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Research article

Some stable and closed-shell structures of anticancer drugs by graph theoretical parameters

Ali N.A. Koam [a], Ali Ahmad [b], Muhammad Azeem [c,*], Khalil Hadi Hakami [a], Kashif Elahi [d]

[a] Department of Mathematics, College of Science, Jazan University, New Campus, Jazan 2097, Saudi Arabia
[b] Department of Information Technology and Security, College of Computer Science and Information Technology, Jazan University, Saudi Arabia
[c] Department of Mathematics, Riphah International University Lahore, Pakistan
[d] Deanship of E-learning and Information Technology, Jazan University, Jazan, Saudi Arabia

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ABSTRACT

The eigenvalues are significant in mathematics, but they are also relevant in other domains like as chemistry, economics, and a variety of others. In terms of our research, eigenvalues are used in chemistry to represent not only the form of energy but also the various physicochemical aspects of a chemical substance. We must comprehend the connection between mathematics and chemistry. The antibonding level is related to positive eigenvalues, the bonding level is associated to negative eigenvalues, and the nonbonding level is linked to zero eigenvalues. In this work, we studied some anticancer drug structures in terms of nullity, matching number, eigenvalues of adjacency matrix, and characteristics polynomials. As a result, Carmustine, Caulibugulone-E, Aspidostomide-E anticancer drug structures are stable, closed-shell molecules since their nullity is equal to zero.

1. Introduction

The rapid proliferation of aberrant cells in the human body is known as cancer. Cancer-causing compounds are known as carcinogens. A carcinogen is a chemical compound found in cigarette smoke that contains certain components. It has the ability to spread throughout the body. A lump, abnormal bleeding, a prolonged cough, and weight loss are some of the symptoms of this condition. Chewing tobacco, obesity, a poor diet, laziness, and excessive alcohol consumption are the main causes of this cancerous condition. Several treatments, including surgery, radiotherapy, chemotherapy, hormone therapy, targeted therapy, and others, can be used to

* Corresponding author.
E-mail addresses: akoum@jazanu.edu.sa (A.N.A. Koam), aimam@jazanu.edu.sa, ahmadsms@gmail.com (A. Ahmad), azeemali7009@gmail.com (M. Azeem), khakami@jazanu.edu.sa (K.H. Hakami), kelahi@jazanu.edu.sa (K. Elahi).

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treat this severe disease. Anticancer medicines, which include alkylates and metabolites, are used to treat the disease known as cancer [1–4].

Chemical graph theory is a branch of mathematics chemistry concerned with chemical graphs that depict chemical systems. The chemical graph theory allows for the definition of numerous anticancer medication properties [5,6]. Several medicational structures are used in this study, by measuring nullity, matching number, eigenvalues of adjacency matrix, and characteristics polynomials.

Nullity is an important factor in molecule stability, and if nullity is zero, the molecule is projected to have a stable, closed-shell electron configuration. The molecule is unstable, extremely reactive, nonexistent, and open shell if nullity is larger than zero [7]. As a result, some of the chosen anticancer drug structures are stable, closed-shell molecules since their nullity is equal to zero.

There are numerous research work is available on the nullity, matching number, eigenvalues of adjacency matrix, characteristics polynomials. Only recent and few important articles are given herewith their importance. A proof is given on the conjecture on the topic of nullity [8]. Rank four graphs are characterized in [9], rank five in [10]. For upper bounds on the nullity $n-2$ and $n-3$, see [11], while further generalizations are given in [12]. For a relation between matching number and rank of a graph given in [13]. Trees are discussed in terms of nullity of a graph found in [14]. On the nullity of a graph with cut-points [15]. Unicyclic graphs in terms of nullity and matching number are found in [16], while for bicyclci graphs are herein [17] and for the line operation of unicyclic graphs and their nullity in [18]. Pure mathematical and abstract theory on nullity is available in [19–21]. Nullity is expressed in terms of maximum degree of a vertex [22,23]. Authors of [24,25], computed the double metric resolvability of convex polytopes, authors of [26], computed the edge version of resolvability and double resolvability of some generalized graphs.

The chemical complex is typically depicted as a graph, with the elements representing vertices and the bonds linking them representing edges. Similarly, the anticancer medications under investigation are treated as chemical compounds, and the parameters are investigated [27]. Graph theory provides methods such as QSAR, QSPR, and QSTR (quantitative structure-activity/property/toxicity relationship) that chemists and pharmacists can employ to enhance their research. Drugs are represented as molecular networks in theoretical chemistry, with each vertex representing an atom and each edge representing a relationship between two atoms [28,29]. Assume that $G(V,E)$ is a molecular graph with vertex and edge sets. Simple graphs with no cycle creation and several edges are considered, while $|V(G)|=n$ and $|E(G)|=m$ are order and size of a graph G, respectively. Adjacency matrix is defined by the elements of the matrix indicate whether pairs of vertices are adjacent or not in the graph and it is denoted by $A(G)$. Characteristics polynomial of a graph is defined by $\mathrm{Char}(A(G);\lambda)=\det(A(G)-\lambda I)=0$, where I is an identity matrix of order same as A-matrix. The values of parameter λ in the equation $\det(A(G)-\lambda I)=0$ are known as eigenvalues and we symbolized as $\mathrm{Eig}\left(\mathrm{Char}(A(G);\lambda)\right)$. While the mulitplicity of $\mathrm{Eig}\left(\mathrm{Char}(A(G);\lambda)\right)=0$ is known as nullity of a graph G, and usually it is denoted by $\eta(G)$ [30]. In [31], the nullity of a bipartite graph is defined by

$$\eta(G)=n-2M(G). \tag{1}$$

In the Equation (1), a parameter $M(G)$ is known as matching number and defined by the size of a largest maximal independent edge set [32,33]. In Fig. 1 to Fig. 10, the wavy edges denoted that edges contributed towards the count of matching number for all anticancer drug structures.

