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Valency-Based Indices for Some Succinct Drugs by Using M-Polynomial

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Abstract: A topological index, which is a number, is connected to a graph. It is often used in chemometrics, biomedicine, and bioinformatics to anticipate various physicochemical properties and biological activities of compounds. The purpose of this article is to encourage original research focused on topological graph indices for the drugs azacitidine, decitabine, and guadecitabine as well as an investigation of the genesis of symmetry in actual networks. Symmetry is a universal phenomenon that applies nature's conservation rules to complicated systems. Although symmetry is a ubiquitous structural characteristic of complex networks, it has only been seldom examined in real-world networks. The $\overline{M}$-polynomial, one of these polynomials, is used to create a number of degree-based topological coindices. Patients with higher-risk myelodysplastic syndromes, chronic myelomonocytic leukemia, and acute myeloid leukemia who are not candidates for intense regimens, such as induction chemotherapy, are treated with these hypomethylating drugs. Examples of these drugs are decitabine (5-aza-20-deoxycytidine), guadecitabine, and azacitidine. The $\overline{M}$-polynomial is used in this study to construct a variety of coindices for the three brief medicines that are suggested. New cancer therapies could be developed using indice knowledge, specifically the first Zagreb index, second Zagreb index, *F*-index, reformulated Zagreb index, modified Zagreb, symmetric division index, inverse sum index, harmonic index, and augmented Zagreb index for the drugs azacitidine, decitabine, and guadecitabine.

Keywords: azacitidine drug; decitabine drug; guadecitabine drug; $\overline{M}$-polynomial; valency-based topological indices

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1. Introduction

Investigating and even forecasting certain features of chemical compounds is performed using the branch of graph theory known as "chemical graph theory" [1–3]. The amount of components a molecule has and their connections may be used to predict a molecule's boiling point, according to molecular graph theory. Understanding this relationship is very helpful when developing chemical processes, synthetic materials, or chemical assembly lines. Chemists make use of a number of physical characteristics to comprehend the structure of molecules. Topological indices (TIs) [4] are used to forecast the physiochemical properties and biological activities of bioactive substances, but their potential

extends far beyond. For example, they can anticipate how dangerous a chemical will be. Because medication performance can now be anticipated based on electrical structure, the TI provides an alternative to empirical testing [5–9].

Transportation, communication network design, manufacturing and inventory planning, facility location and allocation, and VLSI (very large-scale integration) design are just a few of the areas where symmetry is used. Numerous TIs have been created since 1947, and these indices are divided into groups based on the structural properties of the graph [10–12], such as the degree of the vertices, the distance between neighboring vertices, the graph's eigenvalues, and others [13–15]. It is not always possible to compute some TIs directly. Researchers employ polynomials to address this issue. The degree-dependent M-polynomial for the TIs is one of them. The M-polynomial is a polynomial that is the sum of all the various degree-based TI subtypes.

Graph polynomials are graph functions that are independent of graph isomorphism, [16]. They are generally polynomials in one or two variables with integer coefficients. Since certain subgraphs are virtually always counted, graph polynomials may be seen as regular generating functions for the sequences of coefficients. The Hosoya polynomial [17–20] is a significant polynomial in the area of distance-based TIs. In [21–25], more graph polynomials were investigated. Deutsch and Klavzar [26] also proposed the M-polynomial, a degree-based polynomial that may be applied to build a variety of indices. Its high degree of flexibility led to its application in several research works to generate TIs. To calculate additional varieties of graph coindices, a polynomial that takes into account nonadjacent pairs of vertices is required because the M-polynomial only takes into account contributions from pairs of adjacent vertices. The M-polynomial and this polynomial both have comparable modes of operation. The development of polynomials based on non-adjacent pairings of chemical compound vertices was primarily motivated by this. Recently in 2022, a new M-polynomial, namely $\overline{M}$-polynomial, was proposed by Kirmani et al. [27,28] to generalized the widely used M-polynomial. They focused on the degree-based topological coindices (DBTCI). Following it, other authors produced many more works in this manner.

Applications of Graph Theory and Topological Indices

Any graph that mimics a particular molecular structure can be given a topological graph index, also known as a molecular descriptor [29]. From this index, it is possible to analyze numerical numbers and further look into some of a molecule's physical characteristics. As a result, it is a useful technique to eliminate costly and time-consuming laboratory studies. In mathematical chemistry, molecular descriptors are crucial, particularly in studies of quantitative structure–property relationships (QSPR) and quantitative structure–activity relationships (QSAR) [30]. For example, Ghani at all. in [31] started work on entropy by using topological indices. A topological descriptor is an illustration of a molecular descriptor. There are several topological indices available today, some of which are used in chemistry [32,33]. The structural characteristics of the graphs utilized for their computation can be used to categorize them. The Hosoya index, for instance, is determined by counting non-incident edges in a graph. In addition, the degrees of vertices are used to generate the Randi connectivity index, the Zagreb group indices, the Estrada index, and other indices.

1.1. Azacitidine Drug

A medication called azacitidine [34] inhibits DNA methyltransferase. It is an analog of cytidine's pyridine nucleoside. Its chemical name is 4-amino1-D-ribofuranosyl-s-triazin-2(1H)-one. Azacitidine has the empirical formula $C_8H_{12}N_4O_5$ (see Figure 1). Myelodysplastic syndrome, acute myeloid leukemia, and chronic myelomonocytic leukemia are all treated with it.

