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ON METRIC DIMENSION OF PIBRENTASVIR AND VANCOMYCIN

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Abstract:

Let $\zeta = (V,E)$ be a nth order connected graph. If the distance vectors to the vertices in an ordered subset H_r of vertices can uniquely identify each vertex of the graph ζ, then the set H_r is known as resolving set for the graph ζ. The resolving set H_r with smallest cardinality serves as the metric dimension of graph ζ and this resolving set serves as the metric basis for ζ. Since very early times, medicinal drugs have played a significant part in human civilization. In this article, we study the metric dimension for the typical molecular structures of two important drugs namely pibrentasvir (P_{80}) and vancomycin (V_{101}). **MSC(2020):** 05C10, 05C12, 68R10.

Keywords: Molecular graph, pibrentasvir, metric dimension, vancomycin, independent set.

1 Introduction

The notion metric dimension was found to be applicable in a variety of science and technology sectors. It can be used in a variety of fields, including chemistry, industrial chemistry, computer science, networking, molecular topology, etc. Assigning an identity to a specific set, or resolving set, allows one to more easily determine the location of vertices in an intriguing network [7, 16]. The least cardinality of such a specific set is known as the metric dimension of a given graph, denoted by dim(ζ), and that specific set is known as the metric basis for ζ. Chemical graph theory (CGT) is branch of mathematical chemistry that extends conventional graph theory to chemical entities and phenomena. CGT aids in the analysis of various chemical networks, complex structures, and topologies in the form of a graph which are difficult to analyse in its original shape [20]. In CGT, atom are replaced by vertices and the bond between the atoms are depicted by edges between the vertices. Medicial drugs are the vital chemical compounds used to enhance physical or mental health of humans/animals by treating, curing, preventing, and diagnosing various perilous diseases. In this work, we determine the metric basis and dimension for certain significant drugs (viz., pibrentasvir and vancomycin).

AbbVie has created the medication pibrentasvir (P_{80}) with molecular formula $C_{57}H_{65}F_5N_{10}O_8$, and is used to treat hepatitis C virus (HCV) infection [13]. Pibrentasvir was approved in the EU, Iceland, Liechtenstein and Norway on 28 July 2017 for the treatment of HCV infection in adults [14]. Nonstructural protein 5A (NS5A) inhibitors are a direct-acting antiviral agent used to treat HCV. The NS5A has an important role in viral replication, packaging, assembly, and complex interactions with cellular functions. Vancomycin (V_{101}) was isolated in 1957 by Dr. E.C Kornfield, an organic chemist with Eli Lilly in the deep jungles of Borneo from a fungus named streptomyces orientalis. Vancomycin was initially prescribed to treat pencillin-resistant staphylococcus aureus. The drug was previously known as compound 05865, but subsequently

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received the generic name vancomycin, derived from the term "vanquish". The molecular formula of vancomycin is $C_{66}H_{75}Cl_2N_9O_{24}$. Vancomycin is a branched tricyclic glycosylated nonribosomal peptide produced by the antinomycetota species amycolatopsis orientalis (formerly designated nacardia orientalis). Due to the rotational constraint of certain bonds, vancomycin exhibits atropisomerism, having several chemically rotamers. The drug's form is the more thermodynamically stable conformer. Next, we will provide an applicative review regarding these two aforesaid chemically significant drugs i.e., for P_{80} and V_{101}.

1.1 Application

Pibrentasvir belongs to the class of medication called HCV NS5A inhibitors. It works by stopping the virus that causes hepatitis C to spread inside the body. Pibrentasvir is a direct acting antiviral agent for HCV, and NS5A inhibitor present in P_{80} targets the viral RNA replication and viron assembly. Vancomycin is in a class of medication called glycopeptide antibiotics. It works by killing bacteria in the intestines. When treating life-threatening infections brought on by important gram-positive human pathogens like staphylococcus aureus, clostridium difficle, etc., glycopeptides are the antibiotics of last resort.

A glycopeptide antibiotic called vancomycin is prescribed to treat several bacterial infections. It is advised to inject it intravenously to treat methicillin-resistant Staphylococcus aureus-caused severe bloodstream infections, skin infections, bone and joint infections, meningitis, and endocarditis. The ideal dose can be determined by measuring blood levels. It is among the few antibiotics that are utilised in plant tissue culture to get rid of Gram-positive bacterial infections and has comparatively low toxicity to plants.In 1958, the United States government authorised vancomycin for medical use. It has marked a place in the World health Organization's List of Essential Medicines. Vancomycin is regarded by the World Health Organization as being of vital importance to human medicine. Next, we discuss about the most active research domain and topic known as chemical graph theory and metric dimension respectively.

1.2 Chemical Graph Theory and Parameters of Resolvability

A branch of mathematical chemistry called chemical graph theory examines all the consequences of connectedness in a chemical graph. Chemical graph theory is an interdisciplinary field where relevant mathematical questions are investigated into using graph theoretical and computational methods, where the molecular structure of a chemical substance is examined as a graph. In the previous few decades, this discipline has experienced remarkable growth, giving us access to a variety of new and innovative ideas for such studies. In other words, all facets of applying graph theory to chemistry are addressed by chemical graph theory. By using the word chemical, it is made clear that, in contrast to graph theory, one is free to rely on a conceptual grasp of numerous ideas and theorems rather than on rigorous mathematical proofs.

The molecular structure of a compound is frequently represented by a graph in chemical graph theory, where atoms and bonds are represented by vertices and edges respectively. Note that the distinction between single and double bonds is often neglected. As a result, there are usually

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no multiple edges (no two vertices serve as the endpoints of more than one edge). The atoms of hydrogen will automatically be dropped in such a representation because the valence of a hydrogen atom is one, corresponding to its vertex degree. As a result, we often eliminate the vertices that correspond to hydrogens. Consequently, we have what is called as the molecular graph. CGT is used to simplify chemical structures that are difficult to analyse in their original form because they are large and complex. After converting a molecular structure into a graph, a thorough study of structures can be carried out [18]. Detail structural analysis is easily accomplished after translating molecular structure to a graph. Pibrentasvir and vancomycin and are two most important chemical compounds that have their application in medicinal drugs of fatal diseases. The most important and extensively researched parameters in graph theory are metric dimension and its more recently developed versions. So, keeping with the theme, in this work we investigate metric dimension for the molecular structure of piberentasvir and vancomycin.

