJ)\ f(u,v) = 286u^3 + 248u^4 + 30u^4 + 51u^5 + 16u^6$

Now these data in Table.1 immediately yied the aforementioned.

$\overline{M_1}(\mathscr{H}) = (\phi_u + \phi_v)f(u,v)|_{u=v=1} = 1945$

$\overline{M_2}(\mathscr{H}) = (\phi_u.\phi_v)f(u,v)|_{u=v=1} = 1883$

$\overline{ReZ}(\mathscr{H}) = (\phi_u\phi_v)(\phi_u + \phi_v)f(u,v)|_{u=v=1} = 8532$

${}^m\overline{M_2}(\mathscr{H}) = (S_uS_v)f(u,v)|_{u=v=1} = 155.17$

$\overline{F}(\mathscr{H}) = (\phi_u^2 + \phi_v^2)f(u,v)|_{u=v=1} = 4525$

$\overline{ISI}(\mathscr{H}) = (S_uJ\phi_u\phi_v)f(u,v)|_{u=v=1} = 1226$

$\overline{H}(\mathscr{H}) = (2S_uJ)f(u,v)|_{u=v=1} = 747$

Hence the proof. □

Theorem 2.9. *Let $\mathscr{H}$ be the molecular graph of Clofarabine . The $\bar{M}$ polynomial for $\mathscr{H}$ is* $\bar{M}(,\mathscr{H}u,v)$=$13uv^2$+$18uv^3$+$20u^2v^2$+$68u^2v^3$+$48u^3v^3$.

Proof. Consider the graph $\mathscr{H}$ of clofarabine which contains 20 vertices and 22 edges. The edge set of $\mathscr{H}$ based on the degree of vertices. Here $\omega_{12} = |E_{12}| = 1$, $\omega_{13} = |E_{13}| = 4$, $\omega_{22} = |E_{22}| = 1$, $\omega_{23} = |E_{23}| = 9$, $\omega_{33} = |E_{33}| = 7$. And the partition of vertices that depend on their degrees are given as $\sigma_1 = |V_1| = 2$, $\sigma_2 = |V_2| = 7$, $\sigma_3 = |V_3| = 11$, we attain

$$\overline{\omega_{12}} = \sigma_1\rho_2 \text{ - } \omega_{12} = 2(7) - 1 = 13$$
$$\overline{\omega_{13}} = \sigma_1\rho_3 \text{ - } \omega_{13} = 2(11) - 4 = 18$$
$$\overline{\omega_{22}} = \frac{\sigma_2(\sigma_2 - 1)}{2} \text{ - } \omega_{22} = \frac{7(6)}{2} \text{ - } 1 = 20$$
$$\overline{\omega_{23}} = \sigma_2\sigma_3 \text{ - } \omega_{23} = 7(11) - 9 = 68$$
$$\overline{\omega_{33}} = \frac{\sigma_3(\sigma_3 - 1)}{2} \text{ - } \omega_{33} = \frac{11(10)}{2} \text{ - } 7 = 48$$

By the definition of polynomial, we have

$$\begin{aligned}\overline{M}(\mathscr{H},u,v) &= \sum_{i\leq j}\bar{\omega}_{ij}(\mathscr{H})u^iv^j \\ &= \sum_{1\leq 2}\bar{\omega}_{12}(\mathscr{H})uv^2 + \sum_{1\leq 3}\bar{\omega}_{13}(\mathscr{H})uv^3 + \sum_{2\leq 2}\bar{\omega}_{22}(\mathscr{H})u^2v^2 \\ &+ \sum_{2\leq 3}\bar{\omega}_{23}(\mathscr{H})u^2v^3 + \sum_{3\leq 3}\bar{\omega}_{33}(\mathscr{H})u^3v^3 \\ \overline{M}(\mathscr{H},u,v) &= 13uv^2 + 18uv^3 + 20u^2v^2 + 68u^2v^3 + 48u^3v^3.\end{aligned}$$

□

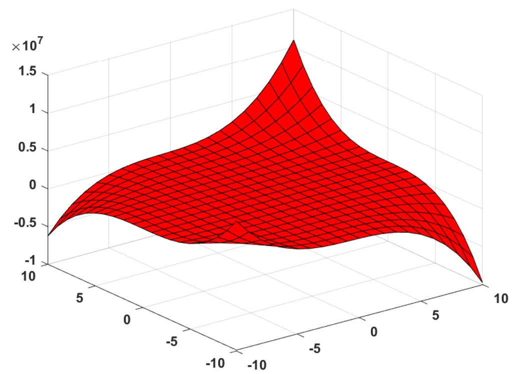

FIGURE 6. M-Polynomial of Clofarabine

Theorem 2.10. *Let $\mathscr{H}$ be the molecular graph of clofarabine, then*
(1) $\overline{M_1}(\mathscr{H}) = 819$ (2) $\overline{M_2}(\mathscr{H}) = 1000$ (3) $\overline{ReZ}(\mathscr{H}) = 5246$ (4) $\overline{^mM_2}(\mathscr{H}) = 34.17$ (5) $\overline{F}(\mathscr{H}) = 2153$ (6)$\overline{ISI}(\mathscr{H}) = 468$ (7) $\overline{H}(\mathscr{H}) = 182$

Proof. For determing the DBTI, we consider
$\bar{M}(,\mathscr{H}u,v)$=$13uv^2$+$18uv^3$+$20u^2v^2$+$68u^2v^3$+$48u^3v^3$. $\phi_u\ f(u,v) = 13uv^2 + 18uv^3 + 40u^2v^2 + 136u^2v^3 + 144u^3v^3$

$\phi_v\ f(u,v) = 26uv^2 + 54uv^3 + 40u^2v^2 + 204u^2v^3 + 144u^3v^3$

$\phi_u + \phi_v\ f(u,v) =$$39uv^2 + 72uv^3 + 80u^2v^2 + 340u^2v^3 + 288u^3v^3$

$\phi_u.\phi_v\ f(u,v) =$$26uv^2 + 54uv^3 + 80u^2v^2 + 408u^2v^3 + 432u^3v^3$

$(\phi_u\phi_v)(\phi_u + \phi_v)\ f(u,v) = 78uv^2 + 216uv^3 + 320u^2v^2 + 2040u^2v^3 + 2592u^3v^3$

$(S_uS_v)\ f(u,v) = \frac{13}{2}uv^2 + 6uv^3 + 5u^2v^2 + \frac{34}{3}u^2v^3 + \frac{16}{3}u^3v^3$

$(\phi_u^2 + \phi_v^2)\ f(u,v) = 117uv^2 + 504uv^3 + 240u^2v^2 + 544u^2v^3 + 864u^3v^3$

$(S_{uu}J\phi_x\phi_v)\ f(u,v) = 26u^3 + 54u^4 + 40u^4 + 204u^5 + 144u^6$

$(2S_uJ)\ f(u,v) = 26u^3 + 36u^4 + 20u^4 + 128u^5 + 32u^6$

Now these data in Table.1 immediately yied the aforementioned.

