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Edge Resolvability of Certain Chemical Compounds used in Hepatitis-C treatment

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Abstract

The representation of molecules by graphs, where the vertices and edges of the graphs are the atoms and the valence bonds between a pair of atoms, respectively, is the most successful use of graph theory in chemistry. Graph theory encompasses various parameters, with the dimension of edge metric being a distinct and significant parameter. The edge metric dimension is a fundamental concept in graph theory that extends the notion of metric dimension from vertices to edges. This notion involves selecting specific vertices, wherein each graph edge possesses a distinct location or identification. Resolving sets were specifically applied in pharmaceutical research to find patterns shared by several different drugs. Since very early times, medicinal drugs have played a significant part in human civilization. In this article, we study the edge metric dimension for the typical molecular structures of two important drugs namely pibrentasvir (P_{80}) and vancomycin (V_{101}).

Keywords: Pibrentasvir, chemical graph, edge metric dimension, vancomycin, independent set.

1. Introduction

The concept of metric dimension has proven to be applicable across various sectors within the fields of science and technology. Image processing, sonar and coastguard loran [1], combinatorial optimization [2], computer networks [3], weighing problems [4], robot navigation [5], facility location problems, etc are some of the areas in which metric resolvability parameters have applications. Due to the wide range of application, the notion of metric dimension is usually applied to address many complex issues. It may be used in a variety of fields, including computer science, networking, molecular topology, industrial chemistry, and chemistry. Chemical graph theory (CGT) examines all facets of how graph theory is used to many branches of chemistry, such as computational, theoretical, and organic chemistry, as well as bioinformatics and computational biology. CGT makes it easier to examine numerous chemical networks, complicated structures, and topologies that take the form of a graph and are challenging to analyse in their natural state [6]. In CGT, vertices stand in for atoms, while edges connecting the vertices represent the bonds that hold the atoms together. Medicinal 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 edge metric basis and dimension of certain significant drugs (namely 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 [7]. The Chemical Structure of pibrentasvir is presented in Figure 1. Pibrentasvir was approved in the EU, Iceland, Liechtenstein and Norway on 28 July 2017 for the treatment of HCV infection in adults [8]. Non-structural 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 received the generic name vancomycin, derived

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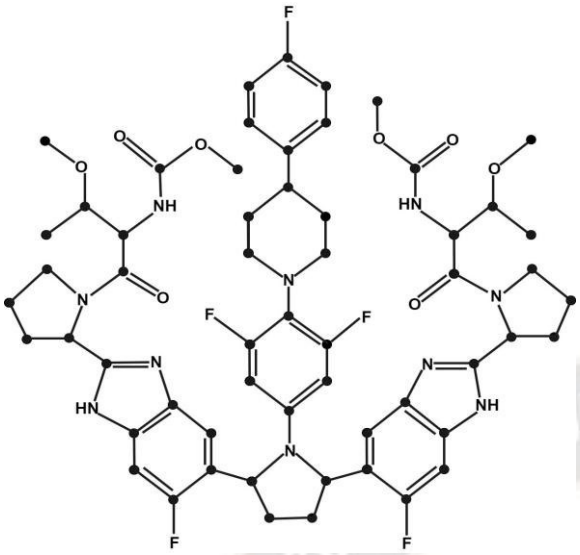

Figure 1. Chemical Structure of Pibrentasvir

from the term "vanquish". The molecular formula of vancomycin is $C_{66}H_{75}Cl_2N_9O_{24}$ and its chemical structure is shown in Figure 2. 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}.

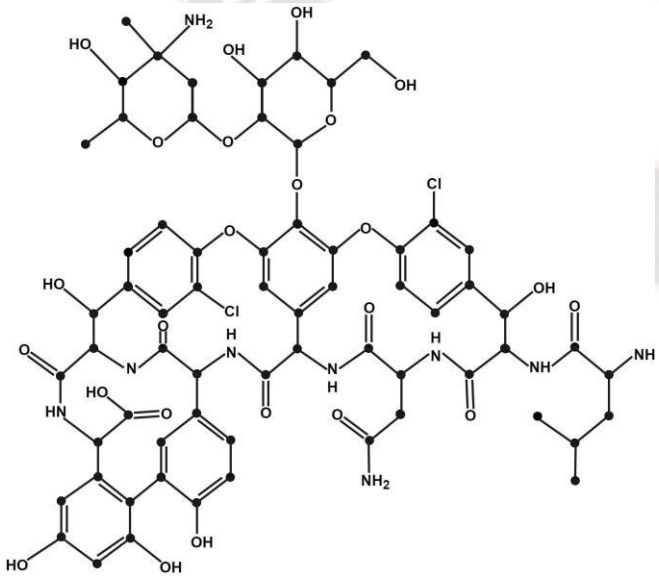

Figure 2. Chemical Structure of Vancomycin

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 difficile, 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, metric dimension and edge metric dimension respectively.