Applications of metric dimensions include identifying the origin of a spread in a network, canonically labelling graphs, and embedding symbolic data in lower dimensional Euclidean spaces [21]. The term “locating set” was first used by Slater in 1975 to refer to the problem of uniquely identifying or differentiating the position of invaders in a network, and it is where the concept of metric dimension was first presented. On the other hand, the identical idea was separately introduced by Harary and Melter in 1976, however this time, a specific set was referred to as a “resolving set”. After the publication of these two foundational works, a sizable amount of research on the theoretical characteristics and certain applications of this invariant has been done. For instance, Chvatal [22], Erdos and Renyi [19] investigated a number of significant connections between the coin weighing or mastermind game and graph-resolving sets. The idea was used to image processing and pattern recognition by Melter and Tomescu [20] and Chartrand et al. [9] demonstrated the applications in the field of chemistry. Metric dimension was studied in terms of combinatorial optimization by Sebo and Tannier [4]. Robot navigation is one area in which Khuller et al. [23] discovered a use for the metric dimension. Sound Navigation and Ranging (SONAR) problems, facility location problems, and coast guard LORAN problems(Long-Range Navigation) were all studied by Slater [16].

To gain a greater understanding of the concept of metric dimension, a number of different resolving set variations have also been developed in the literature. Similar to resolving set, it is possible to imagine that two edges can also be resolved with respect to the specific set of vertices that have been selected, rather than just two individual vertices of a graph. The edge metric dimension was suggested by Kelenc et al. [3] as a new version to describe this idea. Similar to this, Kelenc et al. [2] present a new type of dimension termed mixed metric dimension, which combines metric and edge metric dimensions. Mixed resolving sets identify the elements (vertices and edges) of a connected graph by using vector distances to a predetermined specific set of vertices in the graph.

Researchers have looked into the resolvability parameters for a number of graph families with significant impact. For example, Koam and Ahmad [1] investigated the EMD of Cayley graph’s barycentric subdivision. Raza and Bataineh [28] compared the MD and EMD of a few graph

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related to wheel graphs. For certain families of convex polytope graphs, MD & EMD were obtained by Ahsan et al. [15], Sharma and Bhat [25]. Xing et al. [4] investigated MMD for a few graphs including wheels. Additionally, recent research has examined the conceptions of the MD, EMD, and MMD for a number of significant molecular graphs. For instance, Hussain et al. [27] and Sharma and Bhat [24], respectively, examined the notions of the metric dimension and edge-metric dimension of 1-pentagonal carbon nanocone networks. The MD of networks like silicate star was acquired by Simonraj and George [8]. This idea was also examined by Yang et al. [6] for a number of chemical structures related to wheel graphs. Siddiqui and Imran [11] looked into the MD of H-Naphtalenic and V C_5C_7 nanotubes. One can turn to Khuller et al. [23]; Sharma and Bhat [24]; Xing et al. [5] for additional literature on metric dimesion, edge metric dimesion and mixed metric dimension.

2 Preliminaries

We discuss some fundamental concepts, definitions, and proved results about the metric dimension of graphs in this particular section.

Let $\zeta = (V,E)$ be a connected, simple and undirected graph, where V and E are the sets of vertices and edges respectively. The shortest path between two vertices a and b determines the topological distance d(a,b) between them in a non-trivial connected network. The degree (valency) of a vertex is the number of all edges that incident to that vertex.

Definition 1. Resolving Set: [16] Let $H_r = \{t_1,t_2,t_3,...,t_p\}$ be a ordered subset of vertices in the graph $\zeta = (V,E)$ then the p-vector $\varsigma(k|H_r) = ((d(k|t_1),d(k|t_2),d(k|t_3),...,d(k|t_p))$ is the metric representation of a vertex k with respect to the set H_r. Then the subset H_r is said to resolve two vertices $r,q \in V$ if $\varsigma(r|H_r) \neq \varsigma_t(q|H_r)$. If every pair of different vertices in ζ is resolved by H_r, then H_r is known as resolving set for ζ.

Definition 2. Metric Dimension: [16] The resolving set with smallest possible cardinality serves as metric basis for the graph ζ and number of elements in metric basis for the graph ζ is known as metric dimension of the graph ζ and is denoted by $\dim(\zeta)$.

Definition 3. Independent Set: [10] A subset of vertices in a graph in which there is no pair of vertices that are adjacent is called as independent set.

Definition 4. Independent resolving set: [10] A subset B of vertices in a graph which is both independent and resolving is known as independent resolving set.

In this study, we particularly focus on two drugs viz., pibrentasvir (P_{80}) and vancomycin (V_{101}).

3 Metric Dimension of Pibrentasvir

The structure of P_{80} is discussed in this section. We examine some of its fundamental attributes and determine its metric dimension.

Structure of Molecular Graph P_{80}**:** The molecular graph of P_{80} consists of 80 vertices and 89 edges. It contains five 6 cycles and five 5 cycles. The number of vertices and edges to the left

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of c_{26} are equal to the number of vertices and edges to the right of c_{23} in the molecular graph of P_{80}. This symmetry helps in finding of metric codes for the structure.

