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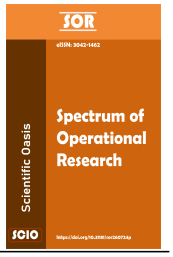

On the Anticancer Drug Structures and Their Locating Numbers

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ABSTRACT

Cancer is the rapid proliferation of unwanted cells in the body. Carcinogens are chemicals that can cause cancer. A carcinogen is a type of chemical compound found in cigarette smoke. It has the ability to spread to many parts of the body. Some of the signs and symptoms of this disease include lumps, irregular bleeding, chronic cough, weight gain or loss, and so on. Tobacco chewing is a major factor in this deadly disease. Obesity, a poor diet, physical inactivity, and increased alcohol consumption are also contributing factors. Anticancer drugs are used to treat this condition. In this work, we studied some anticancer medicines in terms of locating sets, where a locating set is a set used to resolve the entire atom set of a graph in a unique way, allowing each atom to be accessed independently. By locating numbers, a particular resolving set is chosen, and this resolving set, or locating set, transforms the entire structure into a unique form. This helps in studying the chemical structure in greater depth and detail. Thus, the locating number helps to understand the chemical structure more comprehensively. The locating number is part of resolvability parameters and also plays a role in developing a unique way to access each node or vertex of a network. When each vertex is easily accessible with a unique code, working with a network becomes easier. Therefore, this method makes the structures of anticancer drugs more understandable and allows researchers to further extend their work on these structures in medical diagnostics.

Keywords:
Anticancer Drug Structures; Vertex Metric Dimension; Locating Number; Locating Set.

1. Introduction

The explosive growth of unwanted cells in the human body is cancer. Symptom substances are classified as carcinogens. A carcinogen is an organic compound found in cigarette smoke that contains specific components. It has the ability to spread to other places of the body. Some of the signs and symptoms of this illness cause a lump, abnormal bleeding, a prolonged cough, weight gain or loss, etc.

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Chewing tobacco is one of the main causes of this cancerous condition. Obesity, poor diet, laziness, and increased alcohol consumption are all factors. Several treatments for this deadly disease, like surgery, radiation, and chemotherapy, can be used to treat it. Hormone therapy, targeted therapy, and other options are available. In these articles [**1**, **2**, **3**], anticancer medications are used to treat the so-called cancer sickness.

In [**4**], authors discussed some medicinal structures of COVID-19 antiviral disease in terms of graph theoretical parameters. This work motivates us to study some anti-cancer drugs given in [**5**], in terms of some graph theoretical parameters such as metric dimension. For this study, we need some assumptions to take care of before investigations or any type of calculations. In theoretical chemistry, drug structures are denoted by a molecular graph, an atom of a structure called a vertex, and an edge labeled from the links between atoms. Let $D(A, L)$ be a molecular graph of drug structure with atoms set A and links set L. All the chosen graphs or drug structures are simple i.e. without any vertex to itself or any edge and without two edges in any two vertices. For further assumptions, basic definitions, and theoretical study of the molecular graphs we refer to see [**6**, **7**, **8**, **9**].

1.1 Literature Review

The research work of [**10**], stated the metric basis of and generalization of windmill graphs. In [**11**], authors studied the metric dimension graph's modified form and defined this attribute using two variables. In [**12**], authors computed metrics and their upper bounds on some generalized families of graphs. In [**13**], authors discussed the generalization and concept of metric in polycyclic hydrocarbons. In [**14**], the Rooted product was used to create the symmetric graphs generated by the author, along with metrics and their generalizations were explored. In [**15**], authors give the idea of generalization and metric dimension in Hollow Coronoid. In [**16**], in particular, creators derived metric parameters for the structure of quartz without taking into account the pendant nodes beyond the circle provided a way to determine the resolvability of quartz structure. In [**17**], authors detail the rough graphs on the topics of metric dimensions and their generalized parameters. In [**18**], authors discussed hereditary bipartite and computing the metric basis of this generalized class of complex networks. From [**19**], authors gave the idea of pseudo-valuation on KU-algebras and investigated, The relationship between pseudo-valuations and KU-algebras and their generalizations. More recent articles on chemical networks and metric parameters of different chemical structures and networks are available in [**20**, **21**, **22**, **23**, **24**, **25**, **26**, **27**, **28**]. Some interesting results can be found in [**29**, **30**, **31**].

1.2 Methodology: Preliminaries and Background

In this section, we will discuss the methodology of our chosen topic in the form of pure mathematical definitions. The very first, the locating set is laid down its foundation by Slater in 1975 [**32**], and later two independent researchers Melter and Harary 1976 renamed this parameter from locating set to resolving set by Harary et al. in [**33**]. For more advance study of this topic we refer to see [**34**, **35**, **36**, **37**, **38**] and its applications one can see [**39**, **40**, **41**, **42**]. After the applied study of this topic, in 2000 Chartrand again renamed this parameter for pure graph theoretical study and called as metric basis [**43**, **44**]. Now given below are the basic and necessary concepts of this study.

Definition 1.1. *In [4]*" Suppose $D(A(D), L(D))$ is a chemical structure of undirected graph with $A(D)$ is called as set of principal nodes (vertex set) and the set of branches (edge set) is $L(D)$. The principal nodes $v_1, v_2 \in A(D)$, of distance is denoted as $d(v_1, v_2)$ is the minimum count of branches between $v_1 - v_2$ path."

Definition 1.2. *In [4]* "Suppose $R \subset A(D)$ is the subset of principal nodes set and defined as $R =$

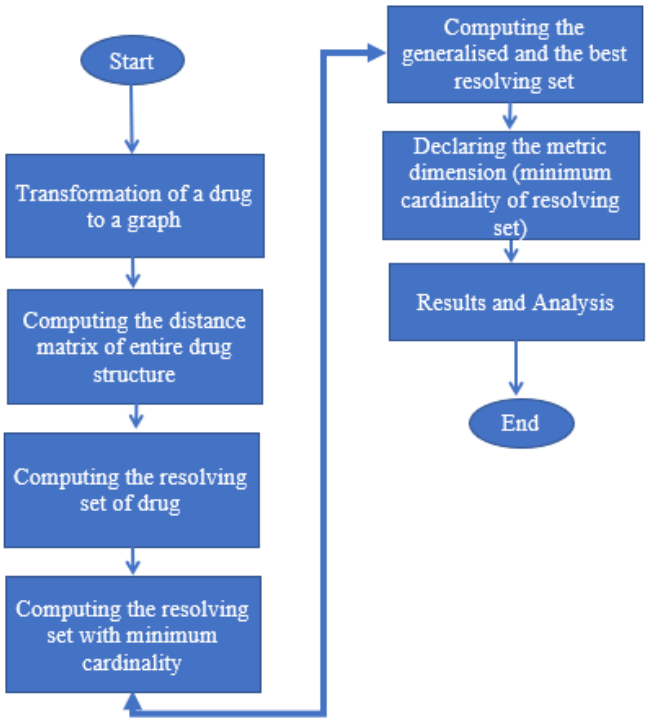

Fig. 1. Flowchart of metric dimension

$\{v_1, v_2, \ldots, v_s\}$, and let a principal node $v \in A(D)$. The identification or locations $r(v|R)$ of a principal node v with respect to R is actually a $s-$ordered distances $(d(v, v_1), d(v, v_2), \ldots, d(v, v_s))$. If each principal node from $A(D)$ have unique identification according to the ordered subset R, then this subset renamed as a resolving set of network D. The minimum numbers of the elements in the subset R is actually the metric dimension of D and it is denoted by the term $dim(D)$."