The positive inertia index is represented by the number of positive eigenvalues $p(G)$, whereas the negative inertia index is represented by the number of negative eigenvalues $q(G)$. An energy of the graph G is the absolute sum of all the eigenvalues. It is written as $E=\sum_{i=1}^{k}=|\lambda_i|$ in mathematics [7,34].

2. Results on matching number and nullity of anticancer drug structures

Several medicational structures are used in this study, by measuring nullity, matching number, eigenvalues of adjacency matrix, and characteristics polynomials.

2.1. Results of matching number and nullity of Amathas-Piramide-E anticancer drug structure

The order of graph obtained from Amathas-Piramide-E $|V(G_1)|=22$, while the size is counted in $|E(G_1)|=24$. Moreover, the vertex and edge set is defined by

$$V(G_1)=\{v_i : 1\le i\le 22\},$$

$$E(G_1)=\{v_iv_j : i,j=1,2,\ldots,7\}\cup\{v_iv_j : i,j=8,9,\ldots,15\}\cup\{v_{14}v_{15},v_{11}v_{16},v_8v_{16},v_6v_{12},$$

$$v_5v_{19},v_{12}v_{20},v_{14}v_{21},v_{15}v_{22},v_1v_{17},v_3v_{18}\}$$

Lemma 2.1. *Let G_1 be a graph obtained by an anticancer drug structure Amathas-Piramide-E. Then $\eta(G_1)=1$.*

Proof. Observe that G_1 is the graph of Amathas-Piramide-E an anticancer drug structure developed by some pendant vertices, two pentagons, and a single hexagon. Fig. 1, shows that it is not a bipartite graph. So to compute the nullity of G_1, we can not follow the Equation (1). Therefore, using the definition of nullity, we will determine the characteristics polynomial $\mathrm{Char}\left(A(G_1);\lambda\right)$ of the adjacency matrix $A(G_1)$ of graph G_1, characteristics polynomial is described as;

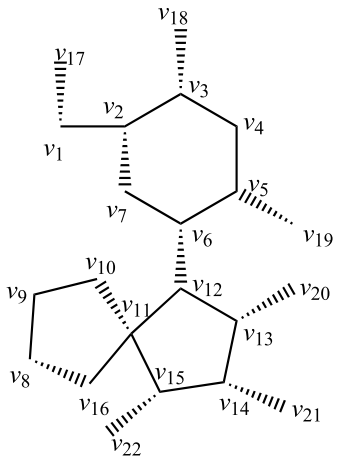

Fig. 1. Anticancer drug structure Amathas-Piramide-E.

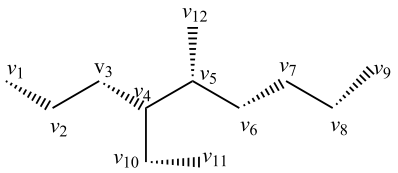

Fig. 2. Anticancer drug structure Carmustine.

$$\begin{aligned}&\mathrm{Char}\left(A\left(G_1\right);\lambda\right)=\\&\lambda^{22}-23\lambda^{20}+220\lambda^{18}-2\lambda^{17}-1146\lambda^{16}+32\lambda^{15}+3577\lambda^{14}-200\lambda^{13}-6932\lambda^{12}\\&+632\lambda^{11}+8353\lambda^{10}-1092\lambda^{9}-6088\lambda^{8}+1040\lambda^{7}+2513\lambda^{6}-518\lambda^{5}-507\lambda^{4}\\&+114\lambda^{3}+33\lambda^{2}-6\lambda.\end{aligned}$$

Now, by solving $\mathrm{Char}\left(A\left(G_1\right);\lambda\right)=0$ for λ, the eigenvalues $\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_1\right);\lambda\right)\right)$ of determined polynomials are

$$\begin{aligned}\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_1\right);\lambda\right)\right)=&\{0,-2.4727,-2.1834,-1.7631,-1.6180,-1.6063,-1.3109,\\&-0.9348,-0.8836,-0.7166,-0.3071,0.1585,0.5259,0.6180,\\&0.7480,0.9260,1.2615,1.3524,1.6064,1.8599,2.2338,2.5061\}.\end{aligned}$$

Observing that there is only a single value of $\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_1\right);\lambda\right)\right)=0$ and which is concluding that $\eta\left(G_1\right)=1$.