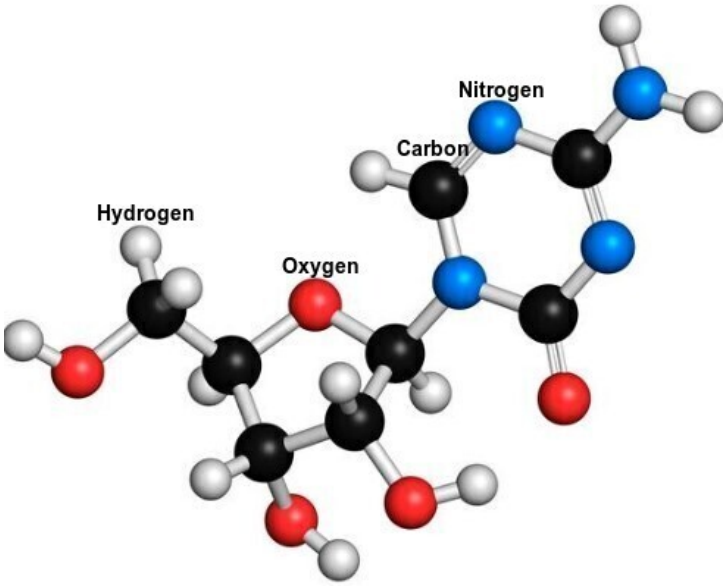

Figure 1. Azacitidine drug ($C_8H_{12}N_4O_5$).

1.2. Decitabine Drug

Myelodysplastic syndromes can be treated with the chemotherapeutic medication decitabine [34]. It achieves this by modifying gene expression and increasing the likelihood that DNA will not be protected. For people with significant MDS, refractory anemia, refractory anemia with ringed sideroblasts, refractory anemia with excess blasts and refractory anemia with excess blasts in transform, decidetabine is prescribed. Patients who have an International Prognostic Scoring System risk score of intermediate-1, intermediate-2, or high risk may also benefit from this medication. Decitabine's (see Figure 2) empirical formula is $C_8H_{12}N_4O_4$.

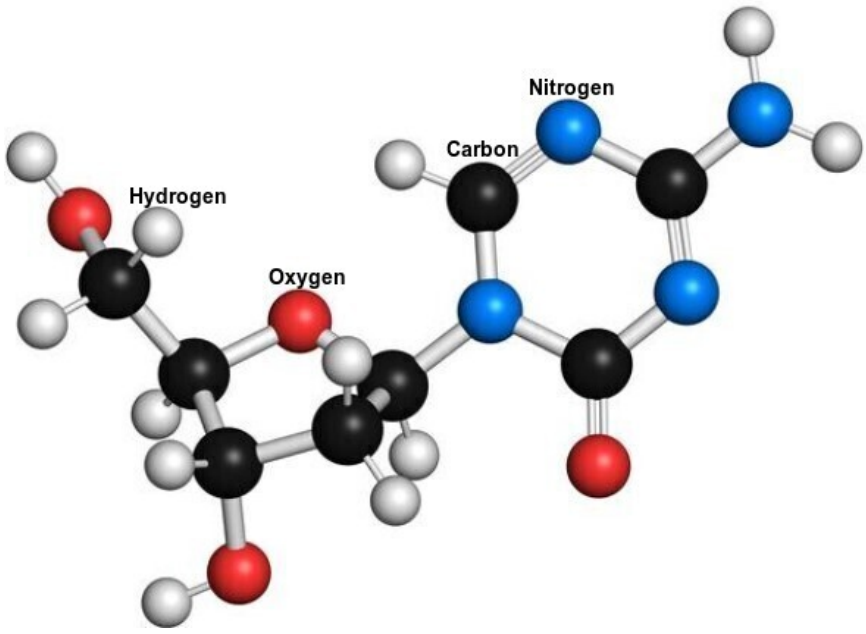

Figure 2. Decitabine drug ($C_8H_{12}N_4O_4$).

1.3. Guadecitabine Drug

The next-generation hypomethylating drug is guadecitabine [35]. More potent hypomethylating drugs are required for the treatment of MDS. The active metabolite of guadecitabine, decitabine, has a longer in vivo exposure period than decitabine given intravenously. Guadecitabine (see Figure 3) is used to treat myelodysplastic syndromes with intermediate or high risk because it is a more effective hypomethylating drug as a consequence. The bone marrow does not mature or become healthy in patients with myelodysplastic syndromes. It is also known as a collection of cancers.

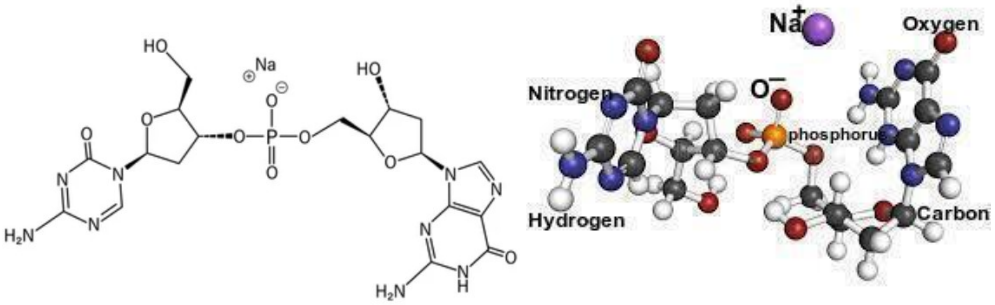

Figure 3. Guadecitabine drug ($C_{18}H_{24}N_9O_{10}P$).

The Figure 4 represent the chemical structure of azacitidine drug.