For further understanding its flowchart given in the Figure 1.

Due to its vast applied look and usage, there are many abstract applications are also found since 1975, such as combinatorial optimization by Sebo and Tainner in [**45**], robot roving by Khuller et al. in [**46**], complicated games, image processing, pharmaceutical chemistry, the polymer sector, and the electric field are just a few areas where the metric dimension is used. One can find all of these applications in [**47**, **48**] by Nadeem et al. and Ahmad et al. Robot roving is related to the idea of applications of a set of vertices partitioning according to metrics, whereas the Djokovic Winkler relationship [**49**], network identification and confirmation, chemistry [**50**], Puzzles with argument [**51**], the dimensions of a structure are relevant for visual analyzing, pattern identification, and complex data structures [**52**]. There is some other interesting literature and links to the application [**53**].

In the above literature, one can see that all the work is on either general graphs or on the chemical networks. There is no work on the disease or medicinal based structures, therefore we choose to work on the anticancer disease structures. We have chosen molecular graphs of Amathaspiramide E, Carmustine, Caulibugulone E, Aspidostomide E, Convolutamide A, Convolutamine F, Convolutamydine A, Perfragilin A, Melatonin, and Tambjamine K medicinal structures to study metric dimension of locating numbers.

1.3 Application of resolving sets in chemistry

Enantiomers, which are chiral compounds that exist as mirror images of each other, are separated in chemistry using resolving sets, also known as resolving agents or resolving reagents. It is feasible

to separate individual enantiomers from a racemic mixture (a 50:50 mixture of both enantiomers) utilising resolving sets. Here are some chemistry examples where resolving sets is used:

Resolving sets are frequently employed in chiral chromatography, a method that divides enantiomers according to how they interact with a chiral stationary phase. As the mixture moves through the column, the enantiomers interact differently with the chiral stationary phase, causing their separation. The resolving set is then added to the mobile phase.

Resolving sets are used in enantioselective synthesis to synthesise a chiral compound's single enantiomer with high selectivity. A resolving set can be used as a catalyst or reagent to regulate the stereochemistry of a reaction and produce a certain enantiomer. Resolving sets can be used to separate the enantiomers during the crystallisation process. The resolving set preferentially interacts with one enantiomer, enabling its separation from the racemic mixture, by creating diastereomeric salts or co-crystals with it.

Derivatization: To transform enantiomers into diastereomers, which have different physical characteristics, derivatization procedures frequently use resolving sets. The resulting diastereomers can be divided according to their various characteristics, such as solubility or boiling point, by treating the racemic mixture with a resolving set. Nuclear magnetic resonance (NMR) spectroscopy: Resolving sets can be used to distinguish between enantiomers. The enantiomeric makeup of a mixture can be determined by creating diastereomeric compounds with the resolving set because the resulting diastereomers' NMR spectra show unique signals.

These are only a few instances of how resolving sets are used in chemistry. The nature of the enantiomers and the preferred separation technique determine the precise choice of resolving set.

In this study, we looked at a few anti-cancer drugs from the perspective of locating sets, which are sets that organise the whole set of atoms in a graph in a way that makes it possible to access each atom separately. A specific resolving set is picked by locating numbers, and this resolving set or locating set transforms the entire structure into a distinctive shape, making it easier to examine the chemical structure in greater depth and detail. So, we may conclude that the locating number aids in a more thorough and detailed understanding of the chemical structure.

2. Main Results: Anticancer Drugs and their Locating sets

The discipline of finding and developing anticancer drugs can benefit from the use of graph theory, a part of mathematics. Several applications of graph theory to anticancer medications are listed below:

Molecular graphs: The structure of molecules, including anticancer medications, can be represented and examined using graph theory. Atoms and chemical bonds are represented as vertices and edges, respectively, in the molecular graph theory. Researchers can investigate the molecular connectivity, symmetry, and characteristics of anticancer medications by using graph algorithms and metrics. This knowledge can help in understanding how they interact with biological targets and making predictions about how effective they will be.

Drug-Target Interaction Networks: Graph theory can be employed to construct and analyze drug-target interaction networks. In these networks, nodes represent drugs and targets (e.g., proteins or receptors), while edges represent interactions between them. Graph algorithms can be applied to identify key targets, predict drug-target interactions, and uncover potential therapeutic targets for anticancer drugs. This network-based approach facilitates the exploration of complex relationships between drugs, targets, and pathways.

Drug Combinations: Combination therapy, which combines several medications to increase effectiveness and combat drug resistance, is a frequent technique in the treatment of cancer. Drug-drug interaction networks, where nodes stand for individual drugs and edges for interactions (such as syner-

gistic or antagonistic effects), can be analysed using graph theory. Graph algorithms can predict synergistic medication pairs, analyse network connectivity, identify subgraphs, and determine the best drug combinations. Pharmacophore Modelling: Pharmacophore modelling entails finding important molecular characteristics accountable for a drug's interaction with a target. Researchers can analyse spatial correlations, pinpoint crucial characteristics, and create structure-activity relationships for anticancer medications by visualising the pharmacophore as a graph. This information is useful for designing and perfecting novel medication candidates.

treatment Resistance Analysis: Graph theory can be used to understand the mechanisms underlying treatment resistance in cancer. Researchers can learn more about the underlying resistance mechanisms by building molecular interaction networks involving drug-resistant proteins, genetic alterations, and signalling pathways. The creation of new anticancer methods can be aided by the identification of key nodes or pathways implicated in drug resistance through graph-based research. These examples show how graph theory can be used to research anticancer medications, comprehend their mechanisms of action, and enhance the drug discovery and development processes by offering insightful analyses and computational tools.