Furthermore, the Fig. 1, it is showing that there are ten counts of wavy edges and which is the matching number $M\left(G_1\right)$ of graph G_1. □

2.2. Results of matching number and nullity of Carmustine anticancer drug structure

The order of graph obtained from Carmustine $|V\left(G_2\right)|=12$, while the size is counted in $|E\left(G_2\right)|=11$. Moreover, the vertex and edge set is defined by

$$\begin{aligned}V(G_2)=&\{v_i:1\le i\le 12\},\\E(G_2)=&\{v_iv_j:i,j=1,2,\ldots,9\}\cup\{v_5v_{12},v_4v_{10},v_{10}v_{11}\}\end{aligned}$$

Lemma 2.2. *Let G_2 be a graph obtained by an anticancer drug structure Carmustine. Then $\eta\left(G_2\right)=0$.*

Proof. Observe that G_2 is the graph of Carmustine an anticancer drug structure developed by some pendant vertices, without any cycle. Fig. 2, shows that it is a bipartite graph. So to compute the nullity of G_2, we will follow the Equation (1). Fig. 1, it is showing that there is six-count of wavy edges and which is the matching number $M\left(G_2\right)$ of graph G_2. So by applying the definition of the nullity of a bipartite graph $\eta\left(G_2\right)=n-2M=12-2(6)=0$.

Furthermore, by using the definition of nullity, we will determine the characteristics polynomial $\mathrm{Char}\left(A\left(G_2\right);\lambda\right)$ of the adjacency matrix $A\left(G_2\right)$ of graph G_2, characteristics polynomial is described as;

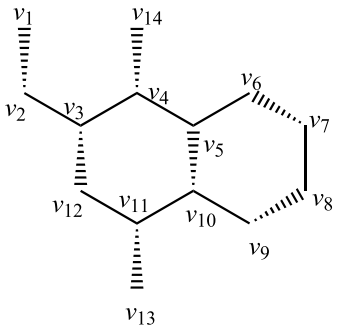

Fig. 3. Anticancer drug structure Caulibugulone-E.

$$\text{Char}\left(A\left(G_2\right);\lambda\right)=\lambda^{12}-11\lambda^{10}+43\lambda^8-74\lambda^6+55\lambda^4-14\lambda^2+1.$$

Now, by solving $\text{Char}\left(A\left(G_2\right);\lambda\right)=0$ for λ, the eigenvalues $\text{Eig}\left(\text{Char}\left(A\left(G_2\right);\lambda\right)\right)$ of determined polynomials are

$$\text{Eig}\left(\text{Char}\left(A\left(G_1\right);\lambda\right)\right)=\{-2.1673,-1.6783,-1.3427,-1.1358,-0.5246,-0.3436,0.3436,$$
$$0.5246,1.1358,1.3427,1.6783,2.1673\}.$$

Observing that there is no value of $\text{Eig}\left(\text{Char}\left(A\left(G_2\right);\lambda\right)\right)=0$ and which is concluding that $\eta\left(G_2\right)=0$. □

2.3. Results of matching number and nullity of Caulibugulone-E anticancer drug structure

The order of graph obtained from Caulibugulone-E $|V\left(G_3\right)|=14$, while the size is counted in $|E\left(G_3\right)|=15$. Moreover, the vertex and edge set is defined by

$$V(G_3)=\{v_i:1\le i\le 14\},$$
$$E(G_3)=\{v_iv_j:i,j=1,2,\ldots,12\}\cup\{v_4v_{14},v_3v_{12},v_5v_{10},v_{11}v_{13}\}$$

Lemma 2.3. *Let G_3 be a graph obtained by an anticancer drug structure Caulibugulone-E. Then $\eta\left(G_3\right)=0$.*

Proof. Observe that G_3 is the graph of Caulibugulone-E an anticancer drug structure developed by some pendant vertices, two cycles of length eight. Fig. 3, shows that it is a bipartite graph. So to compute the nullity of G_3, we will follow the Equation (1). Fig. 3, it is showing that there is seven-count of wavy edges and which is the matching number $M\left(G_3\right)$ of graph G_3. So by applying the definition of the nullity of a bipartite graph $\eta\left(G_3\right)=n-2M=14-2(7)=0$.

Furthermore, by using the definition of nullity, we will determine the characteristics polynomial $\text{Char}\left(A\left(G_3\right);\lambda\right)$ of the adjacency matrix $A\left(G_3\right)$ of graph G_3, characteristics polynomial is described as;

$$\text{Char}\left(A\left(G_3\right);\lambda\right)=\lambda^{14}-15\lambda^{12}+84\lambda^{10}-225\lambda^8+304\lambda^6-200\lambda^4+56\lambda^2-4.$$

Now, by solving $\text{Char}\left(A\left(G_3\right);\lambda\right)=0$ for λ, the eigenvalues $\text{Eig}\left(\text{Char}\left(A\left(G_3\right);\lambda\right)\right)$ of determined polynomials are

$$\text{Eig}\left(\text{Char}\left(A\left(G_3\right);\lambda\right)\right)=\{-2.4344,-1.8478,-1.6055,-1.2736,-0.8769,-0.7654,-0.3240,0.3240,$$
$$0.7654,0.8769,1.2736,1.6055,1.8478,2.4344\}.$$

Observing that there is no value of $\text{Eig}\left(\text{Char}\left(A\left(G_3\right);\lambda\right)\right)=0$ and which is concluding that $\eta\left(G_3\right)=0$. □