$\overline{M_1}(\mathscr{H}) = (\phi_u + \phi_v)f(u,v)|_{u=v=1} = 819$

$\overline{M_2}(\mathscr{H}) =$$(\phi_u.\phi_v)f(u,v)|_{u=v=1} = 1000$

$\overline{ReZ}(\mathscr{H}) = (\phi_u\phi_v)(\phi_u + \phi_v)f(u,v)|_{u=v=1} = 5246$

$\overline{^mM_2}(\mathscr{H}) = (S_uS_v)f(u,v)|_{u=v=1} = 34.17$

$\overline{F}(\mathscr{H}) = (\phi_u^2 + \phi_v^2)f(u,v)|_{u=v=1} = 2153$

$\overline{ISI}(\mathscr{H}) = (S_uJ\phi_u\phi_v)f(u,v)|_{u=v=1} = 468$

$\overline{H}(\mathscr{H}) = (2S_uJ)f(u,v)|_{u=v=1} = 182$

Hence the proof. □

Theorem 2.11. *Let $\mathscr{H}$ be the molecular graph of Cytarabine . The $\bar{M}$ polynomial for $\mathscr{H}$ is* $\bar{M}(\mathscr{H},u,v)$=$13uv^2$+$12uv^3$+$20u^2v^2$+$49u^2v^3$+$23u^3v^3$.

Proof. Consider the graph $\mathscr{H}$ of cyfarabine which contains 17 vertices and 18 edges. We have the partition of edge sets of $\mathscr{H}$ based on the degree of vertices. Here $\omega_{12} = |E_{12}| = 1$, $\omega_{13} = |E_{13}| = 4$, $\omega_{22} = |E_{22}| = 1$, $\omega_{23} = |E_{23}| = 7$, $\omega_{33} = |E_{33}| = 5$. And the partition of vertices that depend on their degrees are given as $\sigma_1 = |V_1| = 2$, $\sigma_2 = |V_2| = 7$, $\sigma_3 = |V_3| = 8$, we obtain

$$\overline{\omega_{12}} = \sigma_1\sigma_2 \text{ - } \omega_{12} = 2(7) - 1 = 13$$
$$\overline{\omega_{13}} = \sigma_1\sigma_3 \text{ - } \omega_{13} = 2(8) - 4 = 12$$
$$\overline{\omega_{22}} = \frac{\sigma_2(\sigma_2-1)}{2} \text{ - } \omega_{22} = \frac{7(6)}{2} \text{ - } 1 = 20$$
$$\overline{\omega_{23}} = \sigma_2\sigma_3 \text{ - } \omega_{23} = 7(8) - 7 = 49$$
$$\overline{\omega_{33}} = \frac{\sigma_3(\sigma_3-1)}{2} \text{ - } \omega_{33} = \frac{8(7)}{2} \text{ - } 5 = 23$$

Bythe definition of polynomial, we have

$$\begin{aligned}\overline{M}(\mathscr{H},u,v) &= \sum_{i\leq j}\bar{\omega}_{ij}(\mathscr{H})u^iv^j \\ &= \sum_{1\leq 2}\bar{\omega}_{12}(\mathscr{H})uv^2 + \sum_{1\leq 3}\bar{\omega}_{13}(\mathscr{H})uv^3 + \sum_{2\leq 2}\bar{\omega}_{22}(\mathscr{H})u^2v^2 \\ &+ \sum_{2\leq 3}\bar{\omega}_{23}(\mathscr{H})u^2v^3 + \sum_{3\leq 3}\bar{\omega}_{33}(\mathscr{H})u^3v^3 \\ \overline{M}(\mathscr{H},u,v) &= 13uv^2 + 12uv^3 + 20u^2v^2 + 49u^2v^3 + 23u^3v^3.\end{aligned}$$

□

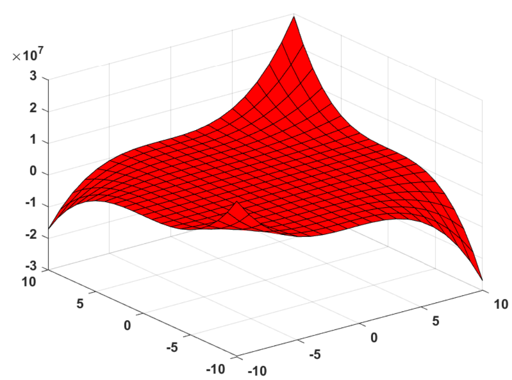

FIGURE 7. M-Polynomial of Cytarabine

Theorem 2.12. *Let $\mathscr{H}$ be the molecular graph of cytarabine, then*
(1) $\overline{M_1}(\mathscr{H}) = 550$ (2) $\overline{M_2}(\mathscr{H}) = 643$ (3) $\overline{ReZ}(\mathscr{H}) = 3254$ (4) $\overline{{}^mM_2}(\mathscr{H}) = 26.3$ (5) $\overline{F}(\mathscr{H}) = 1396$ (6)$\overline{ISI}(\mathscr{H}) = 318$ (7) $\overline{H}(\mathscr{H}) = 134.4$

Proof. For determing the DBTI, we consider

$\bar{M}(\mathscr{H},u,v)$= $13uv^2$+$12uv^3$+$20u^2v^2$+$49u^2v^3$+$23u^3v^3$.