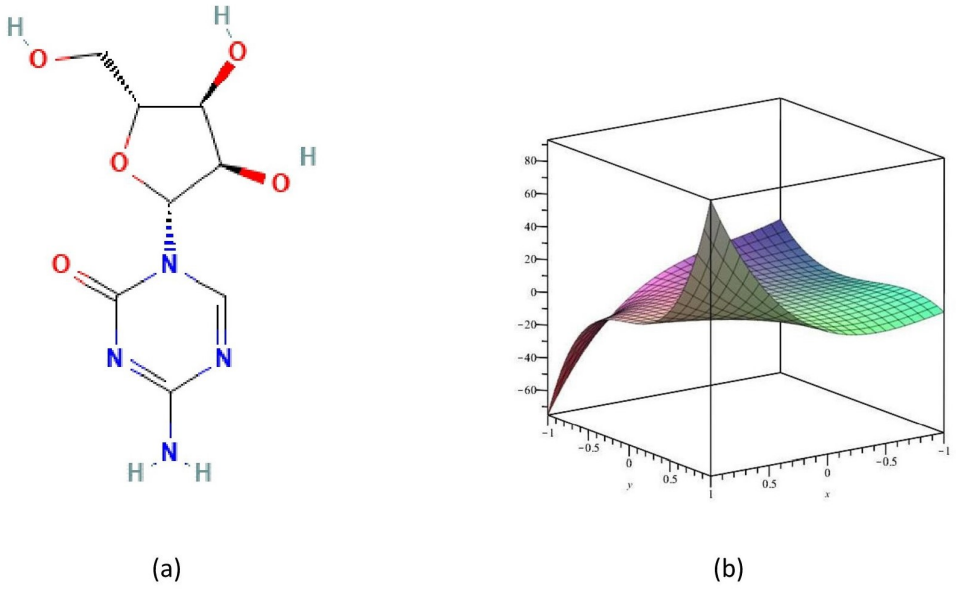

Figure 4. (**a**) The chemical structure of azacitidine (**b**) The 3D plots for $\overline{M}$-polynomial of azacitidine.

Figure 5 represents the chemical structure of decitabine.

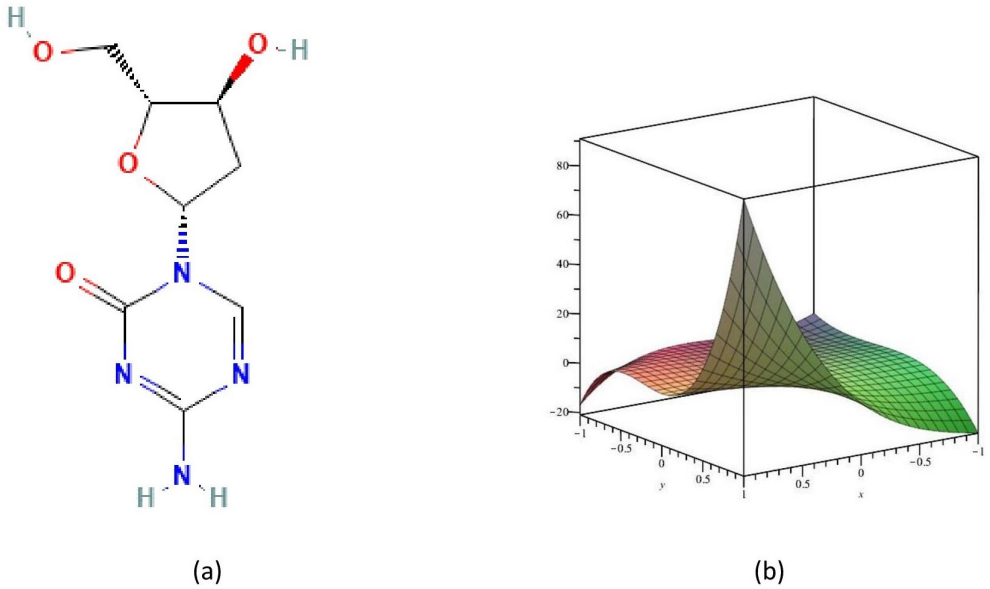

Figure 5. (**a**) The chemical structure of decitabine. (**b**) The 3D plots for $\overline{M}$-polynomial of decitabine.

Figure 6 represents the chemical structure of guadecitabine.

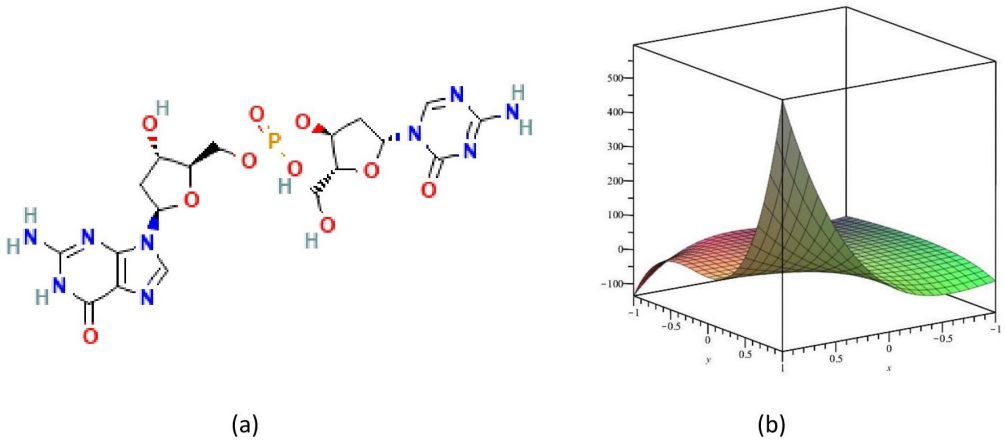

Figure 6. (**a**) The chemical structure of guadecitabine. (**b**) The 3D plots for $\overline{M}$-polynomial of guadecitabine.

2. Preliminaries

Let us use the following notation for the rest of the paper. Let $G = (V, E)$ be a graph, where $V = V(G)$ and $E = E(G)$ represent the vertex set and edge set, respectively. A molecular graph is a straightforward finite graph, where the edges represent chemical bonds and the vertices represent atoms. The degree of a vertex x is the number of edges incident to x, denoted by d_x. The notation $|V_i|$ denotes the number of vertices in the set V_i. The notation $|E(G)|$ denotes the number of edges in graph G or the size of a graph. Define

$$\begin{aligned}\rho_i &= |V_i|, \text{ where } V_i = \{x \in V(G) \,|\, d_x = i\}.\\ \omega_{ij} &= \left|E_{ij}\right|, \text{ where } E_{ij} = \{xy \in V(G) \,|\, d_x = i,\ d_y = j\}.\\ \overline{\omega}_{ij} &= \left|\overline{E}_{ij}\right|, \text{ where } \overline{E}_{ij} = \{xy \in V(\overline{G}) \,|\, d_x = i,\ d_y = j\}.\end{aligned}$$

We concentrate the concept of the M-polynomial for a non-adjacent pair of vertices and define $\overline{M}$-polynomial as follows:

$$\overline{M}(G,x,y) = \sum_{i\leq j} \overline{\omega}_{ij}(G)\, x^i\, y^j,$$

where $\overline{\omega}_{ij}$, is the number of edges $xy \notin E(G)$ such that $\{d(x), d(y)\} = \{i, j\}$.