2.4. Results of matching number and nullity of Aspidostomide-E anticancer drug structure

The order of graph obtained from Aspidostomide-E $|V\left(G_4\right)|=26$, while the size is counted in $|E\left(G_4\right)|=29$. Moreover, the vertex and edge set is defined by

$$V(G_4)=\{v_i:1\le i\le 26\},$$
$$E(G_4)=\{v_iv_j:i,j=1,2,\ldots,11\}\cup\{v_iv_j:i,j=12,13,\ldots,20\}\cup\{v_3v_{11},v_2v_3,v_1v_2,v_5v_{22},$$
$$v_6v_{10},v_7v_{23},v_8v_{24},v_9v_{25},v_{11}v_{15},v_{12}v_{21},v_{12}v_{20},v_{14}v_{18},v_{16}v_{26}\}$$

Lemma 2.4. *Let G_4 be a graph obtained by an anticancer drug structure Aspidostomide-E. Then $\eta\left(G_4\right)=0$.*

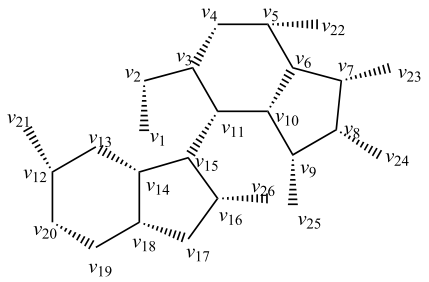

Fig. 4. Anticancer drug structure Aspidostomide-E.

Proof. Observe that G_4 is the graph of Aspidostomide-E an anticancer drug structure developed by some pendant vertices, two pentagons the same count of hexagons. Fig. 4, shows that it is not a bipartite graph. So to compute the nullity of G_4, we can not follow the Equation (1). Therefore, using the definition of nullity, we will determine the characteristics polynomial $\mathrm{Char}\left(A\left(G_4\right);\lambda\right)$ of the adjacency matrix $A\left(G_4\right)$ of graph G_4, characteristics polynomial is described as;

$$\begin{aligned}&\mathrm{Char}\left(A\left(G_4\right);\lambda\right)=\\&\lambda^{26}-29\lambda^{24}+361\lambda^{22}-4\lambda^{21}-2536\lambda^{20}+78\lambda^{19}+11121\lambda^{18}-618\lambda^{17}-31803\lambda^{16}\\&+2588\lambda^{15}+60177\lambda^{14}-6230\lambda^{13}-74914\lambda^{12}+8780\lambda^{11}+59908\lambda^{10}-7076\lambda^{9}\\&-29435\lambda^{8}+3058\lambda^{7}+8260\lambda^{6}-628\lambda^{5}-1177\lambda^{4}+50\lambda^{3}+69\lambda^{2}-1.\end{aligned}$$

Now, by solving $\mathrm{Char}\left(A\left(G_4\right);\lambda\right)=0$ for λ, the eigenvalues $\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_4\right);\lambda\right)\right)$ of determined polynomials are

$$\begin{aligned}\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_4\right);\lambda\right)\right)=\{&-2.4787,-2.2370,-2.1237,-1.9502,-1.7048,-1.5638,-1.3400,\\&-1.0401,-0.8788,-0.5584,-0.5177,-0.2512,-0.1650,0.1340,\\&0.3667,0.4500,0.7540,1.0000,1.1111,1.2313,1.3402,1.6019,\\&1.8261,1.9975,2.3929,2.6038\}.\end{aligned}$$

Observing that there is no value of $\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_4\right);\lambda\right)\right)=0$ and which is concluding that $\eta\left(G_4\right)=0$.

Furthermore, the Fig. 4, it is showing that there are 13 counts of wavy edges and which is the matching number $M\left(G_4\right)$ of graph G_4. □

2.5. Results of matching number and nullity of Convolutamide-A anticancer drug structure

The order of graph obtained from Convolutamide-A $|V\left(G_5\right)|=31$, while the size is counted in $|E\left(G_5\right)|=32$. Moreover, the vertex and edge set is defined by

$$\begin{aligned}V(G_5)=&\{v_i:1\le i\le 31\},\\E(G_5)=&\{v_iv_j:i,j=1,2,\ldots,6\}\cup\{v_iv_j:i,j=7,8,\ldots,11\}\cup\{v_iv_j:i,j=12,13,\ldots,25\}\\&\cup\{v_1v_{30},v_1v_6,v_6v_{29},v_5v_{28},v_3v_{11},v_{11}v_{27},v_{10}v_{26},v_7v_{11},v_9v_{12},v_{12}v_{31}\}\end{aligned}$$

Lemma 2.5. *Let G_5 be a graph obtained by an anticancer drug structure Convolutamide-A. Then $\eta\left(G_5\right)=3$.*

Proof. Observe that G_5 is the graph of Convolutamide-A an anticancer drug structure developed by some pendant vertices, 1 pentagon, and a single hexagon. Fig. 5, shows that it is not a bipartite graph. So to compute the nullity of G_5, we can not follow the Equation (1). Therefore, using the definition of nullity, we will determine the characteristics polynomial $\mathrm{Char}\left(A\left(G_5\right);\lambda\right)$ of the adjacency matrix $A\left(G_5\right)$ of graph G_5, characteristics polynomial is described as;

$$\begin{aligned}&\mathrm{Char}\left(A\left(G_5\right);\lambda\right)=\\&\lambda^{31}-32\lambda^{29}+453\lambda^{27}-2\lambda^{26}-3749\lambda^{25}+46\lambda^{24}+20191\lambda^{23}-456\lambda^{22}-74531\lambda^{21}\\&+2560\lambda^{20}+193407\lambda^{19}-8988\lambda^{18}-356043\lambda^{17}+20548\lambda^{16}+463363\lambda^{15}-30848\lambda^{14}\\&-419835\lambda^{13}+29904\lambda^{12}+257357\lambda^{11}-17904\lambda^{10}-101942\lambda^{9}+6096\lambda^{8}+24282\lambda^{7}\\&-1024\lambda^{6}-3074\lambda^{5}+64\lambda^{4}+156\lambda^{3}.\end{aligned}$$