$\phi_u\ f(u,v) = 13uv^2 + 12uv^3 + 40u^2v^2 + 98u^2v^3 + 69u^3v^3$

$\phi_v\ f(u,v) = 26uv^2 + 36uv^3 + 40u^2v^2 + 147u^2v^3 + 69u^3v^3$

$\phi_u + \phi_v\ f(u,v)$ =$39uv^2 + 48uv^3 + 80u^2v^2 + 245u^2v^3 + 138u^3v^3$

$\phi_u.\phi_v\ f(u,v)$ =$26uv^2 + 36uv^3 + 80u^2v^2 + 294u^2v^3 + 207u^3v^3$

$(\phi_u\phi_v)(\phi_u + \phi_v)\ f(u,v) = 78uv^2 + 144uv^3 + 320u^2v^2 + 1470u^2v^3 + 1242u^3v^3$

$(S_uS_v)\ f(u,v) = \frac{13}{2}uv^2 + 4uv^3 + 5u^2v^2 + \frac{49}{6}u^2v^3 + \frac{23}{9}u^3v^3$

$(\phi_u^2 + \phi_v^2)\ f(u,v) = 65uv^2 + 120uv^3 + 160u^2v^2 + 637u^2v^3 + 414u^3v^3$

$(S_uJ\phi_u\phi_v)\ f(u,v) = 26u^3 + 36u^4 + 40u^4 + 147u^5 + 69u^6$

$(2S_uJ)\ f(u,v) = 26u^3 + 24u^4 + 20u^4 + 49u^5 + \frac{46}{3}u^6$

Using Table.1, we get the results $\overline{M_1}(\mathscr{H}) = (\phi_u + \phi_v)f(u,v)|_{u=v=1} = 550$

$\overline{M_2}(\mathscr{H})$ =$(\phi_u.\phi_v)f(u,v)|_{u=v=1} = 643$

$\overline{ReZ}(\mathscr{H}) = (\phi_u\phi_v)(\phi_u + \phi_v)f(u,v)|_{u=v=1} = 3254$

$\overline{^mM_2}(\mathscr{H}) = (S_uS_v)f(u,v)|_{u=v=1} = 26.3$

$\overline{F}(\mathscr{H}) = (\phi_u^2 + \phi_v^2)f(u,v)|_{u=v=1} = 1396$

$\overline{ISI}(\mathscr{H}) = (S_uJ\phi_u\phi_v)f(u,v)|_{u=v=1} = 318$

$\overline{H}(\mathscr{H}) = (2S_uJ)f(u,v)|_{u=v=1} = 134.4$

Hence the proof. □

Theorem 2.13. *Let $\mathscr{H}$ be the graph of Melphalan . The $\bar{M}$ polynomial for $\mathscr{H}$ is*
$\bar{M}(\mathscr{H},u,v)$=$10uv^2$+$40uv^3$+$11u^2v^2$+$34u^2v^3$+$19u^3v^3$.

Proof. Consider the graph $\mathscr{H}$ of melphalan which contains 19 vertices and 19 edges. We have the edge set of $\mathscr{H}$ based on the degree of vertices. Here $\omega_{12} = |E_{12}| = 2$, $\omega_{13} = |E_{13}| = 3$, $\omega_{22} = |E_{22}| = 4$, $\omega_{23} = |E_{23}| = 8$, $\omega_{33} = |E_{33}| = 2$. The vertices are divided based on their degrees.as $\sigma_1 = |V_1| = 6$, $\sigma_2 = |V_2| = 6$, $\sigma_3 = |V_3| = 7$, we get

$$\overline{\omega_{12}} = \sigma_1\sigma_2 - \omega_{12} = 6(6) - 2 = 10$$
$$\overline{\omega_{13}} = \sigma_1\sigma_3 - \omega_{13} = 6(7) - 2 = 40$$
$$\overline{\omega_{22}} = \frac{\sigma_2(\sigma_2-1)}{2} - \omega_{22} = \frac{6(5)}{2} - 4 = 11$$
$$\overline{\omega_{23}} = \sigma_2\sigma_3 - \omega_{23} = 6(7) - 8 = 38$$
$$\overline{\omega_{33}} = \frac{\sigma_3(\sigma_3-1)}{2} - \omega_{33} = \frac{7(6)}{2} - 2 = 19$$

By the definition of polynomial, we have

$$\begin{aligned}\overline{M}(\mathscr{H},u,v) &= \sum_{i\leq j}\bar{\omega}_{ij}(\mathscr{H})u^i v^j \\ &= \sum_{1\leq 2}\bar{\omega}_{12}(\mathscr{H})uv^2 + \sum_{1\leq 3}\bar{\omega}_{13}(\mathscr{H})uv^3 + \sum_{2\leq 2}\bar{\omega}_{22}(\mathscr{H})u^2v^2 \\ &+ \sum_{2\leq 3}\bar{\omega}_{23}(\mathscr{H})u^2v^3 + \sum_{3\leq 3}\bar{\omega}_{33}(\mathscr{H})u^3v^3 \\ \overline{M}(\mathscr{H},u,v) &= 10uv^2 + 40uv^3 + 11u^2v^2 + 34u^2v^3 + 19u^3v^3.\end{aligned}$$

□

Hence the proof

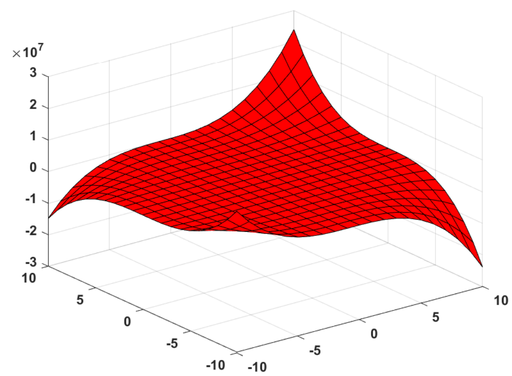

FIGURE 8. M-Polynomial of Melphalan

Theorem 2.14. *Let $\mathscr{H}$ be the molecular graph of melphalan, then*

(1) $\overline{M_1}(\mathscr{H}) = 518$ (2) $\overline{M_2}(\mathscr{H}) = 559$ (3) $\overline{ReZ}(\mathscr{H}) = 2762$ (4) $\overline{^mM_2}(\mathscr{H}) = 28.86$ (5) $\overline{F}(\mathscr{H}) = 1322$ (6)$\overline{ISI}(\mathscr{H}) = 321$ (7) $\overline{H}(\mathscr{H}) = 157.67$

Proof. For determing the DBTI, we consider

$\bar{M}(\mathscr{H},u,v)= 10uv^2+40uv^3+11u^2v^2+34u^2v^3+19u^3v^3.$

$\phi_u\ f(u,v) = 10uv^2 + 40uv^3 + 22u^2v^2 + 68u^2v^3 + 57u^3v^3$

$\phi_v\ f(u,v) = 20uv^2 + 120uv^3 + 22u^2v^2 + 102u^2v^3 + 57u^3v^3$

$\phi_u + \phi_v\ f(u,v) =30uv^2 + 160uv^3 + 44u^2v^2 + 170u^2v^3 + 114u^3v^3$

$\phi_u.\phi_v\ f(u,v) =20uv^2 + 120uv^3 + 44u^2v^2 + 204u^2v^3 + 171u^3v^3$

$(\phi_u\phi_v)(\phi_u + \phi_v)\ f(u,v) = 60uv^2 + 480uv^3 + 176u^2v^2 + 1020u^2v^3 + 1026u^3v^3$