On the edge set $E(G)$ of a graph G, the DBTCI can be stated as

$$DBCI(G) = \sum_{xy\notin E(G)} z(x,y).$$

Formulation of Certain Coindices from $\overline{M}$-Polynomial

In Table 1, a few DBTCI are listed along with their connections to the $\overline{M}$-polynomial of a graph G.

$\phi_x(z(x,y)) = x\left(\frac{\partial(z(x,y))}{\partial x}\right)$, $\phi_y(z(x,y)) = y\left(\frac{\partial(z(x,y))}{\partial y}\right)$, $S_x(z(x,y)) = \int_0^x \frac{z(t,y)}{t}dt$, $S_y(z(x,y)) = \int_0^y \frac{z(x,t)}{t}dt$ and $J(z(x,y)) = z(x,x)$.

Table 1. Derivation of DBTCI using $\overline{M}$-polynomial.

DBCI	$z(d_u, d_v)$	**Derivation from $\overline{M}(G,x,y)$**
First Zagreb coindex $\overline{\omega}_1$	$\left(d_u + d_v\right)$	$\left(\phi_x + \phi_y\right)(\overline{M}(G))$ at $x = y = 1$
Second Zagreb coindex $\overline{\omega}_2$	$d_u\, d_v$	$\left(\phi_x\, \phi_y\right)(\overline{M}(G))$ at $x = y = 1$
F- coindex $\overline{F}$	$\left(d_u^2 + d_v^2\right)$	$\left(\phi_x^2 + \phi_y^2\right)(\overline{M}(G))$ at $x = y = 1$
Reformulated Zagreb coindex $\overline{RZ}$	$\left(d_u + d_v\right)d_u\, d_v$	$\left(\phi_x\, \phi_y(\phi_x + \phi_y)\right)(\overline{M}(G))$ at $x = y = 1$
Modified Zagreb coindex $\overline{M}^*$	$\frac{1}{d_u\, d_v}$	$(S_x\, S_y)(\overline{M}(G))$ at $x = y = 1$
Symmetric deg devision coindex $\overline{SDD}$	$\frac{d_u^2+d_v^2}{d_u\, d_v}$	$(\phi_x\, S_y + S_x\, \phi_y))(\overline{M}(G))$ at $x = y = 1$
Inverse sum indeg coindex $\overline{ISI}$	$\frac{d_u\, d_v}{d_u+d_v}$	$(S_x\, J\, \phi_x\, \phi_y)(\overline{M}(G))$ at $x = y = 1$
Harmonic coindex $\overline{H}$	$\frac{2}{d_u+d_v}$	$(2S_x\, J)(\overline{M}(G))$ at $x = 1$
Augmented Zagreb coindex $\overline{AZ}$	$\left(\frac{d_u\, d_v}{d_u+d_v-2}\right)^3$	$(S_x^3\, \psi_{-2}\, J\, \phi_x^3\, \phi_y^3)(\overline{M}(G))$ at $x = 1$

The proof of the following observation is due to Berhe [36].

We have the following for a connected graph G with n vertices:

(i) If $i = j$ then $\overline{\omega}_{ij} = \left|\overline{E}_{ij}\right| = \frac{\rho_i(\rho_i-1)}{2} - \omega_{ii}$.

(ii) If $i < j$ then $\overline{\omega}_{ij} = \left|\overline{E}_{ij}\right| = \rho_i\rho_j - \omega_{ij}$.

Theorem 1. *Let A be the molecular graph of Azacitidine. The $\overline{M}$ polynomial for A is $\overline{M}(A;x,y) = 9xy^2 + 31xy^3 + 9x^2y^2 + 28x^2y^3 + 16x^3y^3$.*

Proof. For the molecular graph of azacitidine (see Figures 1, 4 and 7), we can easily calculate the edge partition given in the main theorems by using the hand shake lemma [37]. According to the "handshaking theorem," a graph's vertex total is equal to twice as many edges as it has edges, as in Equation (1). Since a vertex's degree is determined by how many edges intersect it, the sum of degrees determines how frequently an edge intersects a vertex overall:

$$\sum_{i=1}^{n} dx = 2 \times |E(G)| \tag{1}$$

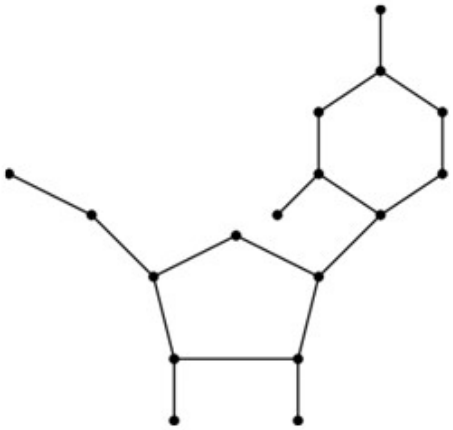

Figure 7. The molecular graph of azacitidine.

There are 17 vertices and 18 edges from the construction of azacitidinen (Figure 7), we have five categories of edge set of A based on the degree of vertices. $\omega_{12} = |E_{12}| = 1$, $\omega_{13} = |E_{13}| = 4$, $\omega_{22} = |E_{22}| = 1$, $\omega_{23} = |E_{23}| = 7$ and $\omega_{33} = |E_{33}| = 5$. In addition, $V(A)$ may be divided into three groups according on the number of vertices, that is, $\rho_1 = |V_1| = 5$, $\rho_2 = |V_2| = 5$ and $\rho_3 = |V_3| = 7$. Using Observation 1, we obtain

$$\begin{gathered}\overline{\omega}_{12} = \rho_1\rho_2 - \omega_{12} = 5(5) - 1 = 9\\ \overline{\omega}_{13} = \rho_1\rho_3 - \omega_{13} = 5(7) - 4 = 31\\ \overline{\omega}_{22} = \frac{\rho_2(\rho_2-1)}{2} - \omega_{22} = \frac{5(4)}{2} - 1 = 9\\ \overline{\omega}_{23} = \rho_2\rho_3 - \omega_{23} = 5(7) - 7 = 28\\ \overline{\omega}_{33} = \frac{\rho_3(\rho_3-1)}{2} - \omega_{33} = \frac{7(6)}{2} - 5 = 21 - 5 = 16.\end{gathered}$$