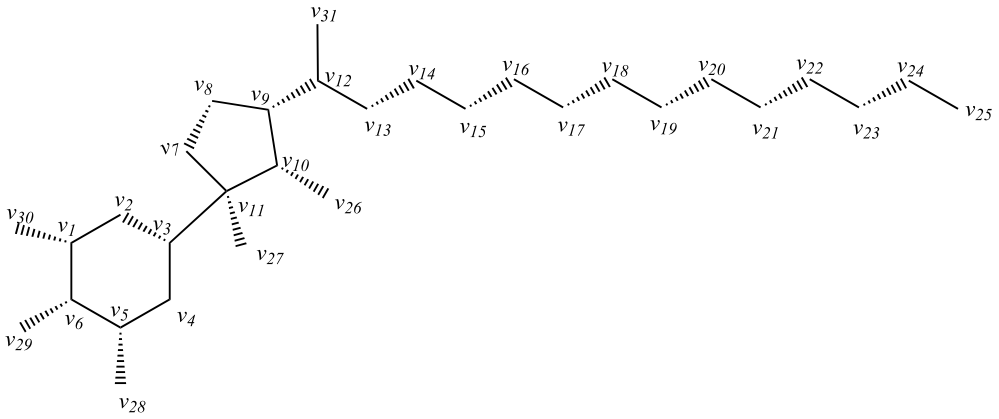

Fig. 5. Anticancer drug structure Convolutamide-A.

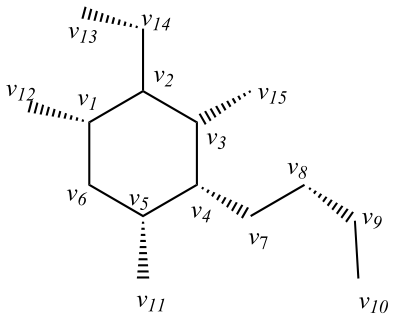

Fig. 6. Anticancer drug structure Convolutamine-F.

Now, by solving $\mathrm{Char}\left(A\left(G_5\right);\lambda\right)=0$ for λ, the eigenvalues $\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_5\right);\lambda\right)\right)$ of determined polynomials are

$$\begin{aligned}\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_5\right);\lambda\right)\right)=&\{0,0,0,-2.4356,-2.1859,-2.0217,-1.9405,-1.7932,-1.5856,\\&-1.4142,-1.3550,-1.2082,-1.0995,-0.7777,-0.5774,-0.4289,\\&-0.3963,0.3925,0.4613,0.7137,0.8663,1.0000,1.1379,1.3320,\\&1.4142,1.5357,1.7466,1.8915,1.9701,2.2327,2.5248\}.\end{aligned}$$

Observing that there are three count of $\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_1\right);\lambda\right)\right)=0$ and which is concluding that $\eta\left(G_5\right)=3$.

Furthermore, the Fig. 5, it is showing that there are fourteen counts of wavy edges and which is the matching number $M\left(G_5\right)$ of graph G_5. □

2.6. Results of matching number and nullity of Convolutamine-F anticancer drug structure

The order of graph obtained from Convolutamine-F $|V\left(G_6\right)|=15$, while the size is counted in $|E\left(G_6\right)|=15$. Moreover, the vertex and edge set is defined by

$$\begin{aligned}V(G_6)=&\{v_i:1\le i\le 15\},\\E(G_6)=&\{v_iv_j:i,j=1,2,\ldots,6\}\cup\{v_iv_j:i,j=7,8,\ldots,10\}\cup\{v_1v_{12},v_2v_{14},v_{13}v_{14},v_3v_{15},\\&v_4v_7,v_5v_{11},v_1v_6,v_3v_4\}\end{aligned}$$

Lemma 2.6. *Let G_6 be a graph obtained by an anticancer drug structure Convolutamine-F. Then $\eta\left(G_6\right)=3$.*

Proof. Observe that G_3 is the graph of Convolutamine-F an anticancer drug structure developed by some pendant vertices, single cycle of length eight. Fig. 6, shows that it is a bipartite graph. So to compute the nullity of G_6, we will follow the Equation (1). Fig. 6, it is showing that there is six-count of wavy edges and which is the matching number $M\left(G_6\right)$ of graph G_6. So by applying the definition of the nullity of a bipartite graph $\eta\left(G_6\right)=n-2M=15-2(6)=3$.

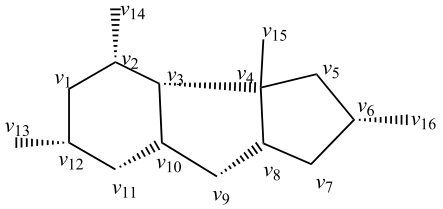

Fig. 7. Anticancer drug structure Convolutamydine-A.