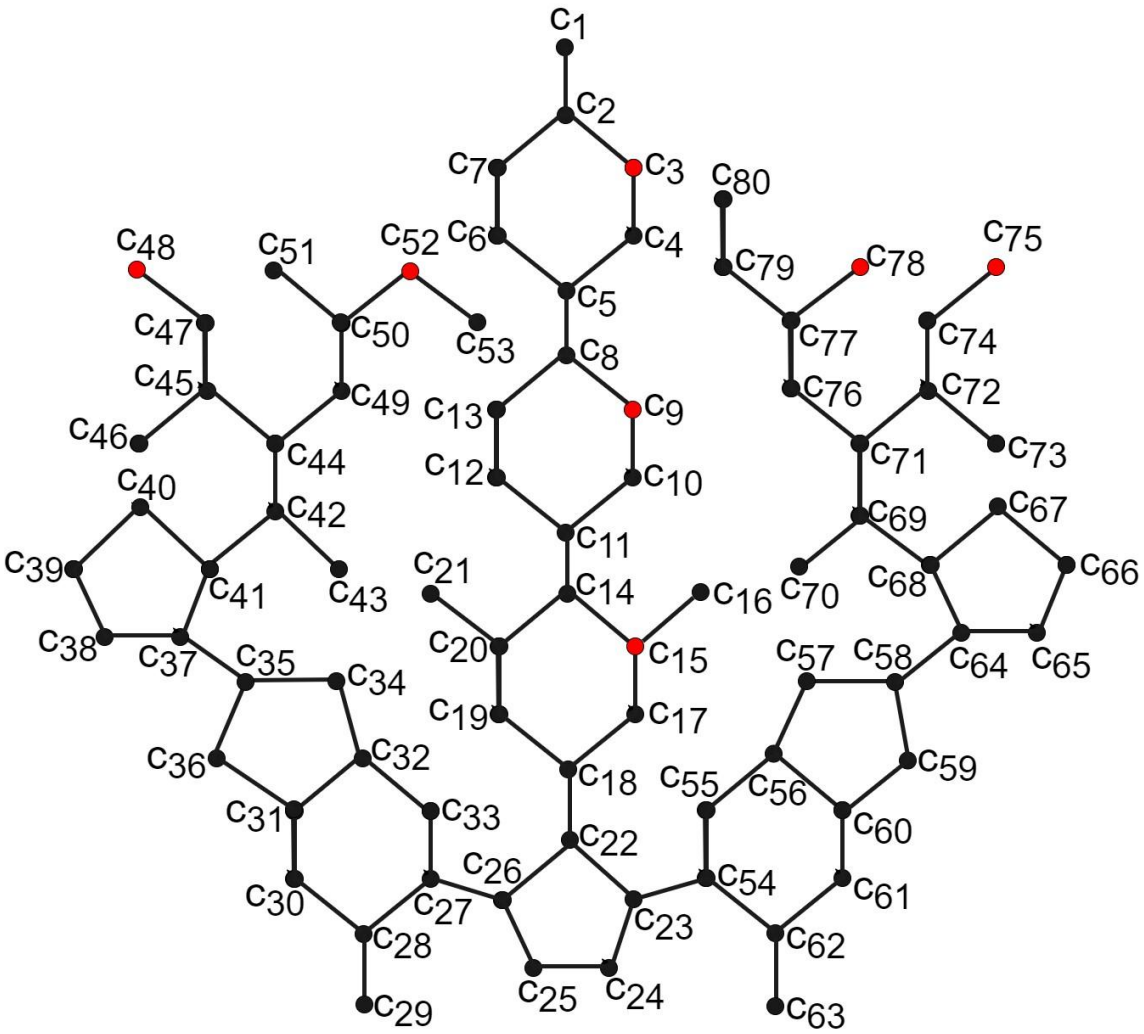

Figure 1: Molecular graph P_{80}

Theorem 1. The metric dimension of the molecular graph P_{80} is 7

Proof. Let $H_r = \{c_3, c_9, c_{15}, c_{48}, c_{52}, c_{75}, c_{78}\}$ be a subset of vertices of P_{80}. The metric co-ordinates for the vertices $\{c_l : 1 \leq l \leq 80\}$ with respect to the set H_r are given below

Metric codes	Corresponding values	Metric codes	Corresponding values
$\varsigma(c_1\|H_r)$	(2,6,10,26,26,26,26)	$\varsigma(c_{41}\|H_r)$	(19,15,11,5,5,21,21)
$\varsigma(c_2\|H_r)$	(1,5,9,25,25,25,25)	$\varsigma(c_{42}\|H_r)$	(20,16,12,4,4,22,22)
$\varsigma(c_3\|H_r)$	(0,4,8,24,24,24,24)	$\varsigma(c_{43}\|H_r)$	(21,17,13,5,5,23,23)