Hence , by the definition of $\overline{M}$ polynomial, we have

$$\begin{aligned}\overline{M}(A;x,y) &= \sum_{i\leq j}\overline{\omega}_{ij}(A)\, x^i\, y^j\\ &= \sum_{1\leq 2}\overline{\omega}_{12}(A)xy^2 + \sum_{1\leq 3}\overline{\omega}_{13}(A)xy^3 + \sum_{2\leq 2}\overline{\omega}_{22}(A)x^2y^2 + \sum_{2\leq 3}\overline{\omega}_{23}(A)x^2y^3\\ &+ \sum_{3\leq 3}\overline{\omega}_{33}(A)x^3y^3\\ &= 9xy^2 + 31xy^3 + 9x^2y^2 + 28x^2y^3 + 16x^3y^3.\end{aligned}$$

Now we present some DBTCI of azacitidine using $\overline{M}$-polynomial. □

Theorem 2. *Let A be the molecular graph of azacitidine. Then*
(1) $\overline{\omega}_1(A) = 423$ (2) $\overline{\omega}_2(A) = 459$ (3) $\overline{F}(A) = 1079$ (4) $\overline{RZ}(A) = 2274$ (5) $\overline{\omega}^*_2(A) = 23.528$ (6) $\overline{SDD}(A) = 236.5$ (7) $\overline{H}(A) = 21.267$ (8) $\overline{ISI}(A) = 95.85$ (9) $\overline{AZ}(A) = 654.875$.

Proof. For computing the DBTCI, we consider $\overline{M}(A;x,y) = 9xy^2 + 31xy^3 + 9x^2y^2 + 28x^2y^3 + 16x^3y^3$.

$\phi_x(z(x,y)) = 9xy^2 + 31xy^3 + 18x^2y^2 + 56x^2y^3 + 48x^3y^3$.
$\phi_y(z(x,y)) = 18xy^2 + 63xy^3 + 18x^2y^2 + 84x^2y^3 + 48x^3y^3$.
$(\phi_x + \phi_y)(z(x,y)) = 27xy^2 + 124xy^3 + 36x^2y^2 + 140x^2y^3 + 96x^3y^3$.
$\phi_x\phi_y(z(x,y)) = 18xy^2 + 93xy^3 + 36x^2y^2 + 168x^2y^3 + 144x^3y^3$.
$(\phi_x^2 + \phi_y^2)(z(x,y)) = 45xy^2 + 310xy^3 + 72x^2y^2 + 364x^2y^3 + 288x^3y^3$.
$(\phi_x + \phi_y)\phi_x\phi_y(z(x,y)) = 54xy^2 + 372xy^3 + 144x^2y^2 + 840x^2y^3 + 864x^3y^3$.
$S_xS_y(z(x,y)) = \frac{9}{2}xy^2 + \frac{31}{3}xy^3 + \frac{9}{4}x^2y^2 + \frac{28}{6}x^2y^3 + \frac{16}{9}x^3y^3$.
$(S_x\phi_y + S_y\phi_x)(z(x,y)) = \frac{45}{2}xy^2 + \frac{310}{3}xy^3 + \frac{72}{4}x^2y^2 + \frac{364}{6}x^2y^3 + \frac{288}{9}x^3y^3$.

$S_xJ(z(x,y)) = \frac{9}{3}x^3 + \frac{40}{4}x^4 + \frac{28}{5}x^5 + \frac{16}{6}x^6$.
$S_xJ\phi_x\phi_y(z(x,y)) = 6x^3 + \frac{129}{4}x^4 + \frac{168}{5}x^5 + 24x^6$.
$(S_x^3\,\psi_{-2}\,J\,\phi_x^3\,\phi_y^3)(z(x,y)) = 72x + \frac{1413}{8}x^2 + 224x^3 + \frac{729}{4}x^4$.

Now, these data in Table 1 immediately yield the aforementioned results:

$\overline{\omega}_1(A) = (\phi_x + \phi_y)((z(x,y)))|_{x=y=1} = 423$.
$\overline{\omega}_2(A) = (\phi_x\,\phi_y)((z(x,y)))|_{x=y=1} = 459$.
$\overline{F}(A) = (\phi_x^2 + \phi_y^2)((z(x,y)))|_{x=y=1} = 1079$.
$\overline{RZ}(A) = ((\phi_x + \phi_y)\phi_x\phi_y)((z(x,y)))|_{x=y=1} = 2274$.
$\overline{\omega}_2^*(A) = (S_xS_y)((z(x,y)))|_{x=y=1} = 23.528$.
$\overline{SDD}(A) = (S_x\phi_y + S_y\phi_x)((z(x,y)))|_{x=y=1} = 236.5$.
$\overline{H}(A) = (S_xJ)((z(x,y)))|_{x=1} = 21.267$.
$\overline{ISI}(A) = (S_xJ\phi_x\phi_y)((z(x,y)))|_{x=1} = 95.85$.
$\overline{AZ}(A) = (S_x^3\,\psi_{-2}\,J\,\phi_x^3\,\phi_y^3)(z(x,y))|_{x=1} = 654.875$. □

Theorem 3. *Let T be the molecular graph of decitabine. Then* $\overline{M}(T;x,y) = 23xy^2 + 21xy^3 + 14x^2y^2 + 21x^2y^3 + 12x^3y^3$.