Furthermore, by using the definition of nullity, we will determine the characteristics polynomial $\mathrm{Char}\left(A\left(G_6\right);\lambda\right)$ of the adjacency matrix $A\left(G_6\right)$ of graph G_6, characteristics polynomial is described as;

$$\mathrm{Char}\left(A\left(G_6\right);\lambda\right)=\lambda^{15}-15\lambda^{13}+85\lambda^{11}-233\lambda^{9}+323\lambda^{7}-211\lambda^{5}+50\lambda^{3}.$$

Now, by solving $\mathrm{Char}\left(A\left(G_6\right);\lambda\right)=0$ for λ, the eigenvalues $\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_6\right);\lambda\right)\right)$ of determined polynomials are

$$\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_6\right);\lambda\right)\right)=\{0,0,0,-2.3991,-1.8061,-1.5606,-1.4142,-1.0000,-0.7394,$$
$$0.7394,1.0000,1.4142,1.5606,1.8061,2.3991\}.$$

Observing that there are three values of $\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_2\right);\lambda\right)\right)=0$ and which is concluding that $\eta\left(G_6\right)=3$. □

2.7. Results of matching number and nullity of Convolutamydine-A anticancer drug structure

The order of graph obtained from Convolutamydine-A $|V\left(G_7\right)|=16$, while the size is counted in $|E\left(G_7\right)|=18$. Moreover, the vertex and edge set is defined by

$$V(G_7)=\{v_i:1\le i\le 16\},$$
$$E(G_7)=\{v_iv_j:i,j=1,2,\ldots,12\}\cup\{v_2v_{14},v_4v_{15},v_6v_{16},v_{12}v_{13},$$
$$v_3v_{10},v_4v_8,v_1v_{12}\}$$

Lemma 2.7. *Let G_7 be a graph obtained by an anticancer drug structure Convolutamydine-A. Then $\eta\left(G_7\right)=4$.*

Proof. Observe that G_7 is the graph of Convolutamydine-A an anticancer drug structure developed by some pendant vertices, two pentagons, and a single hexagon. Fig. 7, shows that it is not a bipartite graph. So to compute the nullity of G_7, we can not follow the Equation (1). Therefore, using the definition of nullity, we will determine the characteristics polynomial $\mathrm{Char}\left(A\left(G_7\right);\lambda\right)$ of the adjacency matrix $A\left(G_7\right)$ of graph G_7, characteristics polynomial is described as;

$$\mathrm{Char}\left(A\left(G_7\right);\lambda\right)=$$
$$\lambda^{16}-18\lambda^{14}+124\lambda^{12}-4\lambda^{11}-415\lambda^{10}+34\lambda^{9}+700\lambda^{8}-90\lambda^{7}-542\lambda^{6}+76\lambda^{5}+133\lambda^{4}.$$

Now, by solving $\mathrm{Char}\left(A\left(G_7\right);\lambda\right)=0$ for λ, the eigenvalues $\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_7\right);\lambda\right)\right)$ of determined polynomials are

$$\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_7\right);\lambda\right)\right)=\{0,0,0,0,-2.3958,-2.1148,-1.8930,-1.4927,-1.3535,-0.5272,$$
$$0.9296,1.1075,1.4992,1.5584,2.0790,2.6033\}.$$

Observing that there are four counts of the values of $\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_1\right);\lambda\right)\right)=0$ and which is concluding that $\eta\left(G_7\right)=4$.

Furthermore, the Fig. 7, it is showing that there are six counts of wavy edges and which is the matching number $M\left(G_7\right)$ of graph G_7. □

2.8. Results of matching number and nullity of Perfragilin-A anticancer drug structure

The order of graph obtained from Perfragilin-A $|V\left(G_8\right)|=17$, while the size is counted in $|E\left(G_8\right)|=18$. Moreover, the vertex and edge set is defined by

$$V(G_8)=\{v_i:1\le i\le 17\},$$
$$E(G_8)=\{v_iv_j:i,j=1,2,\ldots,13\}\cup\{v_1v_{11},v_{11}v_{12},v_5v_6,v_2v_{13},$$
$$v_5v_{14},v_6v_{15},v_9v_{16},v_{10}v_{17},v_1v_{10},v_3v_8\}$$

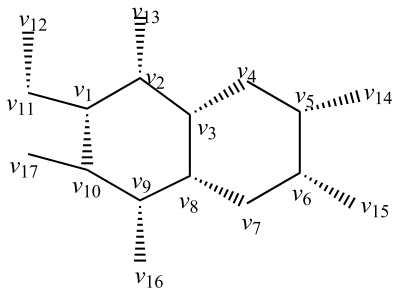

Fig. 8. Anticancer drug structure Perfragilin-A.

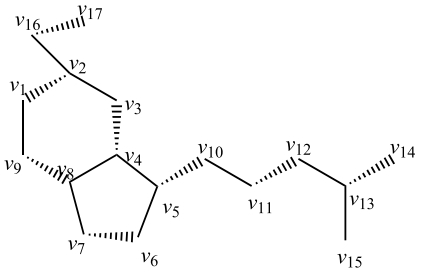

Fig. 9. Anticancer drug structure Melatonin.