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$\varsigma(c_4\|H_r)$	(1,3,7,23,23,23,23)	$\varsigma(c_{44}\|H_r)$	(21,17,13,3,3,23,23)
$\varsigma(c_5\|H_r)$	(2,2,6,22,22,22,22)	$\varsigma(c_{45}\|H_r)$	(22,18,14,4,2,24,24)
$\varsigma(c_6\|H_r)$	(3,3,7,23,23,23,23)	$\varsigma(c_{46}\|H_r)$	(23,19,15,5,3,25,25)
$\varsigma(c_7\|H_r)$	(2,4,8,24,24,24,24)	$\varsigma(c_{47}\|H_r)$	(23,19,15,5,1,25,25)
$\varsigma(c_8\|H_r)$	(3,1,5,21,21,21,21)	$\varsigma(c_{48}\|H_r)$	(24,20,16,6,0,26,26)
$\varsigma(c_9\|H_r)$	(4,0,4,20,20,20,20)	$\varsigma(c_{49}\|H_r)$	(22,18,14,2,4,24,24)
ς(c10Hr)	(5,1,3,19,19,19,19)	$\varsigma(c_{50}\|H_r)$	(23,19,15,1,5,25,25)
ς(c11Hr)	(6,2,2,18,18,18,18)	$\varsigma(c_{51}\|H_r)$	(24,20,16,2,6,26,26)
ς(c12Hr)	(5,3,3,19,19,19,19)	$\varsigma(c_{52}\|H_r)$	(24,20,16,0,6,26,26)
$\varsigma(c_{13}\|H_r)$	(4,2,4,20,20,20,20)	$\varsigma(c_{53}\|H_r)$	(25,21,17,1,7,27,27)
$\varsigma(c_{14}\|H_r)$	(7,3,1,17,17,17,17)	$\varsigma(c_{54}\|H_r)$	(13,9,5,15,15,11,11)
$\varsigma(c_{15}\|H_r)$	(8,4,0,16,16,16,16)	$\varsigma(c_{55}\|H_r)$	(14,10,6,16,16,10,10)
$\varsigma(c_{16}\|H_r)$	(9,5,1,17,17,17,17)	$\varsigma(c_{56}\|H_r)$	(15,11,7,17,17,9,9)
$\varsigma(c_{17}\|H_r)$	(9,5,1,15,15,15,15)	$\varsigma(c_{57}\|H_r)$	(16,12,8,18,18,8,8)
$\varsigma(c_{18}\|H_r)$	(10,6,2,14,14,14,14)	$\varsigma(c_{58}\|H_r)$	(17,13,9,19,19,7,7)
$\varsigma(c_{19}\|H_r)$	(9,5,3,15,15,15,15)	$\varsigma(c_{59}\|H_r)$	(17,13,9,19,19,8,8)
$\varsigma(c_{20}\|H_r)$	(8,4,2,16,16,16,16)	$\varsigma(c_{60}\|H_r)$	(16,12,8,18,18,9,9)
$\varsigma(c_{21}\|H_r)$	(9,5,3,17,17,17,17)	$\varsigma(c_{61}\|H_r)$	(15,11,7,17,17,10,10)
$\varsigma(c_{22}\|H_r)$	(11,7,3,13,13,13,13)	$\varsigma(c_{62}\|H_r)$	(14,10,6,16,16,11,11)
$\varsigma(c_{23}\|H_r)$	(12,8,4,14,14,12,12)	$\varsigma(c_{63}\|H_r)$	(15,11,7,17,17,22,22)
$\varsigma(c_{24}\|H_r)$	(13,9,5,14,14,13,13)	$\varsigma(c_{64}\|H_r)$	(18,14,10,20,20,6,6)
$\varsigma(c_{25}\|H_r)$	(13,9,5.13,13,14,14)	$\varsigma(c_{65}\|H_r)$	(19,15,11,21,21,7,7)
$\varsigma(c_{26}\|H_r)$	(12,8,4,12,12,14,14)	$\varsigma(c_{66}\|H_r)$	(20,16,12,22,22,7,7)

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$\varsigma(c_{27}\|H_r)$	(13,9,5,11,11,15,15)	$\varsigma(c_{67}\|H_r)$	(20,16,12,22,22,6,6)
$\varsigma(c_{28}\|H_r)$	(14,10,6,11,11,16,16)	$\varsigma(c_{68}\|H_r)$	(19,15,11,21,21,5,5)
$\varsigma(c_{29}\|H_r)$	(15,11,7,12,12,17,17)	$\varsigma(c_{69}\|H_r)$	(20,16,12,22,22,4,4)
$\varsigma(c_{30}\|H_r)$	(15,11,7,10,10,17,17)	$\varsigma(c_{70}\|H_r)$	(21,17,13,23,23,5,5)
$\varsigma(c_{31}\|H_r)$	(16,12,8,9,9,18,18)	$\varsigma(c_{71}\|H_r)$	(21,17,13,23,23,3,3)
$\varsigma(c_{32}\|H_r)$	(15,11,7,9,9,17,17)	$\varsigma(c_{72}\|H_r)$	(22,18,14,24,24,2,4)
$\varsigma(c_{33}\|H_r)$	(14,10,6,10,10,16,16)	$\varsigma(c_{73}\|H_r)$	(23,19,15,25,25,3,5)
$\varsigma(c_{34}\|H_r)$	(16,12,8,8,8,18,18)	$\varsigma(c_{74}\|H_r)$	(23,19,15,25,25,1,5)
$\varsigma(c_{35}\|H_r)$	(17,13,9,7,7,19,19)	$\varsigma(c_{75}\|H_r)$	(24,20,16,26,26,0,6)
$\varsigma(c_{36}\|H_r)$	(17,13,9,8,8,19,19)	$\varsigma(c_{76}\|H_r)$	(22,18,14,24,24,4,2)
$\varsigma(c_{37}\|H_r)$	(18,14,10,6,6,20,20)	$\varsigma(c_{77}\|H_r)$	(23,19,15,25,25,5,1)
$\varsigma(c_{38}\|H_r)$	(19,15,11,7,7,21,21)	$\varsigma(c_{78}\|H_r)$	(24,20,16,26,26,6,0)
$\varsigma(c_{39}\|H_r)$	(20,16,12,7,7,22,22)	$\varsigma(c_{79}\|H_r)$	(24,20,16,26,26,6,1)
$\varsigma(c_{40}\|H_r)$	(20,16,12,6,6,22,22)	$\varsigma(c_{80}\|H_r)$	(25,21,17,27,27,7,2)

From the above, it is clear that $\dim(P_{80}) \leq 7$. Now, it only remains to show that $\dim(P_{80}) \geq 7$. If none of the vertices among $\{c_3,c_4,c_6,c_7\}$ is not involved in the resolving set H_r then the metric codes for two different vertices in the set $\{c_3,c_4,c_6,c_7\}$ becomes identical. So, one among the vertices $\{c_3,c_4,c_6,c_7\}$ must be included in the resolving set. Similarly, one among the vertices $\{c_9,c_{10},c_{12},c_{13}\}$ must be included inH_r. In the same way, one among the vertices $\{c_{15},c_{17},c_{19},c_{20}\}$ must be included in H_r.