Proof. Consider T to be the molecular graph of decitabine which contains 16 vertices and 17 edges. The following is the distribution of edges based on vertex degrees: $\omega_{12} = |E_{12}| = 1$, $\omega_{13} = |E_{13}| = 3$, $\omega_{22} = |E_{22}| = 1$, $\omega_{23} = |E_{23}| = 9$ and $\omega_{33} = |E_{33}| = 3$. And the partition of vertices that depend on their degrees are given as $\rho_1 = |V_1| = 4$, $\rho_2 = |V_2| = 6$ and $\rho_3 = |V_3| = 6$. By Observation 1, we obtain

$$\begin{aligned}
\overline{\omega}_{12} &= \rho_1\rho_2 - \omega_{12} = 4(6) - 1 = 23\\
\overline{\omega}_{13} &= \rho_1\rho_3 - \omega_{13} = 4(6) - 3 = 21\\
\overline{\omega}_{22} &= \tfrac{\rho_2(\rho_2-1)}{2} - \omega_{22} = \tfrac{6(5)}{2} - 1 = 14\\
\overline{\omega}_{23} &= \rho_2\rho_3 - \omega_{23} = 6(6) - 9 = 27\\
\overline{\omega}_{33} &= \tfrac{\rho_3(\rho_3-1)}{2} - \omega_{33} = \tfrac{6(5)}{2} - 3 = 12.
\end{aligned}$$

Hence, by the definition of the $\overline{M}$-polynomial, we have

$$\begin{aligned}
\overline{M}(T;x,y) &= \sum_{i\le j}\overline{\omega}_{ij}(G)x^iy^j\\
&= \overline{\omega}_{12}xy^2 + \overline{\omega}_{13}xy^3 + \overline{\omega}_{22}x^2y^2 + \overline{\omega}_{23}x^2y^3 + \overline{\omega}_{33}x^3y^3\\
&= 23xy^2 + 21xy^3 + 14x^2y^2 + 27x^2y^3 + 12x^3y^3.
\end{aligned}$$

□

Theorem 4. *For a decitabine graph, we have*
(1) $\overline{\omega}_1(T) = 386$ (2) $\overline{\omega}_2(T) = 399$ (3) $\overline{F}(T) = 926$ (4) $\overline{RZ}(T) = 1892$ (5) $\overline{\omega}_2^*(T) = 26.833$ (6) $\overline{SDD}(T) = 225$ (7) $\overline{H}(T) = 22.617$ (8) $\overline{ISI}(T) = 88.283$. (9) $\overline{AZ}(T) = 1455.5625$.

Proof. For computing the DBTCI of decitabine (Figure 8), we consider $\overline{M}(T;x,y) = 23xy^2 + 21xy^3 + 14x^2y^2 + 21x^2y^3 + 12x^3y^3$.

$\phi_x(z(x,y)) = 23xy^2 + 21xy^3 + 28x^2y^2 + 42x^2y^3 + 36x^3y^3$.
$\phi_y(z(x,y)) = 46xy^2 + 63xy^3 + 28x^2y^2 + 63x^2y^3 + 36x^3y^3$.
$(\phi_x + \phi_y)(z(x,y)) = 69xy^2 + 84xy^3 + 56x^2y^2 + 105x^2y^3 + 72x^3y^3$.
$\phi_x\phi_y(z(x,y)) = 46xy^2 + 63xy^3 + 56x^2y^2 + 126x^2y^3 + 108x^3y^3$.
$(\phi_x^2 + \phi_y^2)(z(x,y)) = 115xy^2 + 210xy^3 + 112x^2y^2 + 273x^2y^3 + 216x^3y^3$.
$(\phi_x + \phi_y)\phi_x\phi_y(z(x,y)) = 138xy^2 + 252xy^3 + 224x^2y^2 + 630x^2y^3 + 648x^3y^3$.
$S_xS_y(z(x,y)) = \frac{23}{2}xy^2 + \frac{21}{3}xy^3 + \frac{14}{4}x^2y^2 + \frac{21}{6}x^2y^3 + \frac{12}{9}x^3y^3$.
$(S_x\phi_y + S_y\phi_x)(z(x,y)) = \frac{115}{2}xy^2 + \frac{210}{3}xy^3 + \frac{112}{4}x^2y^2 + \frac{273}{6}x^2y^3 + \frac{216}{9}x^3y^3$.
$S_xJ(z(x,y)) = \frac{23}{3}x^3 + \frac{35}{4}x^4 + \frac{21}{5}x^5 + \frac{12}{6}x^6$.

$S_xJ\phi_x\phi_y(z(x,y)) = \frac{46}{3}x^3 + \frac{119}{4}x^4 + \frac{126}{5}x^5 + 108x^6$.
$(S_x^3\,\psi_{-2}\,J\,\phi_x^3\,\phi_y^3)(z(x,y)) = 184x + \frac{1463}{8}x^2 + 168x^3 + \frac{2187}{16}x^4$.
Now, these data in Table 1 immediately yield the aforementioned results.
$\overline{\omega}_1(T) = (\phi_x + \phi_y)((z(x,y)))|_{x=y=1} = 386$.
$\overline{\omega}_2(T) = (\phi_x\,\phi_y)((z(x,y)))|_{x=y=1} = 399$.
$\overline{F}(T) = (\phi_x^2 + \phi_y^2)((z(x,y)))|_{x=y=1} = 926$.
$\overline{RZ}(T) = ((\phi_x + \phi_y)\phi_x\phi_y)((z(x,y)))|_{x=y=1} = 1892$.
$\overline{\omega}_2^*(T) = (S_xS_y)((z(x,y)))|_{x=y=1} = 26.833$.
$\overline{SDD}(T) = (S_x\phi_y + S_y\phi_x)((z(x,y)))|_{x=y=1} = 225$.
$\overline{H}(T) = (S_xJ)((z(x,y)))|_{x=1} = 22.617$.
$\overline{ISI}(T) = (S_xJ\phi_x\phi_y)((z(x,y)))|_{x=1} = 88.283$.
$\overline{AZ}(T) = (S_x^3\,\psi_{-2}\,J\,\phi_x^3\,\phi_y^3)(z(x,y))|_{x=1} = 1455.5625$. □

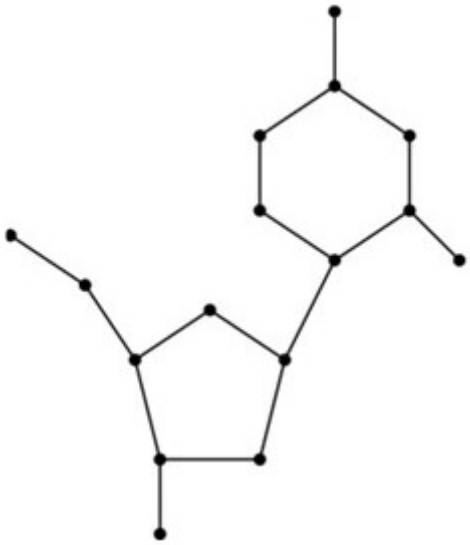

Figure 8. The molecular graph of decitabine.