1.2. Motivation and Novelty:

Assigning unique positions to each edge in a graph with respect to a subset of vertices in that graph is of great interest. In chemistry, there are numerous important compounds which have very complex chemical structure and are not easy to study in their original structure. By assigning unique representation to each edge of the chemical graph obtained from chemical structure, the study of that chemical structure becomes easy.

The drugs like pibrentasvir and vancomycin has been of utmost importance because of their applicability in human life. The chemical structures of both the drugs are very complex to study in their original form. This motivates

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us to work on unique edge identification of these two significant drugs. To the best of our knowledge, no such study related to these drugs has been done in the past. This leads us to work on edge metric basis and dimension of P_{80} and V_{101}.

1.3. Chemical Graph Theory and Parameters of Resolvability:

Chemical graph theory (CGT) is a branch of mathematical chemistry that explores the implications of connectedness within a chemical graph. This interdisciplinary field employs graph theoretical and computational methods to investigate pertinent mathematical inquiries, specifically analyzing the chemical structure of chemical substances as graphs. Over the past few decades, chemical graph theory has witnessed significant growth, offering a plethora of novel and inventive concepts for such investigations. In essence, it encompasses all aspects of applying graph theory to chemistry. Chemical structures that are huge and complicated in their initial form are made simpler via CGT. A detailed analysis of structures may be done after transforming a molecular structure into a graph [9]. Pibrentasvir and vancomycin and are two most important chemical compounds that have their application in medicinal drugs of fatal diseases. Metric dimension and its more recently developed variants are the most significant and well explored graph theory parameters. So, in accordance with this theme, in this study we analyze the edge metric dimension for the chemical graph of pibrentasvir and vancomycin.

Slater [1] coined the term "locating set" in 1975 to illustrate the problem of identifying the position of invaders in a network and this is also where the idea of metric dimension was initially introduced. In a similar vein, Harary and Melter [10] independently introduced the same idea in 1976, but they termed to it as a "resolving set". Many studies on the theoretical properties and numerous applications of this invariant have been done since the publication of these two important papers. As an example, Melter and Tomescu [6] used the concept of resolving set to pattern recognition and image processing. The metric dimension was used by C´aceres et al. [11] to solve problems involving coin weighing and mastermind games. Khuller et al. [5] applied the concept of metric dimension in robot navigation. The use of metric dimension in the domain of chemistry was studied by Chartrand et al. [12]. Sebo and Tannier [13] examined the concept of metric dimension related to combinatorial optimization. Various types of resolving sets have been developed in the literature to enhance comprehension of the metric dimension concept. Similarly to a resolving set, it is conceivable that a pair of edges can be resolved in relation to a specific set of vertices chosen, rather than solely focusing on two individual vertices of a graph. Kelenc et al. [14] introduced a new term namely edge metric dimension to describe this concept. In the same way, Kelenc et al. [15] presented a novel version of dimension called mixed metric dimension, which identify each vertex as well as edge of a connected graph uniquely.

For a number of graph families with substantial significance, researchers have examined the resolvability parameters. For instance, Koam and Ahmad [16] studied the edge resolvability for barycentric subdivision of Cayley graph. The comparison between the vertex resolvability and edge resolvability of some wheel graphs were analyzed by Raza and Bataineh [17]. Ahsan et al. [8], Sharma and Bhat [18] calculated metric dimension and edge metric dimension for some families of convex polytopes. Mixed resolving sets ad mixed metric dimesion for a few graphs including wheels were investigated by Xing et al. [19]. The metric dimension of some network of carbon nanocones was studied by Hussain et al. [20] and edgemetric dimension for network of 1-pentagonal carbon nanocone was examined by Sharma and Bhat [21]. Simonraj and George [2] investigated the vertex resolvability of silicate star was networks. The same idea was also taken into consideration by Yang et al. [22] for some chemical structures which are related to wheel graphs. The vertex resolvability of H-Naphtalenic as well as $V\ C_5C_7$ nanotubes were examined by Siddiqui and Imran [23]. Raza and Bataineh [17] compare metric dimension and edge metric dimension for some sudivisions of wheel graph. One can refer Khuller et al. [5]; Javaid and Rahim [24]; Rashid et al. [25]; Imran et al. [26].

The article is arranged in the following manner: some basic definitions related to resolving set, metric dimension and edge metric dimension have been presented in section 2. The chemical graph of pibrentasvir is discussed in section 3 and edge metric dimension of P_{80} has been computed in the same section. Section 4 consists of chemical graph of

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vancomycin, edge metric dimension of V_{101} and independent resolving number of V_{101}. Conclusion and limitation of the applied technique is discussed in section 5.

2. Preliminaries

We discuss some fundamental ideas and concepts about the edge metric dimension of graphs in this particular section.