If none of the vertices among $\{c_{47},c_{48},c_{50},c_{51}\}$ is not involved in the resolving set H_r then the metric codes for two different vertices in the set $\{c_{47},c_{48},c_{50},c_{51}\}$ is found to be same. So, one among the vertices $\{c_{47},c_{48},c_{50},c_{51}\}$ must be included in H_r. In the same way, one among the vertices $\{c_{74},c_{75},c_{77},c_{78}\}$ must be included in H_r.For each vertex except c_{53} the distance of the vertices c_{51} and c_{52} coincides, so at least one of the vertices in the set c_{51},c_{52} must be taken in resolving set. Similarly, at least one vertex among c_{79} and c_{78} must be taken in H_r. From the above discussion, it follows that $\dim(P_{80}) \geq 7$. This completes the proof of the theorem.

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Corollary 1. The independent resolving number of P_{80} is 7.

4 Metric Dimension of the Molecular graph of Vancomycin

In this section, we start by talking about the structure of V_{101}. We investigate some of its fundamental properties and determine its metric dimension.

Structure of Molecular Graph V_{101} The structure of V_{101} is very complex as it consists of 101 atoms except hydrogen atoms and 110 bonds except the bonds between hydrogen and other atoms. The molecular graph of V_{101} consists of 101 vertices ad 110 edges. It contains seven 6 cycles.

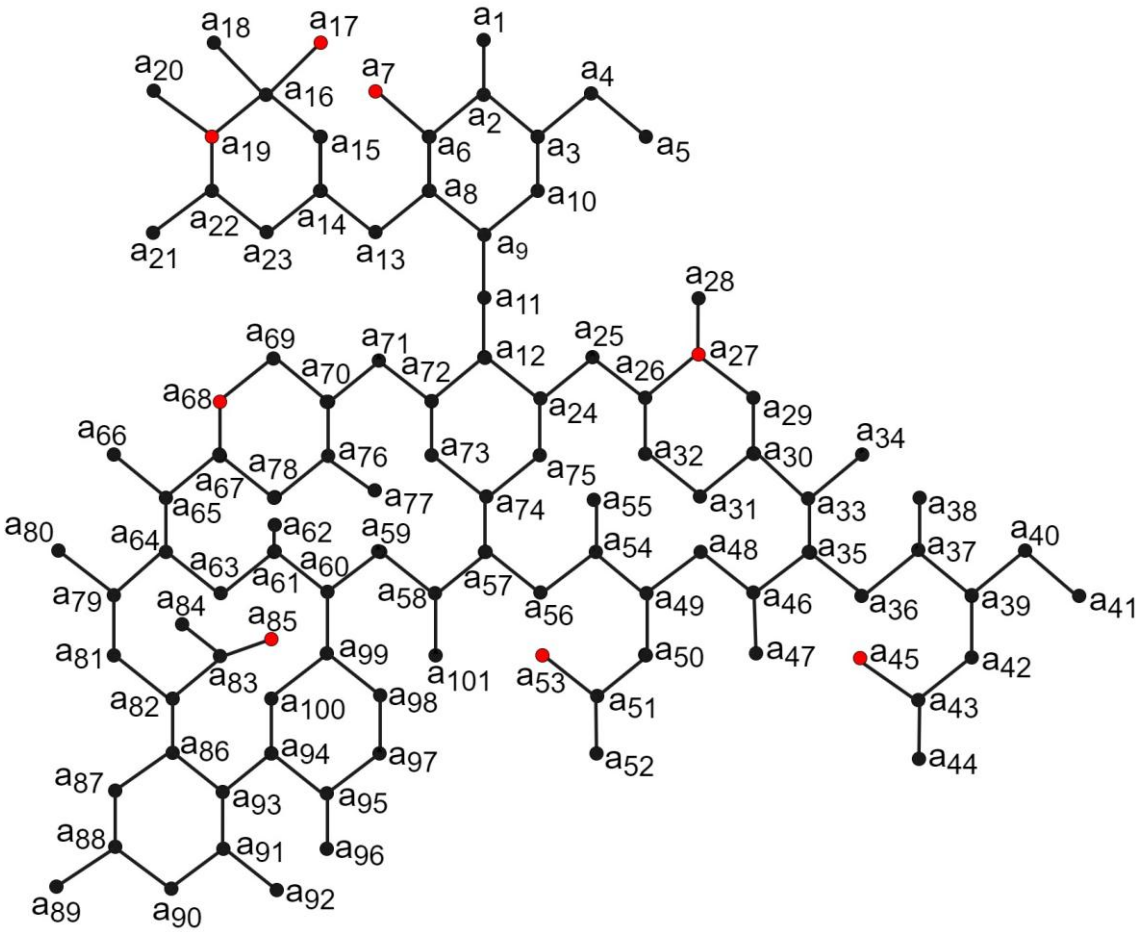

Figure 2: Molecular graph of V_{101}

Theorem 1. The metric dimension of the molecular graph V_{101} is 8.

Proof. Let $H_r = \{a_7, a_{17}, a_{19}, a_{27}, a_{45}, a_{53}, a_{68}, a_{85}\}$ be a subset of vertices of V_{101}. The metric coordinates for the vertices $\{a_l : 1 \leq l \leq 101\}$ with respect to the set H_r are given below

Metric codes	Corresponding values	Metric codes	Corresponding values
$\varsigma(a_1\|H_r)$	(3,8,8,10,20,16,11,19)	$\varsigma(a_7\|H_r)$	(0,7,7,9,19,15,10,18)