We labelled the molecular graph of Amathaspiramide E drug with D_1. The Amathaspiramide E is one of an anticancer drug with molecular formula $C_{15}H_{16}Br_2N_2O_3$, and with molecular weight is 432.11. In graph theoretical study its order (or count of atoms) is $D_1 = 22$ and the size (or count of links) is $D_1 = 24$. The atom and links sets of D_1 as displayed just below. Moreover, the Figure 2, shows the graph of molecules of Amathaspiramide E.

$$\begin{aligned} A(D_1) =& \{v_\zeta : \zeta = 1, 2, \ldots, 22\}, \\ L(D_1) =& \{v_\zeta v_{\zeta+1} : \zeta = 1, 2, \ldots, 6, 8, 9, \ldots, 14\} \cup \{v_{11}v_{15}, \\ & v_{11}v_{16}, v_8v_{16}, v_6v_{12}, v_5v_{19}, v_{13}v_{20}, v_{14}v_{21}, v_{15}v_{22}, \\ & v_1v_{17}, v_3v_{18}, v_2v_7\}. \end{aligned}$$

Theorem 2.1. *Let D_1 be a molecular graph of Amathaspiramide E anticancer drug. Then $dim(D_1)$ is equal to two.*

Proof. To show that $dim(D_1) = 2$, suppose a locating set $R = \{v_8, v_{19}\}$. Using the Definition 1.1 to see the shortest distances and then arranging in the form given in the Definition 1.2, we constructed the following representations of the entire vertex set of (D_1), which is $r(v_\zeta|R) = (d(v_\zeta, v_8), d(v_\zeta, v_{19}))$.

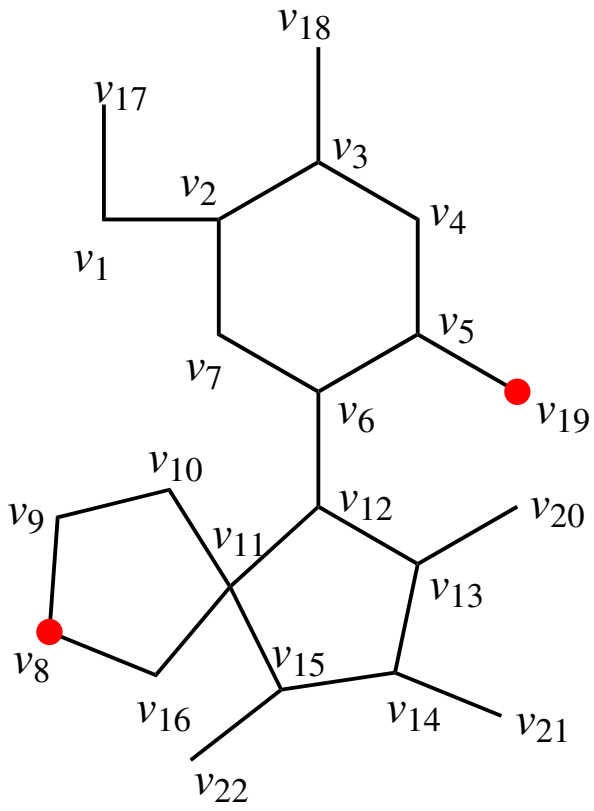

Fig. 2. Molecular graph of Amathaspiramide E with its resolving atoms

$$r(v_\zeta|R) = \begin{cases} (8-\zeta, 6-\zeta), & \text{if } \zeta = 1,2; \\ (10-\zeta, 6-\zeta), & \text{if } \zeta = 3,4,5; \\ (10-\zeta, \zeta-4), & \text{if } \zeta = 6; \\ (5, \zeta-4), & \text{if } \zeta = 7; \\ (\zeta-8, 6), & \text{if } \zeta = 8; \\ (\zeta-8, 15-\zeta), & \text{if } \zeta = 9,10; \\ (\zeta-9, 15_\zeta), & \text{if } \zeta = 11,12; \\ (\zeta-9, 4), & \text{if } \zeta = 13; \\ (18-\zeta, 5), & \text{if } \zeta = 14,15,16; \\ (8, 6), & \text{if } \zeta = 17; \\ (8, 4), & \text{if } \zeta = 18; \\ (25-\zeta, 0), & \text{if } \zeta = 19; \\ (25-\zeta, 5), & \text{if } \zeta = 20; \\ (26-\zeta, 6), & \text{if } \zeta = 21,22; \end{cases}$$

As a result, it follows in the form of a demonstration of the facts stated above that $dim(D_1) \leq 2$ since each and every vertex of (D_1) contain the distinctive representations for resolving set R. Instead of bound, we will now use the contradiction approach for exactness, implies $dim(D_1) > 2$, which is $dim(D_1) = 1$. It is not true, because the only the path graph allows for metric dimension one. and chosen graph is not a path graph. So, $dim(D_1) = 2$, which is required result. □

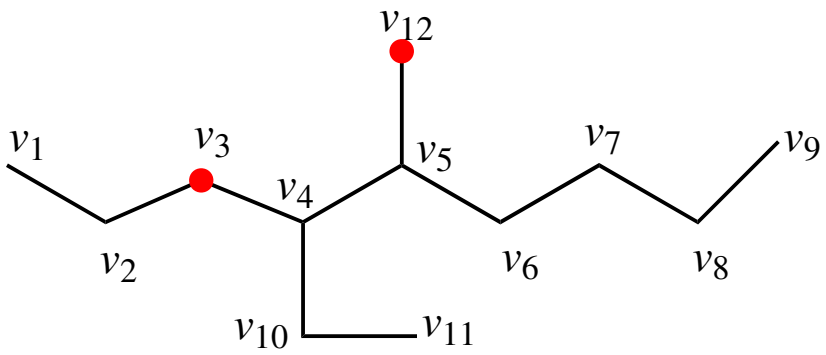

Fig. 3. Molecular graph of Carmustine with its resolving atoms

We labelled the molecular graph of Carmustine drug with D_2. The Carmustine is one of an anticancer drug, in graph theoretical study its order (or count of atoms) is $D_2 = 12$ and the size (or count of links) is $D_2 = 11$. The atom and links sets of D_2 are given below. In addition, the Figure 3, shows the chemical model of Carmustine.

$$\begin{aligned} A(D_2) =& \{v_\zeta : \zeta = 1, 2, \ldots, 12\}, \\ L(D_2) =& \{v_\zeta v_{\zeta+1} : \zeta = 1, 2, \ldots, 8, 10\} \cup \{v_5 v_{12}, v_4 v_{10}\}. \end{aligned}$$

Theorem 2.2. *Let D_2 be a molecular graph of Carmustine anticancer drug. Then $dim(D_2) = 2$.*

Proof. To prove that $dim(D_2) = 2$, assume a locating set $R = \{v_3, v_{12}\}$. Using the Definition 1.1 to see the shortest distances and then arranging in the form given in the Definition 1.2, we constructed the following representations of the entire vertex set of (D_2), which is $r(v_\zeta|R) = (d(v_\zeta, v_3), d(v_\zeta, v_{12}))$.

$$r(v_\zeta|R) = \begin{cases} (3-\zeta, 6-\zeta), & \text{if } \zeta = 1, 2, 3; \\ (\zeta-3, 6-\zeta), & \text{if } \zeta = 4, 5; \\ (\zeta-3, \zeta-4), & \text{if } \zeta = 7, 8, 9; \\ (2, \zeta-7), & \text{if } \zeta = 10; \\ (3, \zeta-7), & \text{if } \zeta = 11; \\ (3, 0), & \text{if } \zeta = 12; \end{cases}$$