$(S_uS_v)\ f(u,v) = 5uv^2 + \frac{40}{3}uv^3 + \frac{11}{4}u^2v^2 + \frac{34}{6}u^2v^3 + \frac{19}{9}u^3v^3$

$(\phi_u^2 + \phi_v^2)\ f(u,v) = 50uv^2 + 400uv^3 + 88u^2v^2 + 442u^2v^3 + 342u^3v^3$

$(S_uJ\phi_u\phi_y)\ f(u,v) = 20u^3 + 120u^4 + 22u^4 + 102u^5 + 95u^6$

$(2S_uJ)\ f(u,v) = 20u^3 + 80u^4 + 11u^4 + 34u^5 + \frac{38}{3}u^6$

Using Table.1, we get the results $\overline{M_1}(\mathscr{H}) = (\phi_u + \phi_v)f(u,v)|_{u=v=1} = 518$
$\overline{M_2}(\mathscr{H}) = (\phi_u.\phi_v)f(u,v)|_{u=v=1} = 559$
$\overline{ReZ}(\mathscr{H}) = (\phi_u\phi_v)(\phi_u + \phi_v)f(u,v)|_{u=v=1} = 2762$
$\overline{^mM_2}(\mathscr{H}) = (S_uS_v)f(u,v)|_{u=v=1} = 28.86$
$\overline{F}(\mathscr{H}) = (\phi_u^2 + \phi_v^2)f(u,v)|_{u=v=1} = 1322$
$\overline{ISI}(\mathscr{H}) = (S_uJ\phi_v\phi_v)f(u,v)|_{u=v=1} = 321$
$\overline{H}(\mathscr{H}) = (2S_uJ)f(u,v)|_{u=v=1} = 157.67$
Hence the proof. □

Theorem 2.15. *Let $\mathscr{H}$ be the molecular graph of Doxorubicine . The $\bar{M}$ polynomial for $\mathscr{H}$ is* $\bar{M}(\mathscr{H},u,v)$=$10uv^2$+$100uv^3$+$53uv^4$+$64u^2v^2$+$132u^2v^3$+$70u^2v^4$+$51u^3v^3$+$71u^3v^4$.

Proof. Consider the graph $\mathscr{H}$ of doxorubicine which contains 39 vertices and 43 edges. We have eight division of edge set of $\mathscr{H}$ based on the degree of vertices. Here $\omega_{12} = |E_{12}| = 2$, $\omega_{13} = |E_{13}| = 8$, $\omega_{14} = |E_{14}| = 1$, $\omega_{22} = |E_{22}| = 2$, $\omega_{23} = |E_{23}| = 12$,$\omega_{24} = |E_{24}| = 2$, $\omega_{33} = |E_{33}| = 15$, $\omega_{34} = |E_{34}| = 1$. And the partition of vertices that depend on their degrees are given as $\rho_1 = |V_1| = 9$, $\sigma_2 = |V_2| = 12$, $\sigma_3 = |V_3| = 12$, $\sigma_4 = |V_4| = 6$, we obtain

$$\overline{\omega_{12}} = \sigma_1\sigma_2 \text{ - } \omega_{12} = 9(12) - 2 = 106$$
$$\overline{\omega_{13}} = \sigma_1\sigma_3 \text{ - } \omega_{13} = 9(12) - 8 = 100$$
$$\overline{\omega_{14}} = \sigma_1\sigma_4 \text{ - } \omega_{14} = 9(6) - 1 = 53$$
$$\overline{\omega_{22}} = \frac{\sigma_2(\sigma_2 - 1)}{2} \text{ - } \omega_{22} = \frac{12(11)}{2} \text{ - } 2 = 64$$
$$\overline{\omega_{23}} = \sigma_2\sigma_3 \text{ - } \omega_{23} = 12(12) - 12 = 132$$
$$\overline{\omega_{24}} = \sigma_2\sigma_4 \text{ - } \omega_{24} = 12(6) - 2 = 70$$
$$\overline{\omega_{33}} = \frac{\sigma_3(\sigma_3 - 1)}{2} \text{ - } \omega_{33} = \frac{12(11)}{2} \text{ - } 15 = 51$$
$$\overline{\omega_{34}} = \sigma_3\sigma_4 \text{ - } \omega_{34} = 12(6) - 1 = 71$$

By the definition of polynomial, we have

$$\begin{aligned}
\overline{M}(\mathscr{H},u,v) &= \sum_{i\leq j} \bar{\omega}_{ij}(\mathscr{H})u^iv^j \\
&= \sum_{1\leq 2} \bar{\omega}_{12}(\mathscr{H})uv^2 + \sum_{1\leq 3} \bar{\omega}_{13}(\mathscr{H})uv^3 + \sum_{1\leq 4} \bar{\omega}_{14}(\mathscr{H})uv^3 + \sum_{2\leq 2} \bar{\omega}_{22}(\mathscr{H})u^2v^2 \\
&+ \sum_{2\leq 3} \bar{\omega}_{23}(G)u^2v^3 + \sum_{2\leq 4} \bar{\omega}_{24}(G)u^2v^3 + \sum_{3\leq 3} \bar{\omega}_{33}(\mathscr{H})u^3v^3 + \sum_{3\leq 4} \bar{\omega}_{34}(\mathscr{H})u^3v^3
\end{aligned}$$
$$\overline{M}(\mathscr{H},u,v) = 10uv^2 + 100uv^3 + 53uv^4 + 64u^2v^2$$

$$+132u^2v^3+70u^2v^4+51u^3v^3+71u^3v^4.$$

□

Hence the proof

We applying these equation, we get the degree-based topological indices as follows

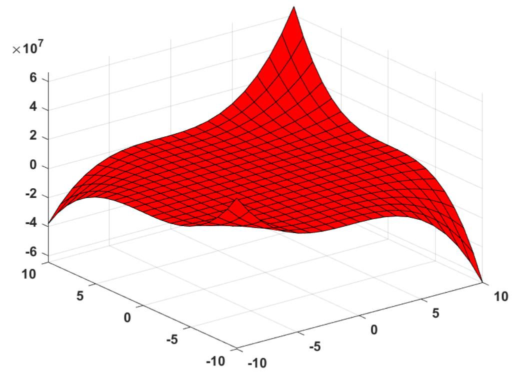

FIGURE 9. M-Polynomial of Doxorubicine

Theorem 2.16. *Let $\mathscr{H}$ be the molecular graph of doxorubicine, then*
(1) $\overline{M_1}(\mathscr{H})=2834$ (2) $\overline{M_2}(\mathscr{H})=3451$ (3) $\overline{ReZ}(\mathscr{H})=19382$ (4) $\overline{^{m}M_2}(\mathscr{H})=109.91$ (5) $\overline{F}(\mathscr{H})=7880$
(6)$\overline{ISI}(\mathscr{H})=1773$ (7) $\overline{H}(\mathscr{H})=673.34$