Lemma 2.8. *Let G_8 be a graph obtained by an anticancer drug structure Perfragilin-A. Then $\eta\left(G_8\right)=1$.*

Proof. Observe that G_8 is the graph of Perfragilin-A an anticancer drug structure developed by some pendant vertices, two cycles of length eight. Fig. 8, shows that it is a bipartite graph. So to compute the nullity of G_8, we will follow the Equation (1). Fig. 8, it is showing that there is eight-count of wavy edges and which is the matching number $M\left(G_8\right)$ of graph G_8. So by applying the definition of the nullity of a bipartite graph $\eta\left(G_8\right)=n-2M=17-2(8)=1$.

Furthermore, by using the definition of nullity, we will determine the characteristics polynomial $\mathrm{Char}\left(A\left(G_8\right);\lambda\right)$ of the adjacency matrix $A\left(G_8\right)$ of graph G_8, characteristics polynomial is described as;

$$\mathrm{Char}\left(A\left(G_8\right);\lambda\right)=\lambda^{17}-18\lambda^{15}+126\lambda^{13}-442\lambda^{11}+833\lambda^{9}-836\lambda^{7}+413\lambda^{5}-82\lambda^{3}+4\lambda.$$

Now, by solving $\mathrm{Char}\left(A\left(G_8\right);\lambda\right)=0$ for λ, the eigenvalues $\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_8\right);\lambda\right)\right)$ of determined polynomials are

$$\begin{aligned}\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_8\right);\lambda\right)\right)=&\{0,-2.4978,-2.0576,-1.6713,-1.4839,-1.1368,-0.9232,\\&-0.5633,-0.2654,0.2654,0.5633,0.9232,1.1368,1.4839,\\&1.6713,2.0576,2.4978\}.\end{aligned}$$

Observing that there is a single value of $\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_8\right);\lambda\right)\right)=0$ and which is concluding that $\eta\left(G_8\right)=1$. □

2.9. Results of matching number and nullity of Melatonin anticancer drug structure

The order of graph obtained from Melatonin $|V\left(G_9\right)|=17$, while the size is counted in $|E\left(G_9\right)|=18$. Moreover, the vertex and edge set is defined by

$$\begin{aligned}V(G_9)=&\{v_i:1\le i\le 17\},\\E(G_9)=&\{v_iv_j:i,j=1,2,\ldots,9\}\cup\{v_iv_j:i,j=10,11,\ldots,14\}\cup\{v_{13}v_{15},v_4v_8,v_2v_{16},\\&v_{16}v_{17}\}\end{aligned}$$

Lemma 2.9. *Let G_9 be a graph obtained by an anticancer drug structure Melatonin. Then $\eta\left(G_9\right)=1$.*

Proof. Observe that G_9 is the graph of Melatonin an anticancer drug structure developed by some pendant vertices, a single pentagon, and a single hexagon. Fig. 9, shows that it is not a bipartite graph. So to compute the nullity of G_9, we can not follow the Equation (1). Therefore, using the definition of nullity, we will determine the characteristics polynomial $\mathrm{Char}\left(A\left(G_9\right);\lambda\right)$ of the adjacency matrix $A\left(G_9\right)$ of graph G_1, characteristics polynomial is described as;

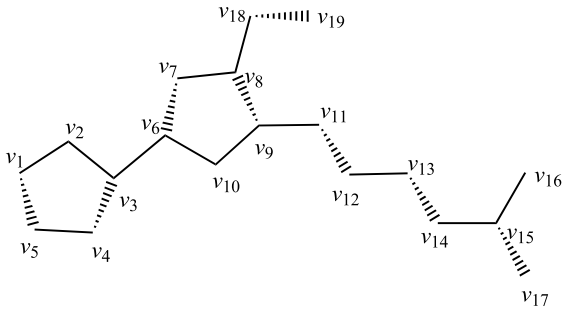

Fig. 10. Anticancer drug structure Tambjamine-K.

$$\begin{aligned}&\mathrm{Char}\left(A\left(G_9\right);\lambda\right)=\\&\lambda^{17}-18\lambda^{15}+129\lambda^{13}-2\lambda^{12}-474\lambda^{11}+20\lambda^{10}+957\lambda^{9}-72\lambda^{8}-1057\lambda^{7}+114\lambda^{6}\\&+598\lambda^{5}-80\lambda^{4}-144\lambda^{3}+20\lambda^{2}+8\lambda.\end{aligned}$$

Now, by solving $\mathrm{Char}\left(A\left(G_9\right);\lambda\right)=0$ for λ, the eigenvalues $\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_9\right);\lambda\right)\right)$ of determined polynomials are

$$\begin{aligned}\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_9\right);\lambda\right)\right)=&\{0,-2.2999,-2.0000,-1.7964,-1.6653,-1.1300,-1.0000,\\&-0.7151,-0.1949,0.4233,0.6396,1.0000,1.0888,1.4530,\\&1.8199,1.9558,2.4211\}.\end{aligned}$$

Observing that there is only a single value of $\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_9\right);\lambda\right)\right)=0$ and which is concluding that $\eta\left(G_9\right)=1$.