As a result, it follows in the form of a representation from the reasons above that $dim(D_2) \leq 2$ as a result of all the vertex (D_2) are represented in an distinctive way with in terms of resolving set R. Instead of bound, we will now use the contradiction approach for exactness, implies $dim(D_2) > 2$, which is $dim(D_2) = 1$. It is not true, due to the fact that the path graph is the only metric dimension one that may exist and chosen graph is not a path graph. So, $dim(D_2) = 2$, which is required result. □

We labelled the molecular graph of Caulibugulone E drug with D_3. The Caulibugulone E is one of an anticancer drug, in graph theoretical study its order (or count of atoms) is $D_3 = 14$ and the size (or count of links) is $D_3 = 15$. The atom and links sets of D_3 are shown below. Meanwhile, the Figure 4, showing a chemical structure of Caulibugulone E.

$$\begin{aligned} A(D_3) =& \{v_\zeta : \zeta = 1, 2, \ldots, 14\}, \\ L(D_3) =& \{v_\zeta v_{\zeta+1} : \zeta = 1, 2, \ldots, 11\} \cup \{v_4 v_{14}, v_3 v_{12}, v_5 v_{10}, \\ & v_{11} v_{13}\}. \end{aligned}$$

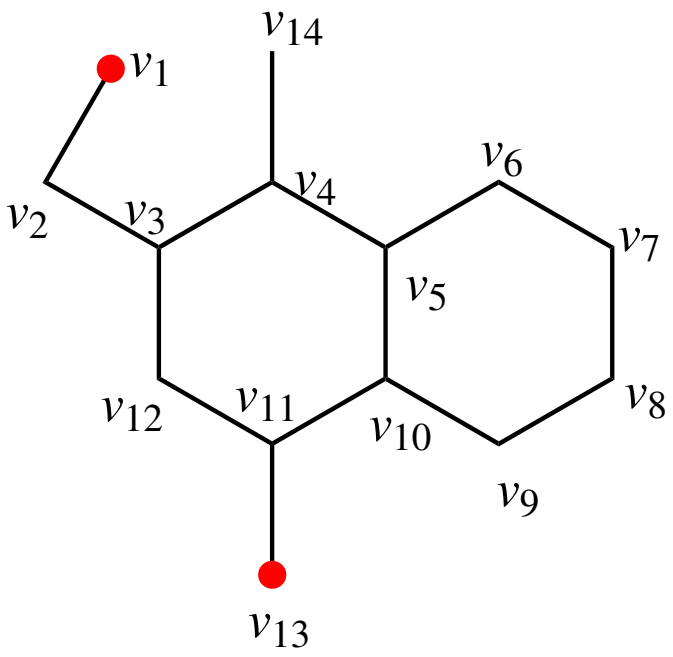

Fig. 4. Molecular graph of Caulibugulone E with its resolving atoms

Theorem 2.3. *Let D_3 be a molecular graph of Caulibugulone E anticancer drug. Then $dim(D_3) = 2$.*

Proof. To prove that $dim(D_3) = 2$, a locating set is assumed $R = \{v_1, v_{13}\}$. Using the Definition 1.1 to see the shortest distances and then arranging in the form given in the Definition 1.2, we constructed the following representations of the entire vertex set of (D_3), which is $r(v_\zeta|R) = (d(v_\zeta, v_1), d(v_\zeta, v_{13}))$.

$$r(v_\zeta|R) = \begin{cases} (\zeta - 1, 6 - \zeta), & \text{if } \zeta = 1, 2, 3; \\ (\zeta - 1, 4), & \text{if } \zeta = 4; \\ (\zeta - 1, \zeta - 2), & \text{if } \zeta = 5, 6, 7; \\ (\zeta - 1, 12 - \zeta), & \text{if } \zeta = 8; \\ (15 - \zeta, 12 - \zeta), & \text{if } \zeta = 9, 10, 11; \\ (15 - \zeta, 2), & \text{if } \zeta = 12; \\ (18 - \zeta, 0), & \text{if } \zeta = 13; \\ (18 - \zeta, 5), & \text{if } \zeta = 14; \end{cases}$$

As a result, it follows in the form of a representation for all the explanations previously stated, $dim(D_3) \leq 2$ due to the fact that all of the vertices of (D_3) are represented in a unique way with regard to resolving set R.Instead of bound, we will now use the contradiction approach for exactness, implies $dim(D_3) > 2$, which is $dim(D_3) = 1$. It is not true, because the one metric dimension is only possible of the path graph and chosen graph is not a path graph. So, $dim(D_3) = 2$, which is required result. □

We labelled the molecular graph of Aspidostomide E drug with D_4. The Aspidostomide E is one of an anticancer drug, in graph theoretical study its order (or count of atoms) is $D_4 = 26$ and the size (or count of links) is $D_4 = 29$. The atom and links sets of D_4 you'll find them below. Additionally, the

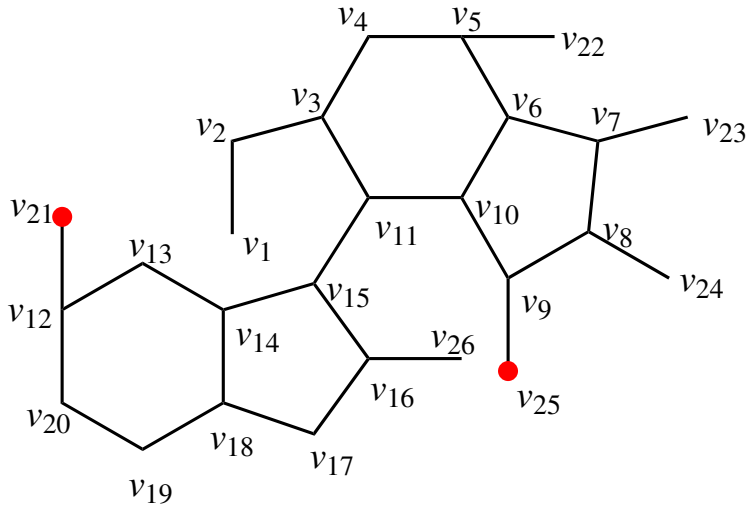

Fig. 5. Molecular graph of Aspidostomide E with its resolving atoms

Figure 5, shows the molecular graph of Aspidostomide E.

$$\begin{aligned}A(D_4) =&\{v_\zeta : \zeta = 1, 2, \ldots, 26\},\\ L(D_4) =&\{v_\zeta v_{\zeta+1} : \zeta = 1, 2, \ldots, 10, 12, 13, \ldots, 19\} \cup \{v_3v_{11},\\ &v_5v_{22}, v_7v_{23}, v_8v_{24}, v_9v_{25}, v_6v_{10}, v_{11}v_{15}, v_{16}v_{26},\\ &v_{14}v_{18}, v_{12}v_{21}, v_{12}v_{20}\}.\end{aligned}$$