Proof. For determing the DBTI, we consider

$\bar{M}(\mathscr{H},u,v)$=$10uv^2$+$100uv^3$+$53uv^4$+$64u^2v^2$+$132u^2v^3$+$70u^2v^4$+$51u^3v^3$+$71u^3v^4$

$\phi_u\ f(u,v)=10uv^2+100uv^3+53uv^4+128u^2v^2+264u^2v^3+140u^2v^4+153u^3v^3+213u^3v^4$

$\phi_v\ f(u,v)=20uv^2+300uv^3+212uv^4+128u^2v^2+396u^2v^3+280u^2v^4+153u^3v^3+284u^3v^4$

$\phi_u+\phi_v\ f(u,v)=30uv^2+400uv^3+265uv^4+256u^2v^2+660u^2v^3+420u^2v^4+306u^3v^3+497u^3v^4$

$\phi_u.\phi_v\ f(u,v)=20uv^2+300uv^3+212uv^4+256u^2v^2+792u^2v^3+560u^2v^4+459u^3v^3+1136u^3v^4$

$(\phi_u\phi_v)(\phi_u+\phi_v)\ f(u,v)=60uv^2+1200uv^3+1060uv^4+1024u^2v^2+3960u^2v^3+3360u^2v^4+2754u^3v^3+5964u^3v^4$

$(S_uS_v)\ f(u,v)=5uv^2+\frac{100}{3}uv^3+\frac{53}{4}uv^4+\frac{32}{2}u^2v^2+\frac{132}{6}u^2v^3+\frac{70}{8}u^2v^4+\frac{51}{9}u^3v^3+\frac{71}{12}u^3v^4$

$(\phi_u^2+\phi_v^2)\ f(u,v)=50uv^2+100uv^3+901uv^4+384u^2v^2+1452u^2v^3+1400u^2v^4+918u^3v^3+1775u^3v^4$

$(S_uJ\phi_u\phi_v)\ f(u,v)=20u^3+428u^4+608u^5+433u^6+284u^7$

$(2S_uJ)\ f(u,v)=20u^3+264u^4+238u^5+104u^6+\frac{142}{3}u^7$

Now these data in Table.1 immediately yied the aforementioned.

$\overline{M_1}(\mathscr{H})=(\phi_u+\phi_v)f(u,v)|_{u=v=1}=2834$

$\overline{M_2}(\mathscr{H})$ =$(\phi_u.\phi_v)f(u,v)|_{u=v=1}$ = 3735

$\overline{ReZ}(\mathscr{H})$ = $(\phi_u\phi_v)(\phi_u+\phi_v)f(u,v)|_{u=v=1}$ = 19382

$^{m}\overline{M_2}(\mathscr{H})$ = $(S_uS_v)f(u,v)|_{u=v=1}$ = 109.91

$\overline{F}(\mathscr{H})$ = $(\phi_u^2+\phi_v^2)f(u,v)|_{u=v=1}$ = 7880

$\overline{ISI}(\mathscr{H})$ = $(S_uJ\phi_u\phi_v)f(u,v)|_{u=v=1}$ = 1773

$\overline{H}(\mathscr{H})$ = $(2S_uJ)f(u,v)|_{u=v=1}$ = 673.34

Hence the proof. □

Theorem 2.17. *Let $\mathscr{H}$ be the molecular graph of Dexamethasone . The $\bar{M}$ polynomial for $\mathscr{H}$ is* $\bar{M}(\mathscr{H},u,v)$=$79uv^2$+$44uv^3$+$28uv^4$+$43u^2v^2$+$51u^2v^3$+$38u^2v^4$+$14u^3v^3$+$18u^3v^4$+$4u^4v^4$.

Proof. Consider the graph $\mathscr{H}$ of dexamethasone which contains 28 vertices and 31 edges. We have eight division of edge set of $\mathscr{H}$ based on the degree of vertices. Here $\omega_{12} = |E_{12}| = 1$, $\omega_{13} = |E_{13}| = 4$, $\omega_{14} = |E_{14}| = 4$, $\omega_{22} = |E_{22}| = 2$, $\omega_{23} = |E_{23}| = 9$,$\omega_{24} = |E_{24}| = 2$, $\omega_{33} = |E_{33}| = 1$, $\omega_{34} = |E_{34}| = 6$, $\omega_{44} = |E_{44}| = 2$.The vertices are divided based on their degrees. $\rho_1 = |V_1| = 8$, $\sigma_2 = |V_2| = 10$, $\sigma_3 = |V_3| = 6$, $\sigma_4 = |V_4| = 4$, we obtain

$$\overline{\omega_{12}} = \sigma_1\sigma_2 \text{ - } \omega_{12} = 8(1)0-1 = 79$$
$$\overline{\omega_{13}} = \sigma_1\sigma_3 \text{ - } \omega_{13} = 5(6)-4 = 44$$
$$\overline{\omega_{14}} = \sigma_1\sigma_4 \text{ - } \omega_{14} = 8()4-4 = 28$$
$$\overline{\omega_{22}} = \frac{\sigma_2(\sigma_2-1)}{2} \text{ - } \omega_{22} = \frac{10(9)}{2} \text{ - } 2 = 43$$
$$\overline{\omega_{23}} = \sigma_2\sigma_3 \text{ - } \omega_{23} = 10(6)-9 = 51$$
$$\overline{\omega_{24}} = \sigma_2\sigma_4 \text{ - } \omega_{24} = 10(4)-2 = 38$$
$$\overline{\omega_{33}} = \frac{\sigma_3(\sigma_3-1)}{2} \text{ - } \omega_{33} = \frac{6(5)}{2} \text{ - } 1 = 14$$
$$\overline{\omega_{34}} = \sigma_3\sigma_4 \text{ - } \omega_{34} = 6(4)-6 = 18$$
$$\overline{\omega_{44}} = \sigma_4\sigma_4 \text{ - } \omega_{44} = 4(3)-2 = 4$$