Furthermore, the Fig. 9, it is showing that there are eight counts of wavy edges and which is the matching number $M\left(G_9\right)$ of graph G_9. □

2.10. Results of matching number and nullity of Tambjamine-K anticancer drug structure

The order of graph obtained from Tambjamine-K $|V\left(G_{10}\right)|=19$, while the size is counted in $|E\left(G_{10}\right)|=20$. Moreover, the vertex and edge set is defined by

$$\begin{aligned}V(G_{10})=&\{v_i:1\le i\le 19\},\\E(G_{10})=&\{v_iv_j:i,j=1,2,\ldots,5\}\cup\{v_iv_j:i,j=6,7,\ldots,10\}\cup\{v_iv_j:i,j=11,12,\ldots,16\}\\&\cup\{v_3v_6,v_8v_{18},v_{18}v_{19},v_9v_{11},v_{15}v_{17}\}\end{aligned}$$

Lemma 2.10. *Let G_{10} be a graph obtained by an anticancer drug structure Tambjamine-K. Then $\eta\left(G_{10}\right)=1$.*

Proof. Observe that G_{10} is the graph of Tambjamine-K an anticancer drug structure developed by some pendant vertices, and two pentagons. Fig. 10, shows that it is not a bipartite graph. So to compute the nullity of G_{10}, we can not follow the Equation (1). Therefore, using the definition of nullity, we will determine the characteristics polynomial $\mathrm{Char}\left(A\left(G_{10}\right);\lambda\right)$ of the adjacency matrix $A\left(G_{10}\right)$ of graph G_{10}, characteristics polynomial is described as;

$$\begin{aligned}&\mathrm{Char}\left(A\left(G_{10}\right);\lambda\right)=\\&\lambda^{19}-20\lambda^{17}+164\lambda^{15}-4\lambda^{14}-714\lambda^{13}+52\lambda^{12}+1785\lambda^{11}-258\lambda^{10}-2581\lambda^{9}+612\lambda^{8}\\&+2045\lambda^{7}-710\lambda^{6}-755\lambda^{5}+360\lambda^{4}+71\lambda^{3}-54\lambda^{2}+6\lambda.\end{aligned}$$

Now, by solving $\mathrm{Char}\left(A\left(G_{10}\right);\lambda\right)=0$ for λ, the eigenvalues $\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_{10}\right);\lambda\right)\right)$ of determined polynomials are

$$\begin{aligned}\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_{10}\right);\lambda\right)\right)=&\{0,-2.1363,-2.1225,-1.9049,-1.6180,-1.5051,-1.2730,\\&-0.9461,-0.4990,0.1673,0.4002,0.6012,0.6180,1.0000,\\&1.3453,1.4991,1.9169,2.0555,2.4014\}.\end{aligned}$$

Observing that there is only a single value of $\mathrm{Eig}\left(\mathrm{Char}\left(A\left(G_{10}\right);\lambda\right)\right)=0$ and which is concluding that $\eta\left(G_{10}\right)=1$.

Furthermore, the Fig. 10, it is showing that there are eight counts of wavy edges and which is the matching number $M\left(G_{10}\right)$ of graph G_{10}. □

Table 1
Energy, positive-negative-Inertia and nullity for various anticancer drug structures.

G	$\eta(G)$	$p(G)$	$q(G)$	E
G_1	1	11	10	27.5929
G_2	0	12	6	14.3847
G_3	0	7	7	18.2550
G_4	0	13	13	33.6189
G_5	3	14	14	38.4390
G_6	3	6	6	17.8389
G_7	4	6	6	19.5540
G_8	1	8	8	21.1985
G_9	1	8	8	21.6032
G_{10}	1	10	8	24.0097

Table 2
Different parameters for various anticancer drug structures.

G	$\eta(G)$	$b_1(G)$	$cn(G)$
G_1	1	3	3
G_2	0	0	0
G_3	0	2	2
G_4	0	4	4
G_5	3	2	2
G_6	3	1	1
G_7	4	3	3
G_8	1	2	2
G_9	1	2	2
G_{10}	1	2	2

3. Conclusion and discussion

Some anticancer drug structures are studied namely, Amathas-Piramide-E, Carmustine, Caulibugulone-E, Aspidostomide-E, Convolutamide-A, Convolutamine-F, Convolutamydine-A, Perfragilin-A, Melatonin, and Tambjamine-K. All these structures are studied in terms of nullity, matching number, eigenvalues of adjacency matrix, and characteristics polynomials. As a result, Carmustine, Caulibugulone-E, Aspidostomide-E anticancer drug structures are stable, closed-shell molecules since their nullity is equal to zero (Table 1).

The first Betti number $b_1(G) = m + |C| - n$. It is also called the cyclomatic number a term introduced by [35]. While in [36], nullity termed referred as first Betti number or cyclomatic number ($cn(G)$). Table 2, compare nullity, first Betti number and cyclomatic number for anticancer drug structures.

From the comparison given in the Table 2, the first betti number and nullity is equal for G_2, otherwise all the anticancer drug structures have different nullity and first Betti number, somehow the count of cyclomatic number and first Betti number are same for all the structures. Moreover, further research direction can be considered for the structures of [37], in the context to this chosen topic.

CRediT authorship contribution statement

Ali. N. A. Koam, A. Ahmad, M. Azeem, Khalil Hadi Hakami, and Kashif Elahi: conceived and designed the experiments; performed the experiments; analyzed and interpreted the data; contributed reagents, materials, analysis tools or data; wrote the paper.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data included in article/supplementary material/referenced in article.

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