Theorem 2.4. *Let D_4 be a molecular graph of Aspidostomide E anticancer drug. Then $dim(D_4) = 2$.*

Proof. To obtained that $dim(D_4) = 2$, consider a locating set $R = \{v_{21}, v_{25}\}$. Using the Definition 1.1 to see the shortest distances and then arranging in the form given in the Definition 1.2, we constructed the following representations of the entire vertex set of (D_4), which is $r(v_\zeta|R) = (d(v_\zeta, v_{21}), d(v_\zeta, v_{25}))$.

$$r(v_\zeta|R) = \begin{cases}(9-\zeta, 7-\zeta), & \text{if } \zeta = 1, 2, 3;\\ (\zeta+3, 9-\zeta), & \text{if } \zeta = 4, 5;\\ (\zeta+1, 9-\zeta), & \text{if } \zeta = 6;\\ (\zeta+1, 10-\zeta), & \text{if } \zeta = 7;\\ (16-\zeta, 10-\zeta), & \text{if } \zeta = 8, 9;\\ (16-\zeta, \zeta-8), & \text{if } \zeta = 10, 11;\\ (\zeta-11, 19-\zeta), & \text{if } \zeta = 12, 13 \ldots 15;\\ (\zeta-11, \zeta-11), & \text{if } \zeta = 16;\\ (22-\zeta, \zeta-11), & \text{if } \zeta = 17;\\ (22-\zeta, \zeta-12), & \text{if } \zeta = 18, 19, 20;\\ (0, 8), & \text{if } \zeta = 21;\\ (9, 27-\zeta), & \text{if } \zeta = 22, 23, 24;\\ (8, 0), & \text{if } \zeta = 25;\\ (6, 6), & \text{if } \zeta = 26;\end{cases}$$

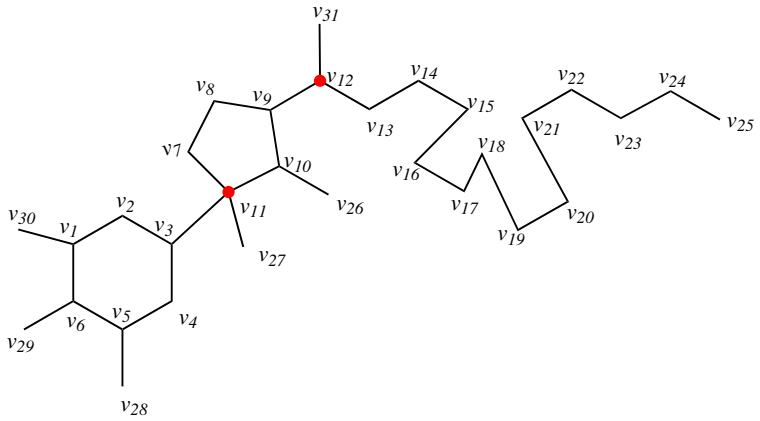

Fig. 6. Molecular graph of Convolutamide A with its resolving atoms

The representation that results from the above-mentioned causes is that $dim(D_4) \leq 2$ since each of the vertices of (D_4) have the unique representations with respect to resolving set R. Instead of bound, we will now use the contradiction approach for exactness, implies $dim(D_4) > 2$, which is $dim(D_4) = 1$. It is incorrect because the chosen graph is not a path graph and the metric dimension 1 only is feasible for path graphs. So, $dim(D_4) = 2$, which is required result. □

We labelled the molecular graph of Convolutamide A drug with D_5. The Convolutamide A is one of an anticancer drug, in graph theoretical study its order (or count of atoms) is $D_5 = 31$ and the size (or count of links) is $D_5 = 32$. The atom and links sets of D_5 appear below. Additionally, the Figure 6, shows the molecular graph of Convolutamide A.

$$\begin{aligned} A(D_5) =& \{v_\zeta : \zeta = 1, 2, \ldots, 31\}, \\ L(D_5) =& \{v_\zeta v_{\zeta+1} : \zeta = 1, 2, \ldots, 5, 6, \ldots 10, 12, 13 \ldots, 24\} \\ & \cup \{v_1v_{30}, v_1v_6, v_6v_{29}, v_5v_{28}, v_3v_{11}, v_{11}v_{27}, v_{10}v_{26}, \\ & v_7v_{11}, v_9v_{12}, v_{12}v_{31}\}. \end{aligned}$$

Theorem 2.5. *Let D_5 be a molecular graph of Convolutamide A anticancer drug. Then $dim(D_5) = 2$.*

Proof. To prove that $dim(D_5) = 2$, assume a locating set $R = \{v_{11}, v_{12}\}$. Using the Definition 1.1 to see the shortest distances and then arranging in the form given in the Definition 1.2, we constructed the following representations of the entire vertex set of (D_5), which is $r(v_\zeta|R) = (d(v_\zeta, v_{11}), d(v_\zeta, v_{12}))$.

$$r(v_\zeta|R) = \begin{cases} (3, \zeta), & \text{if } \zeta = 1; \\ (6-\zeta, \zeta), & \text{if } \zeta = 2, 3, 4; \\ (6-\zeta, 8-\zeta), & \text{if } \zeta = 5; \\ (\zeta-4, 8-\zeta), & \text{if } \zeta = 6; \\ (\zeta-4, \zeta-2), & \text{if } \zeta = 7.8, \ldots, 10; \\ (0, 4), & \text{if } \zeta = 11; \\ (4, 0), & \text{if } \zeta = 12; \\ (19-\zeta, 17-\zeta), & \text{if } \zeta = 13, 14; \\ (19-\zeta, 4), & \text{if } \zeta = 15; \end{cases}$$

As a result, It follows as a justification based on the above-mentioned metrics that $dim(D_5) \leq 2$ because every vertices of (D_5) have distinct representations for resolving sets R. Instead of bound, we