Theorem 5. *Let G be the molecular graph of guadecitabine. Then, we have* $\overline{M}(G;x,y) = 111xy^2 + 107xy^3 + 6xy^4 + 88x^2y^2 + 176x^2y^3 + 13x^2y^4 + 83x^3y^3 + 13x^3y^4$.

Proof. Consider that the graph G of guadecitabine (Figure 9) has 37 vertices and 41 edges. The partition of edges that depends on the vertex degrees is given as $\omega_{12} = |E_{12}| = 1$, $\omega_{13} = |E_{13}| = 5$, $\omega_{14} = |E_{14}| = 2$, $\omega_{22} = |E_{22}| = 3$, $\omega_{23} = |E_{23}| = 20$, $\omega_{24} = |E_{24}| = 1$, $\omega_{33} = |E_{33}| = 8$ and $\omega_{34} = |E_{34}| = 1$. Similarly, the partition of vertices that depends on their degrees is given as $\rho_1 = |V_1| = 8$, $\rho_2 = |V_2| = 14$, $\rho_3 = |V_3| = 14$ and $\rho_4 = |v_4| = 1$. By Observation 1, we obtain

$$\begin{gathered}
\overline{\omega}_{12} = \rho_1\rho_2 - \omega_{12} = 8(14) - 1 = 111 \\
\overline{\omega}_{13} = \rho_1\rho_3 - \omega_{13} = 8(14) - 5 = 107 \\
\overline{\omega}_{14} = \rho_1\rho_4 - \omega_{14} = 8(1) - 2 = 6 \\
\overline{\omega}_{22} = \tfrac{\rho_2(\rho_2-1)}{2} - \omega_{22} = \tfrac{14(13)}{2} - 3 = 88 \\
\overline{\omega}_{23} = \rho_2\rho_3 - \omega_{23} = 14(14) - 20 = 176 \\
\overline{\omega}_{24} = \rho_2\rho_4 - \omega_{24} = 14(1) - 1 = 13 \\
\overline{\omega}_{33} = \tfrac{\rho_3(\rho_3-1)}{2} - \omega_{33} = \tfrac{14(13)}{2} - 8 = 83 \\
\overline{\omega}_{34} = \rho_3\rho_4 - \omega_{34} = 14(1) - 1 = 13.
\end{gathered}$$

By the definition of the $\overline{M}$-polynomial, we obtain

$$\begin{aligned}\overline{M}(G;x,y) &= \overline{\omega}_{12}xy^2+\overline{\omega}_{13}xy^3+\overline{\omega}_{14}xy^4+\overline{\omega}_{22}x^2y^2+\overline{\omega}_{23}x^2y^3+\overline{\omega}_{24}x^2y^4+\overline{\omega}_{33}x^3y^3+\overline{\omega}_{34}x^3y^4\\ &= 111xy^2+107xy^3+6xy^4+88x^2y^2+176x^2y^3+13x^2y^4+83x^3y^3+13x^3y^4.\end{aligned}$$

□

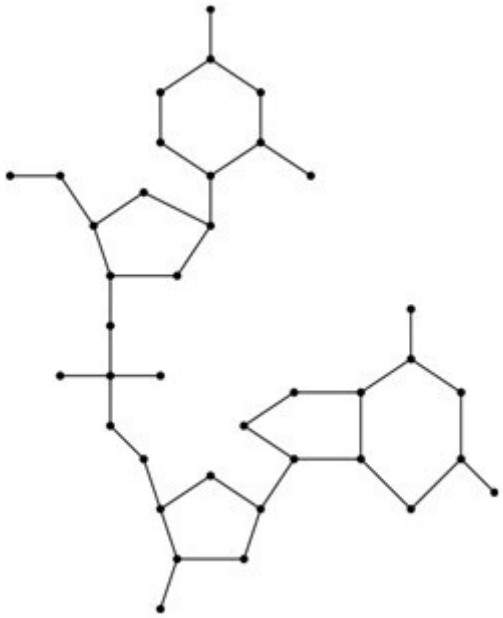

Figure 9. The molecular graph of guadecitabine.

Theorem 6. *For a guadecitabine graph, we have*
$(1)\overline{\omega}_1(G) = 2690$ $(2)\overline{\omega}_2(G) = 2982$ $(3)\overline{F}(G) = 6798$ $(4)\overline{RZ}(G) = 14956$ $(5)\overline{\omega}_2^*(G) = 155.93$ $(6)\overline{SDD}(G) = 1442.583$ $(7)\overline{H}(G) = 140.007$ $(8)\overline{ISI}(G) = 622.369$ $(9)\overline{AZ}(G) = 4604.481$.

Proof. For computing the DBTCI, we consider $\overline{M}(G;x,y) = 111xy^2+107xy^3+6xy^4+88x^2y^2+176x^2y^3+13x^2y^4+83x^3y^3+13x^3y^4$.

$\phi_x(z(x,y)) = 111xy^2+107xy^3+6xy^4+176x^2y^2+352x^2y^3+26x^2y^4+249x^3y^3+39x^3y^4$.

$\phi_y(z(x,y)) = 222xy^2+321xy^3+24xy^4+176x^2y^2+528x^2y^3+52x^2y^4+249x^3y^3+52x^3y^4$.