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$\varsigma(a_2\|H_r)$	(2,7,7,9,19,15,10,18)	$\varsigma(a_8\|H_r)$	(2,5,5,7,17,13,8,16)
$\varsigma(a_3\|H_r)$	(3,8,8,8,18,14,9,17)	$\varsigma(a_9\|H_r)$	(3,6,6,6,16,12,7,15)
$\varsigma(a_4\|H_r)$	(4,9,9,9,19,15,10,18)	$\varsigma(a_{10}\|H_r)$	(4,7,7,7,17,13,8,16)
$\varsigma(a_5\|H_r)$	(5,10,10,10,20,16,11,19)	$\varsigma(a_{11}\|H_r)$	(4,7,7,5,15,11,6,14)
$\varsigma(a_6\|H_r)$	(1,6,6,8,18,14,9,17)	$\varsigma(a_{12}\|H_r)$	(5,8,8,4,14,10,5,13)
$\varsigma(a_{13}\|H_r)$	(3,4,4,8,18,14,9,17)	$\varsigma(a_{58}\|H_r)$	(10,13,13,7,13,7,8,10)
$\varsigma(a_{14}\|H_r)$	(4,3,3,9,19,15,10,18)	$\varsigma(a_{59}\|H_r)$	(11,14,14,8,14,8,7,9)
$\varsigma(a_{15}\|H_r)$	(5,2,2,10,20,16,11,19)	$\varsigma(a_{60}\|H_r)$	(12,15,15,9,15,9,6,8)
$\varsigma(a_{16}\|H_r)$	(6,1,1,11,21,1,12,20)	$\varsigma(a_{61}\|H_r)$	(13,16,16,10,16,10,5,7)
$\varsigma(a_{17}\|H_r)$	(7,0,2,12,22,18,13,21)	$\varsigma(a_{62}\|H_r)$	(14,17,17,11,17,11,6,8)
$\varsigma(a_{18}\|H_r)$	(7,2,2,12,22,18,13,21)	$\varsigma(a_{63}\|H_r)$	(14,17,17,11,17,11,4,6)
$\varsigma(a_{19}\|H_r)$	(7,2,0,12,22,18,13,21)	$\varsigma(a_{64}\|H_r)$	(13,16,16,12,18,12,3,5)
$\varsigma(a_{20}\|H_r)$	(8,3,1,13,23,19,14,22))	$\varsigma(a_{65}\|H_r)$	(12,15,15,11,19,13,2,6)
$\varsigma(a_{21}\|H_r)$	(6,3,1,11,21,17,12,20)	$\varsigma(a_{66}\|H_r)$	(13,16,16,12,20,14,3,7)
$\varsigma(a_{22}\|H_r)$	(7,4,2,12,22,18,13,21)	$\varsigma(a_{67}\|H_r)$	(11,14,14,10,20,14,1,7)
$\varsigma(a_{23}\|H_r)$	(5,4,2,10,20,16,11,19)	$\varsigma(a_{68}\|H_r)$	(10,13,13,9,19,13,0,8)
$\varsigma(a_{24}\|H_r)$	(6,9,9,3,13,9,6,14)	$\varsigma(a_{69}\|H_r)$	(9,12,12,8,18,12,1,9)
$\varsigma(a_{25}\|H_r)$	(7,10,10,2,12,10,7,15))	$\varsigma(a_{70}\|H_r)$	(8,11,11,7,17,11,2,10)
$\varsigma(a_{26}\|H_r)$	(8,11,11,1,11,11,8,16)	$\varsigma(a_{71}\|H_r)$	(7,10,10,6,16,10,3,11)
$\varsigma(a_{27}\|H_r)$	(9,12,12,0,10,10,9,17)	$\varsigma(a_{72}\|H_r)$	(6,9,9,5,15,9,4,12)
$\varsigma(a_{28}\|H_r)$	(10,13,13,1,11,11,10,18)	$\varsigma(a_{73}\|H_r)$	(7,10,10,6,14,8,5,13)
$\varsigma(a_{29}\|H_r)$	(10,13,13,1,9,9,10,18)	$\varsigma(a_{74}\|H_r)$	(8,11,11,5,13,7,6,12)
$\varsigma(a_{30}\|H_r)$	(11,14,14,2,8,8,11,19)	$\varsigma(a_{75}\|H_r)$	(7,10,10,4,14,8,7,13)
$\varsigma(a_{31}\|H_r)$	(10,13,13,3,9,9,10,18)	$\varsigma(a_{76}\|H_r)$	(9,12,12,8,18,12,3,9)
$\varsigma(a_{32}\|H_r)$	(9,12,12,2,10,10,9,17)	$\varsigma(a_{77}\|H_r)$	(10,13,13,9,19,13,4,10)
$\varsigma(a_{33}\|H_r)$	(12,15,15,3,7,7,12,18)	$\varsigma(a_{78}\|H_r)$	(10,13,13,9,19,13,2,8)
$\varsigma(a_{34}\|H_r)$	(13,16,16,4,8,8,13,19)	$\varsigma(a_{79}\|H_r)$	(14,17,17,13,19,13,4,4)
$\varsigma(a_{35}\|H_r)$	(13,16,16,4,6,6,13,17)	$\varsigma(a_{80}\|H_r)$	(15,18,18,14,20,14,5,5)
$\varsigma(a_{36}\|H_r)$	(14,17,17,5,5,7,14,18)	$\varsigma(a_{81}\|H_r)$	(15,18,18,14,20,14,5,3)
$\varsigma(a_{37}\|H_r)$	(15,18,18,6,4,8,15,19)	$\varsigma(a_{82}\|H_r)$	(16,19,19,15,21,15,6,2)