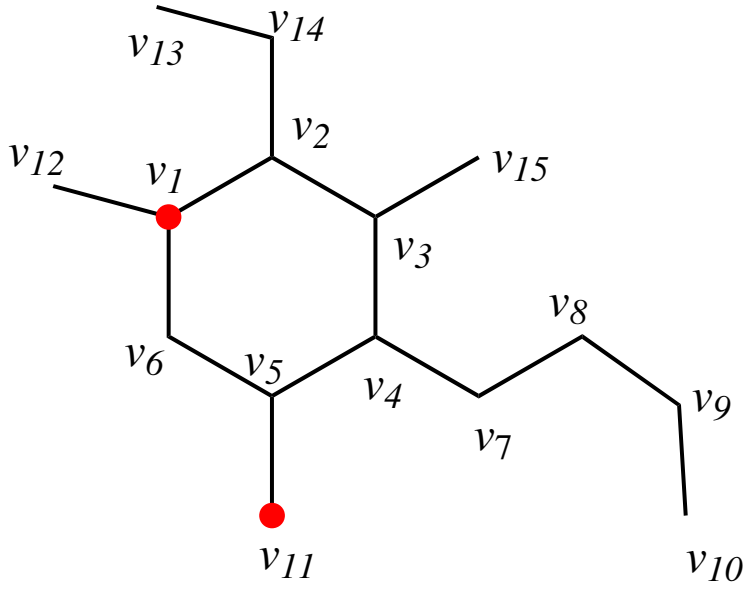

Fig. 7. Molecular graph of Convolutamine F with its resolving atoms

will now use the contradiction approach for exactness, implies $dim(D_5) > 2$, which is $dim(D_5) = 1$. It is not true,because only the path graph can support the metric dimension one and chosen graph is not a path graph. So, $dim(D_5) = 2$, which is required result. □

We labelled the molecular graph of Convolutamine F drug with D_6. The Convolutamine F is one of an anticancer drug, in graph theoretical study its order (or count of atoms) is $D_6 = 15$ and the size (or count of links) is $D_6 = 15$. The sets of linkages and atoms for D_6 are displayed below. The Figure 7, also displays the chemical graph of Convolutamine F.

$$\begin{aligned} A(D_6) =& \{v_\zeta : \zeta = 1, 2, \ldots, 15\}, \\ L(D_6) =& \{v_\zeta v_{\zeta+1} : \zeta = 1, 2, \ldots, 5, 7, 8, 9, 13\} \cup \{v_1v_{12}, v_2v_{14}, \\ & v_3v_{15}, v_4v_7, v_5v_{11}, v_1v_6\}. \end{aligned}$$

Theorem 2.6. *Let D_6 be a molecular graph of Convolutamine F anticancer drug. Then $dim(D_6) = 2$.*

Proof. To prove that $dim(D_6) = 2$, assume a locating set $R = \{v_1, v_{11}\}$. Using the Definition 1.1 to see the shortest distances and then arranging in the form given in the Definition 1.2, we constructed the following representations of the entire vertex set of (D_6), which is $r(v_\zeta|R) = (d(v_\zeta, v_1), d(v_\zeta, v_{11}))$.

$$r(v_\zeta|R) = \begin{cases} (6-\zeta, \zeta+1), & \text{if } \zeta = 1, 2, \ldots, 4; \\ (|\zeta-7|, \zeta+1), & \text{if } \zeta = 5; \\ (|\zeta-7|, 13-\zeta), & \text{if } \zeta = 6, 7, \ldots, 13; \\ (5, 4), & \text{if } \zeta = 14; \\ (18-\zeta, 6), & \text{if } \zeta = 15; \\ (18-\zeta, 8), & \text{if } \zeta = 16; \end{cases}$$

As a result, it follows in the due to the fact that all of the vertices of "(D_6) have unique representations with respect to the resolving set R, it can be concluded from the above justifications that $dim(D_6) \leq 2$.

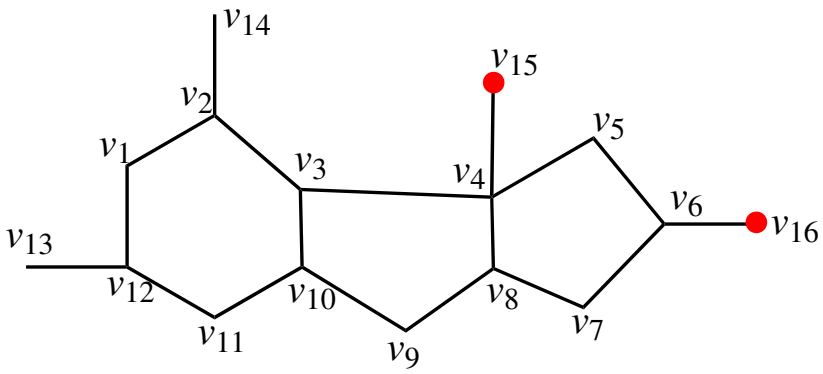

Fig. 8. Molecular graph of Convolutamydine A with its resolving atoms

Instead of bound, we will now use the contradiction approach for exactness, implies $dim(D_6) > 2$, which is $dim(D_6) = 1$. It is not true, since the chosen graph is not a path graph and the metric dimension one is only possible for the path graph. So, $dim(D_6) = 2$, which is required result. □

We labelled the molecular graph of Convolutamydine A drug with D_7. The Convolutamydine A is one of an anticancer drug, in graph theoretical study its order (or count of atoms) is $D_7 = 16$ and the size (or count of links) is $D_7 = 18$. The atom and links sets of D_7appear below. Additionally, Figure 8, displays the chemical graph of Convolutamydine A.

$$\begin{aligned} A(D_7) =& \{v_\zeta : \zeta = 1, 2, \ldots, 16\}, \\ L(D_7) =& \{v_\zeta v_{\zeta+1} : \zeta = 1, 2, \ldots, 12\} \cup \{v_2v_{14}, v_4v_{15}, v_6v_{16}, \\ & v_3v_{10}, v_4v_8, v_1v_{12}\}. \end{aligned}$$

Theorem 2.7. *Let D_7 be a molecular graph of Convolutamydine A anticancer drug. Then $dim(D_7) = 2$.*

Proof. To prove that $dim(D_7) = 2$, assume a locating set $R = \{v_{15}, v_{16}\}$. Using the Definition 1.1 to see the shortest distances and then arranging in the form given in the Definition 1.2, we constructed the following representations of the entire vertex set of (D_7), which is $r(v_\zeta|R) = (d(v_\zeta, v_{15}), d(v_\zeta, v_{16}))$.

$$r(v_\zeta|R) = \begin{cases} (10-\zeta, 4-\zeta), & \text{if } \zeta = 1, 2; \\ (10-\zeta, \zeta), & \text{if } \zeta = 3, 4, 5; \\ (\zeta, \zeta), & \text{if } \zeta = 6; \\ (\zeta, 13-\zeta), & \text{if } \zeta = 7; \\ (\zeta-1, 13-\zeta), & \text{if } \zeta = 8, 9; \\ (14-\zeta, \zeta-4), & \text{if } \zeta = 10, 11, \ldots 13; \\ (2, \zeta-4), & \text{if } \zeta = 14; \\ (0, 10), & \text{if } \zeta = 15; \\ (\zeta-7, 17-\zeta), & \text{if } \zeta = 16; \end{cases}$$

As a result, it follows in the form of a representation derived from all of the above factors $dim(D_7) \leq 2$ due to the fact that each and every vertex of (D_7) has a unique representation in terms of the resolving set R. Instead of bound, we will now use the contradiction approach for exactness, implies $dim(D_7) > 2$, which is $dim(D_7) = 1$. The metric dimension one is only conceivable for path graphs, which chosen graph is not, hence this statement is invalid. So, $dim(D_7) = 2$, which is required result. □