Let $\Gamma = (V,E)$ 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 x and y determines the topological distance $d(x,y)$ between them in a non-trivial connected network. The topological distance $d(x,ab)$ between the vertex x and edge ab in a non-trivial connected network is $min\{d(x,a),d(x,b)\}$. The degree (valency) of a vertex is the number of all edges that incident to that vertex.

Definition 1. Resolving Set: [1] Let $\Gamma = (V,E)$ be a simple connected graph and $L_r = \{z_1,z_2,z_3,...,z_k\}$ be an ordered subset of vertices. Then the k-vector $\varsigma(w|L_r) = ((d(w|z_1),d(w|z_2),d(w|z_3),...,d(w|z_k))$ is the metric code of a vertex w with respect to the set L_r. Then we say L_r resolves two vertices $r,q \in V$ if $\varsigma(r|L_r) \neq \varsigma(q|L_r)$. If each pair of distinct vertices in Γ is resolved by L_r, then L_r is termed as resolving set for Γ.

Definition 2. Edge Resolving Set:[25] Let $\Gamma = (V,E)$ be a simple connected graph and $E_r =$

$\{z_1,z_2,z_3,...,z_k\}$ be an ordered subset of vertices. Then the k-vector $\varsigma(cd|H_r) = ((d(cd|z_1),d(cd|z_2),d(cd|z_3),$ $...,d(cd|z_k))$ is the edge metric code of an edge cd with respect to the set E_r. Then we say E_r resolves two edges $pq,tu \in E$ if $\varsigma(pq|E_r) \neq \varsigma(tu|E_r)$. If each pair of distinct edges in Γ is resolved by E_r, then E_r is termed as edge resolving set for Γ.

Definition 3. Metric Dimension: [1] A resolving set with minimum number of elements in it is termed as metric basis for the graph Γ and cardinality of metric basis is known as metric dimension Γ and it is represented as $dim(\Gamma)$.

Definition 4. Edge Metric Dimension: [25] An edge resolving set with minimum number of elements in it is termed as edge metric basis for the graph Γ and cardinality of edge metric basis is known as edge metric dimension of Γ and it is represented as $edim(\Gamma)$.

Definition 5. Independent Set: [30] A subset of vertices in a graph in which there is no pair of vertices that are adjacent is called as independent set.

Definition 6. Independent edge resolving set: [23] A subset B of vertices in a graph which is both independent and edge 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. Edge Basis and Metric Dimension of (P_{80})

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

The Chemical Graph of P_{80}:

The chemical graph of P_{80} consists of 80 vertices and 89 edges. It contains five 6 cycles and five 5 cycles. The number of vertices as well as edges to the left of c_{26} are equal to the number of vertices as well as edges to the right of c_{23} in the chemical graph of P_{80}. This symmetry helps in finding of edge metric codes for the structure. This chemical graph is represented in Figure 3 and the red coloured vertices in Figure 3 represent those vertices which are present in minimal edge resolving set of P_{80}.

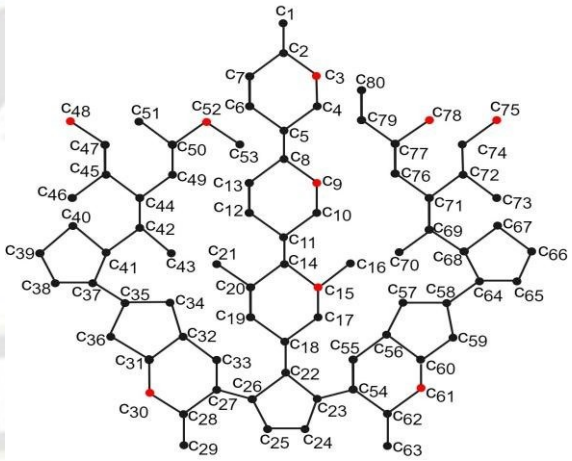

Figure 3. Chemical graph of P_{80}

Theorem 1. *The edge metric dimension of P_{80} is 9 i.e., $edim(P_{80}) = 9$.*

Proof. Let $E_r = \{c_3,c_9,c_{15},c_{30},c_{48},c_{52},c_{61},c_{75},c_{78}\}$ be a subset of vertices of P_{80}. We will show that the set E_r will serve as edge resolving set and is with smallest number of vertices i.e., E_r serves as edge metric basis for P_{80}. The edge metric codes for the edges in P_{80} are presented in Table 1.