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$\varsigma(a_{38}\|H_r)$	(16,19,19,7,5,9,16,20)	$\varsigma(a_{83}\|H_r)$	(17,20,20,16,22,16,7,1)
$\varsigma(a_{39}\|H_r)$	(16,19,19,7,3,9,16,20)	$\varsigma(a_{84}\|H_r)$	(18,21,21,17,23,17,8,2)
$\varsigma(a_{40}\|H_r)$	(17,20,20,8,4,10,17,21)	$\varsigma(a_{85}\|H_r)$	(18,21,21,17,23,17,8,0)
$\varsigma(a_{41}\|H_r)$	(18,21,21,9,5,11,18,22)	$\varsigma(a_{86}\|H_r)$	(17,20,20,14,20,14,7,3)
$\varsigma(a_{42}\|H_r)$	(17,20,20,8,2,10,17,21)	$\varsigma(a_{87}\|H_r)$	(18,21,21,15,21,15,8,4)
$\varsigma(a_{43}\|H_r)$	(18,21,21,9,1,11,18,22)	$\varsigma(a_{88}\|H_r)$	(19,22,22,16,22,16,9,5)
$\varsigma(a_{44}\|H_r)$	(19,22,22,10,2,12,19,23)	$\varsigma(a_{89}\|H_r)$	(20,23,23,17,23,17,10,6)
$\varsigma(a_{45}\|H_r)$	(19,22,22,10,0,12,19,23)	$\varsigma(a_{90}\|H_r)$	(18,21,21,15,21,15,11,6)
$\varsigma(a_{46}\|H_r)$	(14,17,17,5,7,5,12,16)	$\varsigma(a_{91}\|H_r)$	(17,20,20,14,20,14,9,5)
$\varsigma(a_{47}\|H_r)$	(15,18,18,6,8,6,13,17)	$\varsigma(a_{92}\|H_r)$	(18,21,21,15,21,15,10,6)
$\varsigma(a_{48}\|H_r)$	(13,16,16,6,8,4,11,15)	$\varsigma(a_{93}\|H_r)$	(16,19,19,13,19,13,8,4)
$\varsigma(a_{49}\|H_r)$	(12,15,15,7,9,3,10,14)	$\varsigma(a_{94}\|H_r)$	(15,18,18,12,18,12,9,5)
$\varsigma(a_{50}\|H_r)$	(13,16,16,8,10,2,11,15)	$\varsigma(a_{95}\|H_r)$	(16,19,19,13,19,13,10,6)
$\varsigma(a_{51}\|H_r)$	(14,17,17,9,11,1,12,16)	$\varsigma(a_{96}\|H_r)$	(17,20,20,14,20,14,11,7)
$\varsigma(a_{52}\|H_r)$	(15,18,18,10,12,2,13,17)	$\varsigma(a_{97}\|H_r)$	(15,18,18,12,18,12,9,7)
$\varsigma(a_{53}\|H_r)$	(15,18,18,10,12,0,13,17)	$\varsigma(a_{98}\|H_r)$	(14,17,17,11,17,11,8,8)
$\varsigma(a_{54}\|H_r)$	(11,14,14,8,10,4,9,13)	$\varsigma(a_{99}\|H_r)$	(13,16,16,10,16,10,7,7)
$\varsigma(a_{55}\|H_r)$	(12,15,15,9,11,5,10,14)	$\varsigma(a100\|Hr)$	(14,17,17,11,17,11,8,6)
$\varsigma(a_{56}\|H_r)$	(10,13,13,7,11,5,8,12)	$\varsigma(a101\|Hr)$	(11,14,14,8,14,8,9,11)
$\varsigma(a_{57}\|H_r)$	(9,12,12,6,12,6,7,11)		

From the above, it is clear that $\dim(V_{101}) \leq 8$. Now, it only remains to show that $\dim(V_{101}) \geq 8$.If none of the vertices among $\{a_1,a_2,a_6,a_7\}$ is not involved in the resolving set H_r then the metric codes for two different vertices in the set $\{a_1,a_2,a_6,a_7\}$ becomes identical. So, one among the vertices $\{a_1,a_2,a_6,a_7\}$ must be included in H_r. If none of the vertices among $\{a_{18},a_{19},a_{21}\}$ is not involved in the resolving set H_r then the metric codes for two different vertices in the set $\{a_{18},a_{19},a_{21}\}$ becomes identical. So, one among the vertices $\{a_{18},a_{19},a_{21}\}$ must be included in H_r. If none of the vertices among $\{a_{17},a_{18}\}$ is not involved in H_r then the metric codes for two different vertices in the set $\{a_{17},a_{18}\}$ becomes equal. So, one among the vertices $\{a_{17},a_{18}\}$ must be included in H_r.

If none of the vertices among $\{a_{27},a_{29},a_{31},a_{32}\}$ is not involved in the resolving set H_r then the metric codes for two different vertices in the set $\{a_{27},a_{29},a_{31},a_{32}\}$ becomes identical. So, one among the vertices $\{a_{27},a_{29},a_{31},a_{32}\}$ must be included in H_r. Similarly, one among the vertices

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$\{a_{98},a_{69},a_{76},a_{78}\}$ must be included in H_r. If none of the vertices among $\{a_{44},a_{45}\}$ is not involved in the resolving set H_r then the metric codes for two different vertices in the set $\{a_{44},a_{45}\}$ becomes equal. So, one among the vertices $\{a_{44},a_{45}\}$ must be included in H_r. Similarly, one among the vertices $\{a_{52},a_{53}\}$ and one among $\{a_{84},a_{85}\}$ must be included in H_r. From the above discussion, it follows that $\dim(V_{101}) \geq 8$. This completes the proof of the theorem.

Corollary 2. The independent resolving number for the molecular graph V_{101} is 8.

5 Conclusion

This study looks at the metric basis as well as on the respective dimensions of the two famous drugs viz., P_{80} and V_{101}. We have shown for these two drugs that $\dim(P_{80}) = 7$ and $\dim(V_{101}) = 8$. We also proved that the resolving set for both of the structures are independent. In future, we will discuss various other recently introduced variations of the metric dimension (such as, edge metric dimension, local metric dimension, partition dimension, mixed metric dimension, etc.) for the these two globally important significant drugs viz., P_{80} and V_{101}.

Authors contributions

All authors contributed equally in this manuscript.

Conflict of interest

The authors declare that they have no conflict of interest.

Data availability

Not applicable.

References:

[1] A.N. Koam and A. Ahmad Barycentric subdivision of Cayley graphs with constant edge metric dimension, IEEE Access **3** (2020) 80624–80628. https://doi.org/10.1109/ACCESS.2020.2990109.