we have

$$\begin{aligned}\overline{M}(\mathscr{H},u,v) &= \sum_{i\leq j}\bar{\omega}_{ij}(\mathscr{H})u^iv^j\\ &= \sum_{1\leq 2}\bar{\omega}_{12}(\mathscr{H})uv^2 + \sum_{1\leq 3}\bar{\omega}_{13}(\mathscr{H})uv^3 + \sum_{1\leq 4}\bar{\omega}_{14}(\mathscr{H})uv^4 + \sum_{2\leq 2}\bar{\omega}_{22}(\mathscr{H})u^2v^2\\ &+ \sum_{2\leq 3}\bar{\omega}_{23}(\mathscr{H})u^2v^3 + \sum_{2\leq 4}\bar{\omega}_{24}(\mathscr{H})u^2v^4 + \sum_{3\leq 3}\bar{\omega}_{33}(\mathscr{H})u^3v^3\\ &+ \sum_{3\leq 4}\bar{\omega}_{34}(\mathscr{H})u^3v^4 + \sum_{4\leq 4}\bar{\omega}_{44}(\mathscr{H})uv^4\end{aligned}$$

$$\overline{M}(\mathscr{H},u,v) = 79uv^2 + 44uv^3 + 28uv^4 + 43u^2v^2 + 51u^2v^3 + 38u^2v^4 + 14u^3v^3 + 18u^3v^4 + 4u^4v^4$$

.

□

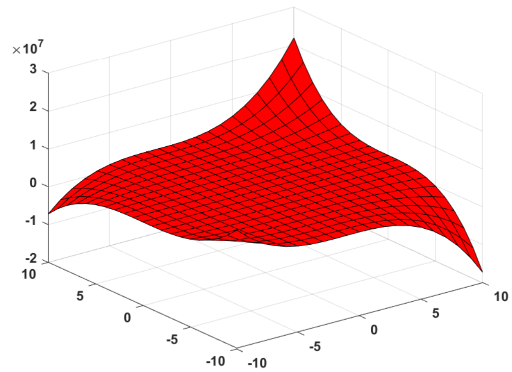

FIGURE 10. M-Polynomial of Dexamethasone

Theorem 2.18. *Let $\mathscr{H}$ be the molecular graph of dexamethasone, then*
(1) $\overline{M_1}(\mathscr{H}) = 1450$ (2) $\overline{M_2}(\mathscr{H}) = 1590$ (3) $\overline{ReZ}(\mathscr{H}) = 8384$ (4) $^{m}\overline{M_2}(\mathscr{H}) = 88.48$ (5) $\overline{F}(\mathscr{H}) = 3908$
(6)$\overline{ISI}(\mathscr{H}) = 923$ (7) $\overline{H}(\mathscr{H}) = 457.4$

Proof. For determing the DBTI, we consider

$\bar{M}(\mathscr{H}, u, v) = 79uv^2+44uv^3+28uv^4+43u^2v^2+51u^2v^3+38u^2v^4+14u^3v^3+18u^3u^4+4u^4v^4$

. $\phi_u\ f(u,v) = 79uv^2 + 44uv^3 + 28uv^4 + 86u^2v^2 + 102u^2v^3 + 46u^2v^4 + 42u^3v^3 + 54u^3v^4 + 16u^4y^4$

$\phi_v\ f(u,v) = 158uv^2 + 132uv^3 + 112uv^4 + 86u^2v^2 + 153u^2v^3 + 152u^2v^4 + 42u^3v^3 + 216u^3v^4 + 64u^4v^4$

$\phi_u + \phi_v\ f(u,v) = 237uv^2 + 176uv^3 + 140uv^4 + 172u^2v^2 + 255u^2v^3 + 198u^2v^4 + 84u^3v^3 + 270u^3v^4 + 80u^4v^4$

$\phi_u.\phi_v\ f(u,v) = 158uv^2 + 132uv^3 + 112uv^4 + 172u^2v^2 + 306u^2v^3 + 304u^2v^4 + 126u^3v^3 + 648u^3v^4 + 256u^4v^4$

$(\phi_u\phi_v)(\phi_u+\phi_v)\ f(u,v) = 474uv^2+528uv^3+560uv^4+344u^2v^2+765u^2v^3+792u^2v^4+252u^3v^3+1080u^3v^4+$
$320u^4v^4$

$(S_uS_v)\ f(u,v) = \frac{79}{2}uv^2 + \frac{44}{3}uv^3 + \frac{28}{4}uv^4 + \frac{43}{4}u^2v^2 + \frac{51}{6}u^2v^3 + \frac{38}{8}u^2v^4 + \frac{14}{9}u^3v^3 + \frac{18}{12}u^3v^4 + \frac{4}{16}u^4v^4$

$(\phi_u^2+\phi_v^2)\ f(u,v) = 395uv^2 + 440uv^3 + 476uv^4 + 344u^2v^2 + 663u^2v^3 + 760u^2v^4 + 252u^3v^3 + 450u^3v^4 80u^4v^4$

$(S_uJ\phi_u\phi_v)\ f(u,v) = 158u^3 + 132u^4 + 112u^5 + 86u^4 + 153u^5 + 152u^6 + 42u^6 + 288u^7 + 64u^8$

$(2S_uJ)\ f(u,v) = 158u^3 + 88u^6 + 56u^5 + 43u^4 + 51u^5 + 38u^6 + \frac{28}{3}u^6 + 12u^7 + 2u^8$

Now the data in Table.1, we get the results

$\overline{M_1}(\mathscr{H}) = (\phi_u + \phi_v)f(u,v)|_{u=v=1} = 1450$

$\overline{M_2}(\mathscr{H}) = (\phi_u.\phi_v)f(u,v)|_{u=v=1} = 1590$

$\overline{ReZ}(\mathscr{H}) = (\phi_u\phi_v)(\phi_u + \phi_v)f(u,v)|_{u=v=1} = 8384$

$^{m}\overline{M_2}(\mathscr{H}) = (S_uS_v)f(u,v)|_{u=v=1} = 88.48$

$\overline{F}(\mathscr{H}) = (\phi_u^2 + \phi_v^2)f(u,v)|_{u=v=1} = 3908$

$\overline{ISI}(\mathscr{H}) = (S_uJ\phi_u\phi_v)f(u,v)|_{u=v=1} = 927$

$\overline{H}(\mathscr{H}) = (2S_u J)f(u,v)|_{u=v=1} = 457.4$

Hence the proof. □

Theorem 2.19. *Let $\mathscr{H}$ be the molecular graph of Bexarotene . The $\bar{M}$ polynomial for $\mathscr{H}$ is* $\bar{M}(\mathscr{H},)$=$76uv^3$+$26uv^4$+$6u^2v^2$+$37u^2v^3$+$13u^2v^4$+$23u^3v^3$+$22u^3v^4$.