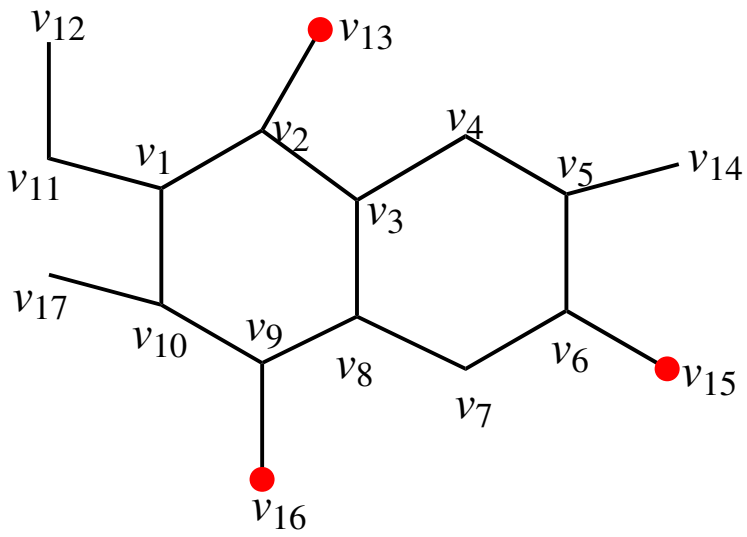

Fig. 9. Molecular graph of Perfragilin A with its resolving atoms

We labelled the molecular graph of Perfragilin A drug with D_8. The Perfragilin A is one of an anticancer drug, in graph theoretical study its order (or count of atoms) is $D_8 = 17$ and the size (or count of links) is $D_8 = 18$. Described below are the D_8 atom and link sets. Moreover, Figure 9 displays the chemical graph of Perfragilin A.

$$\begin{aligned} A(D_8) =& \{v_\zeta : \zeta = 1, 2, \ldots, 17\}, \\ L(D_8) =& \{v_\zeta v_{\zeta+1} : \zeta = 1, 2, \ldots, 9, 11\} \cup \{v_1v_{11}, v_1v_{10}, v_2v_{13}, \\ & v_5v_{14}, v_6v_{15}, v_9v_{16}, v_{10}v_{17}, v_3v_8\}. \end{aligned}$$

Theorem 2.8. *Let D_8 be a molecular graph of Perfragilin A anticancer drug. Then $dim(D_8) = 3$.*

Proof. To prove that $dim(D_8) = 3$, consider a locating set $R = \{v_{13}, v_{15}, v_{16}\}$. Using the Definition 1.1 to see the shortest distances and then arranging in the form given in the Definition 1.2, we constructed the following representations of the entire vertex set of (D_8), which is $r(v_\zeta|R) =$

$(d(v_\zeta, v_{13}), d(v_\zeta, v_{15}), d(v_\zeta, v_{16}))$.

$$r(v_\zeta|R) = \begin{cases} (2, 7-\zeta, \zeta+2), & \text{if } \zeta = 1; \\ (\zeta-1, 7-\zeta, \zeta+2), & \text{if } \zeta = 2; \\ (\zeta-1, 7-\zeta, \zeta), & \text{if } \zeta = 3, 4, 5; \\ (\zeta-1, 7-\zeta, 10-\zeta), & \text{if } \zeta = 6; \\ (11-\zeta, \zeta-5, 10-\zeta), & \text{if } \zeta = 7, 8; \\ (13-\zeta, \zeta-5, 10-\zeta), & \text{if } \zeta = 9; \\ (13-\zeta, \zeta-5, 2), & \text{if } \zeta = 10; \\ (\zeta-9, \zeta-4, \zeta-7), & \text{if } \zeta = 11, 12; \\ (0, 6, \zeta-8), & \text{if } \zeta = 13; \\ (5, 3\zeta-8), & \text{if } \zeta = 14; \\ (21-\zeta, 0, 5), & \text{if } \zeta = 15; \\ (21-\zeta, \zeta-11, 0), & \text{if } \zeta = 16; \\ (21-\zeta, \zeta-11, 3), & \text{if } \zeta = 17; \end{cases}$$

As a result, it follows in the form of a representation from the reasons above that $dim(D_8) \leq 3$ because each of the (D_8) vertices has an individual representation with regard to the resolving set R.

Currently, we are able to show this $dim(D_8) \geq 3$.In the case of contradicting, we suppose $dim(D_8) = 2$. Consider the resolving set R' for this with cardinality 2. The discussion that follows for this supposition.

Case: Assuming $R' = \{v_1, v_2\}$. When it has cardinality 2. The same representation are; $r(v_{13}|R') = r(v_{15}|R')$. Similarly, by taking any possible subset from the atom set of Perfragilin A, the situation becomes: let $r(v_\alpha|R') = r(v_\beta|R')$ if and only if $d(v_\alpha, v_\beta) = 2$. This concludes that $dim(D_8) = 3$. □

We labelled the molecular graph of Melatonin drug with D_9. The Melatonin is one of an anticancer drug, in graph theoretical study its order (or count of atoms) is $D_9 = 17$ and the size (or count of links) is $D_9 = 18$. The atom and links sets of D_9 listed below. Additionally, Figure 10 displays the chemical networks of Melatonin.

$$\begin{aligned} A(D_9) =& \{v_\zeta : \zeta = 1, 2, \ldots, 17\}, \\ L(D_9) =& \{v_\zeta v_{\zeta+1} : \zeta = 1, 2, \ldots, 8, 9, \ldots, 13, 16\} \cup \{v_{13}v_{15}, \\ & v_4v_8, v_2v_{16}, v_1v_9, v_5v_{10}\}. \end{aligned}$$

Theorem 2.9. *Let D_9 be a molecular graph of Melatonin anticancer drug. Then $dim(D_9) = 2$.*

Proof. To show that $dim(D_9) = 2$, suppose a locating set $R = \{v_2, v_{17}\}$. Using the Definition 1.1 to see the shortest distances and then arranging in the form given in the Definition 1.2, we constructed the

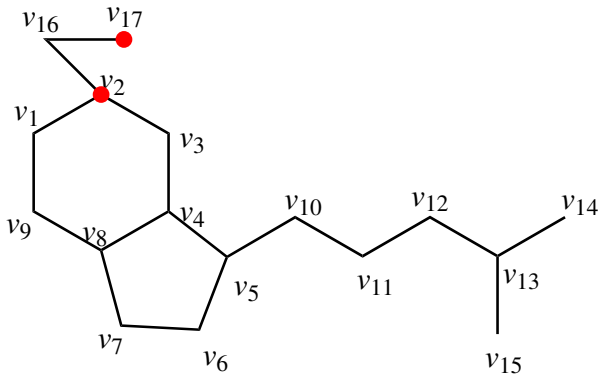

Fig. 10. Molecular graph of Melatonin with its resolving atoms

following representations of the entire vertex set of (D_9), which is $r(v_\zeta|R) = (d(v_\zeta, v_2), d(v_\zeta, v_{17}))$.