$(\phi_x+\phi_y)(z(x,y)) = 333xy^2+428xy^3+6xy^4+30x^2y^2+352x^2y^3+880x^2y^4+78x^3y^3+498x^3y^4$.

$\phi_x\phi_y(z(x,y)) = 222xy^2+321xy^3+24xy^4+352x^2y^2+1056x^2y^3+104x^2y^4+747x^3y^3+156x^3y^4$.

$(\phi_x^2+\phi_y^2)(z(x,y)) = 555xy^2+1070xy^3+102xy^4+704x^2y^2+2288x^2y^3+260x^2y^4+1494x^3y^3+325x^3y^4$.

$(\phi_x+\phi_y)\phi_x\phi_y(z(x,y)) = 666xy^2+1284xy^3+120xy^4+1408x^2y^2+5280x^2y^3+624x^2y^4+4482x^3y^3+1092x^3y^4$.

$S_xS_y(z(x,y)) = \frac{111}{2}xy^2+\frac{107}{2}xy^3+\frac{6}{4}xy^4+\frac{88}{4}x^2y^2+\frac{176}{6}x^2y^3+\frac{13}{8}x^2y^4+\frac{83}{9}x^3y^3+\frac{13}{12}x^3y^4$.

$(S_x\phi_y+S_y\phi_x)(z(x,y)) = \frac{555}{2}xy^2+\frac{1070}{3}xy^3+\frac{102}{4}xy^4+\frac{704}{4}x^2y^2+\frac{2288}{6}x^2y^3+\frac{260}{8}x^2y^4+\frac{1494}{9}x^3y^3+\frac{325}{12}x^3y^4$.

$S_xJ(z(x,y)) = \frac{111}{3}x^3+\frac{107}{4}x^4+\frac{6}{5}x^5+\frac{88}{4}x^4+\frac{176}{5}x^5+\frac{13}{6}x^6+\frac{83}{36}x^6+\frac{13}{7}x^7$.

$S_xJ\phi_x\phi_y(z(x,y)) = \frac{222}{3}x^3+\frac{321}{4}x^4+\frac{24}{5}x^5+\frac{352}{4}x^4+\frac{1056}{5}x^5+\frac{104}{6}x^6+\frac{747}{36}x^6+\frac{156}{7}x^7$.

$(S_x^3\,\psi_{-2}\,J\,\phi_x^3\,\phi_y^3)(z(x,y)) = 888x+\frac{8521}{8}x^2+\frac{38400}{27}x^3+\frac{67163}{64}x^4+\frac{22464}{125}x^5$.

Now, these data in Table 1 immediately yield the aforementioned results.

$\overline{\omega}_1(G) = (\phi_x + \phi_y)((z(x,y)))|_{x=y=1} = 2690.$
$\overline{\omega}_2(G) = (\phi_x\phi_y)((z(x,y)))|_{x=y=1} = 2982.$
$\overline{F}(G) = (\phi_x^2 + \phi_y^2)((z(x,y)))|_{x=y=1} = 6798.$
$\overline{RZ}(G) = ((\phi_x + \phi_y)\phi_x\phi_y)((z(x,y)))|_{x=y=1} = 14956.$
$\overline{\omega}_2^*(G) = (S_xS_y)((z(x,y)))|_{x=y=1} = 155.93.$
$\overline{SDD}(G) = (S_x\phi_y + S_y\phi_x)((z(x,y)))|_{x=y=1} = 1442.583.$
$\overline{H}(G) = (S_xJ)((z(x,y)))|_{x=1} = 140.007.$
$\overline{ISI}(G) = (S_xJ\phi_x\phi_y)((z(x,y)))|_{x=1} = 622.369.$
$\overline{AZ}(G) = (S_x^3\,\psi_{-2}\,J\,\phi_x^3\,\phi_y^3)(z(x,y))|_{x=1} = 4604.481.$ □

Display the graphical representations of the $\overline{M}$-polynomials. We first create a horizontal grid using the x and y parameters, and then we build a surface on top of that grid. These graphs demonstrate diverse polynomial behavior depending on the parameters. By adjusting the polynomials using these parameters, we may regulate topological coindices and, therefore, a large number of features and activities.

3. Application

Consider the treatment for myelodysplastic syndrome (a group of conditions in which the bone marrow produces blood cells that are misshapen and does not produce enough healthy blood cells) with azacitidine. Azacitidine or decitabine belongs to the group of drugs known as demethylation agents. An experimental medication being tested for the treatment of acute myeloid leukemia and myelodysplastic syndrome is guadecitabine. Drug design in medical research depends on the chemical, physiological, biological, and pharmacological aspects of molecular structure. Different mathematical instruments include forecasting certain chemistries' features, such as the topological index. The topological index allows us to link a single number to a molecular graph of a chemical complex. Polygonal forms, trees, graphs, and other geometrical shapes are widely used to represent drugs and other chemical compounds. In this study, we discuss the newly introduced invariants for the drugs azacitidine, decitabine, and guadecitabine (first Zagreb index, second Zagreb index, F-index, reformulated Zagreb index, modified Zagreb, symmetric division index, inverse sum index, harmonic index, and augmented Zagreb index). The goal of this study is to give the reader a current overview of drugs azacitidine, decitabine, and guadecitabines and drugs-based medications that are now used to treat patients as well as information on future therapeutic uses for these medications.

4. Conclusions

Building quantitative structure–activity relationships (QSAR), quantitative structure–property relationships (QSPR), and quantitative structure–toxicity relationships (QSTR) frequently uses topological indices (TIs) as molecular descriptors (QSTRs). In this article, we examine a few topological features of three concise drugs, azacitidine, decitabine, and guadecitabine, in terms of several DBTCIs. These three structures' M-polynomials are first determined, and then specific DBTCIs are derived using these polynomials. We also produce the graphical representations of these polynomials in Figures 4b, 5b and 6b. These figures are 3D plots also known as surface plots used to represent three-dimensional data of the M-polynomial of (i) azacitidine, (ii) decitabine, (iii) guadecitabine. With our obtained results, the F-index and RZ-index, future studies will evaluate how well the DBTCI can forecast the physicochemical properties of various chemical compounds.

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