Proof. Consider the graph $\mathscr{H}$ of bexarotene which contains 26 vertices and 28 edges. We have seven division of edge set of $\mathscr{H}$ based on the degree of vertices. Here $\omega_{13} = |E_{13}| = 4$, $\omega_{14} = |E_{14}| = 4$, $\omega_{22} = |E_{22}| = 3$, $\omega_{23} = |E_{23}| = 8$,$\omega_{24} = |E_{24}| = 2$, $\omega_{33} = |E_{33}| = 5$, $\omega_{34} = |E_{34}| = 2$, $\sigma_1 = |V_1| = 10$, $\sigma_2 = |V_2| = 5$, $\sigma_3 = |V_3| = 8$, $\sigma_4 = |V_4| = 3$, we attain

$$\overline{\omega_{13}} = \sigma_1\sigma_3 \text{ - } \omega_{13} = 10(8) - 4 = 76$$

$$\overline{\omega_{14}} = \sigma_1\sigma_4 \text{ - } \omega_{14} = 10(3) - 4 = 26$$

$$\overline{\omega_{22}} = \frac{\sigma_2(\rho_2 - 1)}{2} \text{ - } \omega_{22} = \frac{5(4)}{2} \text{ - } 4 = 6$$

$$\overline{\omega_{23}} = \sigma_2\sigma_3 \text{ - } \omega_{23} = 5(8) - 3 = 37$$

$$\overline{\omega_{24}} = \sigma_2\sigma_4 \text{ - } \omega_{24} = 5(3) - 2 = 13$$

$$\overline{\omega_{33}} = \frac{\sigma_3(\sigma_3 - 1)}{2} \text{ - } \omega_{33} = \frac{8(7)}{2} \text{ - } 5 = 23$$

$$\overline{\omega_{34}} = \sigma_3\sigma_4 \text{ - } \omega_{34} = 8(3) - 2 = 22$$

By the definition of polynomial, we have

$$\begin{aligned}
\overline{M}(\mathscr{H},u,v) &= \sum_{i\le j} \bar{\omega}_{ij}(\mathscr{H})u^i v^j \\
&= \sum_{1\le 3} \bar{\omega}_{13}(\mathscr{H})uv^3 + \sum_{1\le 4} \bar{\omega}_{14}(\mathscr{H})uv^4 + \sum_{2\le 2} \bar{\omega}_{22}(\mathscr{H})u^2v^2 + \sum_{2\le 3} \bar{\omega}_{23}(\mathscr{H})u^2v^3 \\
&+ \sum_{2\le 4} \bar{\omega}_{24}(\mathscr{H})u^2v^4 + \sum_{3\le 3} \bar{\omega}_{33}(\mathscr{H})u^3v^3 + \sum_{3\le 4} \bar{\omega}_{34}(\mathscr{H})u^3v^4
\end{aligned}$$

$$\overline{M}(\mathscr{H},u,v) = 76uv^3 + 26uv^4 + 6u^2v^2 + 37u^2v^3 + 13u^2v^4 + 23u^3v^3 + 22u^3v^4.$$

□

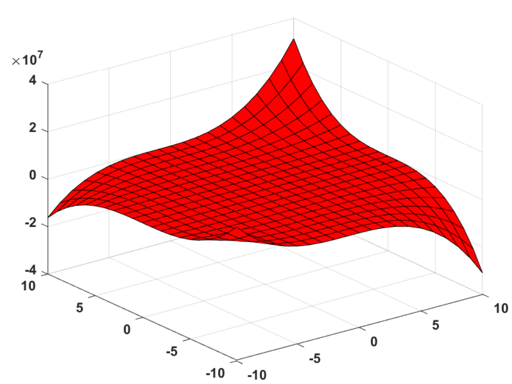

FIGURE 11. M-Polynomial of Bexarotene

Theorem 2.20. *Let $\mathscr{H}$ be the molecular graph of bexarotene, then*
(1) $\overline{M_1}(\mathscr{H}) = 1013$ (2) $\overline{M_2}(\mathscr{H}) = 1153$ (3) $\overline{ReZ}(\mathscr{H}) = 6352$
(4) $\overline{{}^mM_2}(\mathscr{H}) = 45.51$ (5) $\overline{F}(\mathscr{H}) = 2823$ (6)$\overline{ISI}(\mathscr{H}) = 664$
(7) $\overline{H}(\mathscr{H}) = 153$

Proof. For determing the DBTI, we consider

$\bar{M}(\mathscr{H}, u, v)$=$76uv^3$+$26uv^4$+$6u^2v^2$+$37u^2v^3$+$13u^2v^4$+$23u^3v^3$+$22u^3v^4$

. $\phi_u\ f(u, v) = 76uv^3 + 26uv^4 + 12u^2v^2 + 74u^2v^3 + 26u^2v^4 + 69u^3v^3 + 66u^3v^4$

$\phi_v\ f(u, v) = 228uv^3 + 104uv^4 + 12u^2v^2 + 111u^2v^3 + 52u^2v^4 + 69u^3v^3 + 88u^3v^4$

$\phi_u + \phi_v\ f(u, v) =304uv^3 + 130uv^4 + 24u^2v^2 + 185u^2v^3 + 78u^2v^4 + 138u^3v^3 + 154u^3v^4$

$\phi_u.\phi_v\ f(u, v) =228uv^3 + 104uv^4 + 24u^2v^2 + 222u^2v^3 + 104u^2v^4 + 207u^3v^3 + 207u^3v^4$

$(\phi_u\phi_v)(\phi_u + \phi_v)\ f(u, v) = 912uv^3 + 520uv^4 + 96u^2v^2 + 1110u^2v^3 + 624u^2v^4 + 1242u^3v^3 + 1848u^3v^4$

$(S_uS_v)\ f(u, v) = \dfrac{76}{6}uv^3 + \dfrac{26}{4}uv^4 + \dfrac{3}{2}u^2v^2 + \dfrac{37}{6}u^2v^3 + \dfrac{13}{8}u^2v^4 + \dfrac{23}{9}u^3v^3 + \dfrac{22}{12}u^3v^4$

$(\phi_u^2 + \phi_v^2)\ f(u, v) = uv^2 + 440uv^3 + 476uv^4 + 344u^2v^2 + 663u^2v^3 + 760u^2v^4 + 252u^3v^3 + 450u^3v^4 80u^4v^4$

$(S_uJ\phi_u\phi_v)\ f(u, v) = 158u^3 + 132u^4 + 112u^5 + 86u^4 + 153u^5 + 152u^6 + 42u^6 + 288u^7 + 64u^8$