$$r(v_\zeta|R) = \begin{cases} (|\zeta - 2|, 12 - \zeta), & \text{if } \zeta = 1, 2, 3; \\ (2, 6 + \zeta), & \text{if } \zeta = 4, 5; \\ (\zeta - 4, 8), & \text{if } \zeta = 6, 7; \\ (\zeta - 4, 15 - \zeta), & \text{if } \zeta = 8; \\ (13 - \zeta, 15 - \zeta), & \text{if } \zeta = 9; \\ (13 - \zeta, 7), & \text{if } \zeta = 10; \\ (\zeta - 6, 16 - \zeta), & \text{if } \zeta = 11, 12, \ldots 15; \\ (10, 2), & \text{if } \zeta = 16; \\ (10, 0), & \text{if } \zeta = 17; \\ (\zeta - 13, \zeta - 10), & \text{if } \zeta = 18, 19; \end{cases}$$

As a result $dim(D_9) \leq 2$, it follows in the form of a representation from the arguments mention in above, considering the resolving set R, each vertex of (D_9) has a distinctive representation. Instead of bound, we will now use the contradiction approach for exactness, implies $dim(D_9) > 2$, which is $dim(D_9) = 1$. It is incorrect since the chosen graph is not a path graph, which must exist for the presence of the metric dimension 1. So, $dim(D_9) = 2$, which is required result. □

We labelled the molecular graph of Tambjamine K drug with D_{10}. The Tambjamine K is one of an anticancer drug, in graph theoretical study its order (or count of atoms) is $D_{10} = 19$ and the size (or count of links) is $D_{10} = 20$. It is shown in below the links sets and atom of D_{10}. Further, the Figure 11, shows the chemical structure of Tambjamine K.

$$\begin{aligned} A(D_{10}) =& \{v_\zeta : \zeta = 1, 2, \ldots, 19\}, \\ L(D_{10}) =& \{v_\zeta v_{\zeta+1} : \zeta = 1, 2, \ldots, 4, 6, 7, \ldots, 9, 11, 12, \ldots, \\ & 15, 18\} \cup \{v_1v_5, v_3v_6, v_6v_{10}, v_8v_{18}, v_9v_{11}, v_{15}v_{17}\}. \end{aligned}$$

Theorem 2.10. *Let D_{10} be a molecular graph of Tambjamine K anticancer drug. Then $dim(D_{10}) = 2$.*

Proof. To show that $dim(D_{10}) = 2$, suppose a locating set $R = \{v_1, v_{17}\}$. Using the Definition 1.1 to see the shortest distances and then arranging in the form given in the Definition 1.2, we constructed

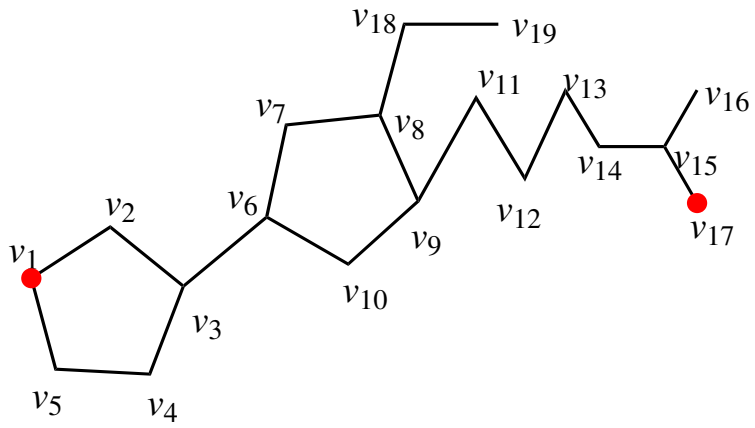

Fig. 11. Molecular graph of Tambjamine K with its resolving atoms

the following representations of the entire vertex set of (D_{10}), which is $r(v_\zeta|R) = (d(v_\zeta, v_1), d(v_\zeta, v_{17}))$.

$$r(v_\zeta|R) = \begin{cases} (\zeta, 8-\zeta), & \text{if } \zeta = 1, 2, 3; \\ (\zeta, \zeta+2), & \text{if } \zeta = 4; \\ (8-\zeta, \zeta+2), & \text{if } \zeta = 5, 6; \\ (\zeta-2, 11-\zeta), & \text{if } \zeta = 7, 8; \\ (15-\zeta, 11-\zeta), & \text{if } \zeta = 9; \\ (15-\zeta, \zeta-7), & \text{if } \zeta = 10, 11; \\ (\zeta-5, \zeta_1 1), & \text{if } \zeta = 12, 13, \ldots 25; \\ (32-\zeta, \zeta-22), & \text{if } \zeta = 26, 27; \\ (32-\zeta, \zeta-20), & \text{if } \zeta = 28, 29; \\ (0, 8), & \text{if } \zeta = 30; \\ (8, 0), & \text{if } \zeta = 31; \end{cases}$$

As a result, it follows in the form of a representation from the reasons above that $dim(D_{10}) \leq 2$ because all the vertices of (D_{10}) have the unique representations with respect to resolving set R. Instead of bound, we will now use the contradiction approach for exactness, implies $dim(D_{10}) > 2$, which is $dim(D_{10}) = 1$. It is false due to the chosen graph is not a path graph, which is required for the metric dimension one to exist. So, $dim(D_{10}) = 2$, which is required result. □

3. Conclusion and Discussion

To cure cancer disease anticancer medications are being used. In this work, we studied some of the anticancer medications in terms of locating set, where locating set is a set to settle the entire atom set of a graph into a unique way to access each atom independently. Additionally, the key outcomes' summary is provided as: the Amathaspiramide E, Carmustine, Caulibugulone E, Aspidostomide E, Convolutamide A, Convolutamine F, Convolutamydine A, Melatonin, and Tambjamine K has two metric dimensions while the only one drug which is Perfragilin A containing three elements in their resolving set.

There are few limitations of this work, like *Computational Complexity:* Certain locating numbers or computational models may exhibit significant computational complexity, rendering them unfeasible for handling extensive datasets or real-time applications. In fuzzy graph theory, generalized classes of

graphs are very complex to compute the locating numbers. It took very complex modeling and time as well.

There are many medicinal structures available for cancer disease. One can choose a few structures and develop its graphs and work the locating numbers of those developed graphs. There are many locating numbers like fault-tolerant locating number, edge locating number and many others, one can study these numbers as well on these chosen structures.

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Conflicts of Interest

The authors declare no conflicts of interest.

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