[2] A. Kelenc, D. Kuziak, A. Taranenko and I.G. Yero, Mixed metric dimension of graphs, Appl. Math. Comput. **314** (2017) 429–438. https://doi.org/10.1016/j.amc.2017.07.027

[3] A. Kelenc, N. Tratnik and I.G. Yero, Uniquely identifying the edges of a graph: the edge metric dimension, Discret. Appl. Math. **31** (2018) 204–220. https://doi.org/10.1016/j.dam.2018.05.052.

[4] A. Seb˜o and E. Tannier, On metric generators of graphs, Math. Oper.Res., **29(2)** (2004) 383–393.

[5] B.H. Xing, S.K. Sharma, V.K. Bhat, H. Raza and J.B. Liu, The vertex edge resolvability of some wheel-related graphs, J Math 1859714 (2021). https://doi.org/10.1155/2021/1859714

[6] B. Yang, M. Rafullah, H.M.A. Siddiqui and S. Ahmad, On resolvability parameters of some wheelrelated graphs, J Chem 9259032 (2019). https://doi.org/10.1155/2019/9259032

Received: Oct 30 2022

International Journal of Applied Mathematics

Volume 35 No. 6, 2022

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version

[7] F. Harary and R. A. Melter, On the metric dimension of a graph, Ars Comb. **2** (1976), 191-195.

[8] F. Simonraj and A. George, On the metric dimension of silicate stars, ARPN J. Eng. Appl. Sci. **5** (2015) 2187–2192.

[9] G. Chartrand, L. Eroh, M.A Johnson and O.R Oellermann, Resolvability in graphs and the metric dimension of a graph, Discrete Appl. Math. **105** (2000) 99–113. https://doi.org/10.1016/S0166218X(00)00198-0.

[10] G. Chartrand, V. Saenpholphat and P. Zhang, The independent resolving number of a graph, Math. Bohem. **128** (2003) 379–393.

[11] H.M. Siddiqui and M. Imran, Computing the metric and partition dimension of H-Naphtalenic and VC5C7 nanotubes, J. Optoelectron Adv. Mater.**7(5)** (2015) 790–794.

[12] I. Javaid, M. T. Rahim and K. Ali, Families of regular graphs with constant metric dimension, Util. Math. **75** (2008) 21-34.

[13] K. Liu, and N. Abu-Ghazaleh, Virtual coordinate back tracking for void travarsalin geographic routing, In International Conference on Ad-Hoc Networks and Wireless,Springer, Berlin, Heidelberg **4104** (2006), 46-59.

[14] Y. N. Lamb, Glecaprevir/pibrentasvir: first global approval, Drugs **77(16)** (2017) 1797-1804.

[15] M. Ahsan, Z. Zahid, S. Zafar, A. Rafq, M.S. Sindhu and M. Umar, Computing the edge metric dimension of convex polytopes related graphs, J Math Computer Sci **22** (2021) 174–188. https://doi.org/10.22436/jmcs.022.02.08.

[16] P. J. Slater, Leaves of trees, Proc. 6th Southeastern Conf. Combinatorics, Graph Theory, Comput., Congressus Numerantium, The Netherlands,**14** (1975) 549–559.

[17] M. Imran, S. A. Bokhary and A. Q. Baig, Families of Rotationally-Symmetric Plane Graphs with Constant Metric Dimension, Southeast Asian Bull. Math. **36** (2012), 663-675.

[18] N. Trinajstic, Chemical graph theory, Routledge World Health Organization (2000) Air quality guidelines for Europe. Copenhagen: World Health Organization, Regional Office for Europe. (2018) https://apps.who.int/iris/handle/10665/107335.

[19] P. Erdos and A. R´enyi, On two problems of information theory, Magyar Tud. Akad. Mat. Kutat´o Int. K¨ozl **8** (1963) 229-243.

[20] R.A. Melter and I. Tomescu, Metric bases in digital geometry, Comput. Gr. Image Process **25** (1984)113–121. https://doi.org/10.1016/0734-189X(84)90051-3.

[21] R.C. Tillquist, R.M. Frongillo and M.E. Lladser, Getting the lay of the land in discrete space: A survey of metric dimension and its applications, (2021) arXiv preprint arXiv:2104.07201.

Received: Oct 30 2022

International Journal of Applied Mathematics

Volume 35 No. 6, 2022

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version

[22] V. Chvatal, Mastermind, Combinatorica **3(3)** (1983),325–329. https://doi.org/10.1007/BF02579188.

[23] S. Khuller, B. Raghavachari and A. Rosenfeld, Landmarks in graphs, Disc. Appl. Math., **70** (1996) 217–229.

[24] S.K. Sharma, H. Raza and V.K. Bhat, Computing edge metric dimension of one-pentagonal carbon nanocone, Front Phys 600 (2021). https://doi.org/10.3389/fphy.2021.749166.

[25] S.K. Sharma and V.K. Bhat Metric dimension of heptagonal circular ladder, Discrete Math Algorithms Appl. **13(1)**:2050095. https://doi.org/10.1142/S1793830920500950.

[26] Z. Beerliova, F. Eberhard, T. Erlebach, A. Hall, M. Hoffman, M. Mihalak and L. S. Ram, Network discovery and verification, IEEE J. Sel. Areas Commun. **24** (2006), 2168-2181.

[27] Z. Hussain, M. Munir, A. Ahmad, M. Chaudhary, J.A Khan and I. Ahmed, Metric basis and metric dimension of 1-pentagonal carbon nanocone networks, Sci Rep **10(1)** (2020) 1–7. https://doi.org/10.1038/s41598-020-76516-1.

[28] Z. Raza and M.S. Bataineh The comparative analysis of metric and edge metric dimension of some subdivisions of the wheel graph, Asian Eur. J. Math **14(4)** (2020) 2150062. https://doi.org/10.1142/S1793557121500625.

Received: Oct 30 2022