$(2S_uJ)\ f(u, v) = 158u^3 + 88u^6 + 56u^5 + 43u^4 + 51u^5 + 38u^6 + \dfrac{28}{3}u^6 + 12u^7 + 2u^8$

Using Table 1. we get the results

$\overline{M_1}(\mathscr{H}) = (\phi_u + \phi_v)f(u, v)|_{u=v=1} = 1013$

$\overline{M_2}(\mathscr{H}) =(\phi_u.\phi_v)f(u, v)|_{u=v=1} = 1153$

$\overline{ReZ}(\mathscr{H}) = (\phi_u\phi_v)(\phi_u + \phi_v)f(u, v)|_{u=v=1} = 6352$

$\overline{{}^mM_2}(\mathscr{H}) = (S_uS_v)f(u, v)|_{u=v=1} = 45.51$

$\overline{F}(\mathscr{H}) = (\phi_u^2 + \phi_v^2)f(u, v)|_{u=v=1} = 2823$

$\overline{H}(\mathscr{H}) = (S_uJ\phi_u\phi_v)f(u, v)|_{u=v=1} = 664$

$\overline{H}(\mathscr{H}) = (2S_uJ)f(u, v)|_{u=v=1} = 153$

Hence the proof. □

A graph is an effective visual aid as it presents data in a concise manner, facilitates comparison, and reveals patterns and connections within the data, such as changes over time, frequency distribution, correlation, or relative proportions. The line graphs use various colors to distinguish between different parameters of drugs. The X-axis displays the names of the drugs, while the Y-axis displays the topological indices.

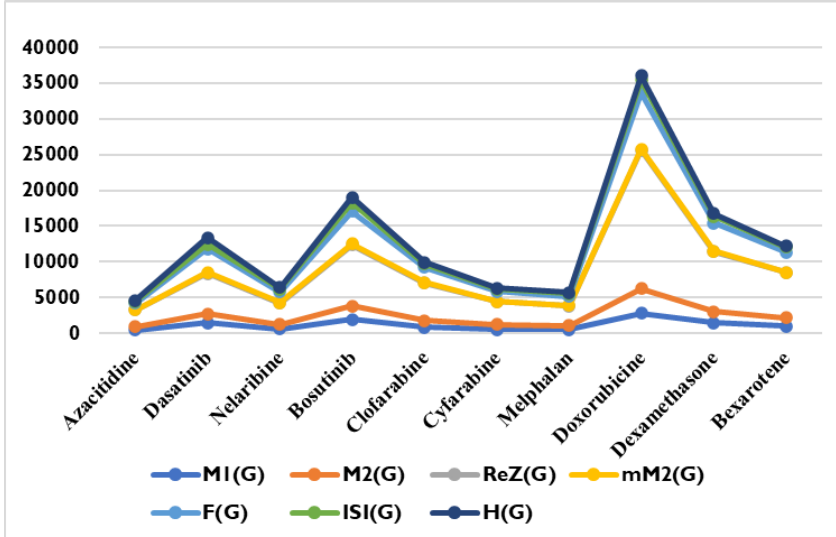

Figure 12. Comparison of degree-based topological indices for some drugs

3. Applications

Cancer is a devastating disease that is becoming increasingly fatal worldwide. There is a need for improved cancer treatment that is free from harmful side effects. The treatment should specifically target cancer cells without harming healthy cells [28,29]. Chemotherapy is the most commonly used treatment for cancer, but it also affects normal cells along with tumor-specific cells. The US food and drug administration has approved 132 cancer chemotherapy drugs, 14 of which are derived from medicinal plants. Research studies have shown that a low-calorie diet can reduce the adverse effects of chemotherapy. One common side effect of chemotherapy for breast cancer is hair loss. Combining chemotherapeutic drugs with bioactive substances from medicinal plants may have anti-cancer effects while causing fewer side effects. Advanced cancer treatments such as nano-medicines, extracellular vesicles, natural antioxidants, targeted immunotherapy, and gene therapy using active phytoconstituents from medicinal plants have also been used to diagnose and treat cancer [30]. Herbal medicines are commonly used to treat various ailments, and their effectiveness in cancer treatment should be explored. A significant percentage of cancer patients use herbal medicines to manage the side effects of chemotherapy or radiation therapy, alleviate sadness and anxiety, and actively participate in their recovery. Breast cancer patients are more likely to use herbal medicines compared to patients with other types of cancer. The main objective of using herbal medicine as an alternative treatment is to target cancer cells, and clinical trials should be conducted to evaluate their efficacy. These drugs not only treat cancer but also prevent its development by interfering with the processes involved in cancer growth [31,32]. They can also boost the immune system and have immunomodulatory and chemopreventive effects. Ganoderma lucidum, Sophora flavescens, Curcuma longa, Amoora rohituka, Angelica sinensis, and Tabebuia avellanedae have been shown to inhibit cancer cell proliferation and block cancer development pathways. These herbal medicines promote survival, improve quality of life, modulate the immune system, and enhance overall well-being.

4. Limitations

Chemists do not publish the range of topological indices on the internet, making it difficult for mathematicians to determine the significance of the values they obtain for various chemical compounds. To address this issue, a potential solution would be for mathematicians, statisticians, chemists, and pharmacists to collaborate on future studies.

5. Conclusion

The ability of a molecule to reach its target and have a biological effect is determined by factors such as potency and concentration. The physical and chemical properties of the molecule, including solubility, hydrogen bonding, and isomerism, also play a role. Topological indices can be used to predict biological activity, such as enzyme inhibition and carcinogenicity. These predictions are important for studying environmental pollution and toxicity. This study focuses on the physicochemical properties of anticancer drugs and how they can be analyzed using topological indices. The findings suggest that these drugs could be further studied and designed using these indices. The correlation between drugs and their impact on cancer treatment is also discussed. The example of treating myelodysplastic syndrome with azacitidine is given. In medical research, the process of drug design takes into account various factors such as the chemical, physical, biological, and pharmaceutical characteristics of molecular structure. Topological indices are mathematical tools used to forecast chemical features. This article presents topological descriptors for blood cancer and their graphical behavior in predicting physical, chemical, and biological qualities. Topological indices are commonly used in quantitative structure-activity relationships, structure-property relationships, and structure-toxicity relationships. The topological features of drugs like azacitidine, dasatinib, and bosutinib are examined using several DBT-CIs. M-polynomials are used to determine the chemical structure, and specific DBTI are derived from these polynomials. The goal of this study is to provide an overview of current drugs and their therapeutic uses, as well as information on future applications.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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