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Table 1. Edge Metric codes for the edges of P_{80}

Edge Metric codes	Corresponding values	Edge Metric codes	Corresponding values
$\varsigma(c_1c_2\|E_r)$	(1,5,9,16,25,25,16,25,25)	$\varsigma(c31c36\|Er)$	(16,12,8,1,8,8,9,18,18)
$\varsigma(c_2c_3\|E_r)$	(0,4,8,15,24,24,15,24,24)	$\varsigma(c35c37\|Er)$	(17,13,9,3,6,6,10,19,19)
$\varsigma(c_3c_4\|E_r)$	(0,3,7,14,23,23,14,23,23)	$\varsigma(c37c41\|Er)$	(18,14,10,4,5,5,11,20,20)
$\varsigma(c_4c_5\|E_r)$	(1,2,6,13,22,22,13,22,22)	$\varsigma(c37c38\|Er)$	(18,14,10,4,6,6,11,20,20)
$\varsigma(c_5c_6\|E_r)$	(2,2,6,13,22,22,13,22,22)	$\varsigma(c38c39\|Er)$	(19,15,11,5,7,7,12,21,21)
$\varsigma(c_6c_7\|E_r)$	(2,3,7,14,23,23,14,23,23)	$\varsigma(c39c40\|Er)$	(20,16,12,6,6,6,13,22,22)
$\varsigma(c_2c_7\|E_r)$	(1,4,8,15,24,15,24,24,24)	$\varsigma(c40c41\|Er)$	(19,15,11,5,5,5,12,21,21)
$\varsigma(c_5c_8\|E_r)$	(2,1,5,12,21,21,12,21,21)	$\varsigma(c41c42\|Er)$	(19,15,11,5,4,4,12,21,21)
$\varsigma(c_8c_9\|E_r)$	(3,0,4,11,20,20,11,20,20)	$\varsigma(c42c43\|Er)$	(20,16,12,6,4,4,13,22,22)
$\varsigma(c9c10\|Er)$	(4,0,3,10,19,19,10,19,19)	$\varsigma(c42c44\|Er)$	(20,16,12,6,3,3,13,22,22)
$\varsigma(c10c11\|Er)$	(5,1,2,9,18,18,9,18,18)	$\varsigma(c44c45\|Er)$	(21,17,13,7,2,3,14,23,23)
$\varsigma(c11c12\|Er)$	(5,2,2,9,18,18,9,18,18)	$\varsigma(c45c46\|Er)$	(22,18,14,8,2,4,15,24,24)
$\varsigma(c12c13\|Er)$	(4,2,3,10,19,19,10,19,19)	$\varsigma(c45c47\|Er)$	(22,18,14,8,1,4,15,24,24)
$\varsigma(c8c13\|Er)$	(3,1,4,11,20,20,11,20,20)	$\varsigma(c47c48\|Er)$	(23,19,15,9,0,5,16,25,25)
$\varsigma(c11c14\|Er)$	(6,2,1,8,17,17,8,17,17)	$\varsigma(c44c49\|Er)$	(21,17,13,7,3,2,14,23,23)
$\varsigma(c14c15\|Er)$	(7,3,0,7,16,16,7,16,16)	$\varsigma(c49c50\|Er)$	(22,18,14,8,4,1,15,24,24)
$\varsigma(c15c16\|Er)$	(8,4,0,7,16,16,7,16,16)	$\varsigma(c50c51\|Er)$	(23,19,15,9,5,1,16,25,25)
$\varsigma(c15c17\|Er)$	(8,4,0,6,15,15,6,15,15)	$\varsigma(c50c52\|Er)$	(23,19,15,9,5,0,16,25,25)
$\varsigma(c17c18\|Er)$	(9,5,1,5,14,14,5,14,14)	$\varsigma(c52c53\|Er)$	(24,20,16,10,6,0,17,26,26)
$\varsigma(c18c19\|Er)$	(9,5,2,5,14,14,5,14,14)	$\varsigma(c23c54\|Er)$	(12,8,4,5,14,14,2,11,11)
$\varsigma(c19c20\|Er)$	(8,4,2,6,15,15,6,15,15)	$\varsigma(c54c62\|Er)$	(13,9,9,6,15,15,1,11,11)
$\varsigma(c14c20\|Er)$	(7,3,1,7,16,16,7,16,16)	$\varsigma(c62c63\|Er)$	(14,10,6,7,16,16,1,11,11)
$\varsigma(c20c21\|Er)$	(8,4,2,7,16,16,7,16,16)	$\varsigma(c61c62\|Er)$	(14,10,6,7,16,16,0,10,10)
$\varsigma(c18c22\|Er)$	(10,6,2,4,13,13,4,13,13)	$\varsigma(c60c61\|Er)$	(15,11,7,8,17,17,0,9,9)
$\varsigma(c22c23\|Er)$	(11,7,3,4,13,13,3,12,12)	$\varsigma(c56c60\|Er)$	(15,11,7,8,17,17,1,9,9)
$\varsigma(c23c24\|Er)$	(12,8,4,5,14,14,3,12,12)	$\varsigma(c55c56\|Er)$	(14,10,6,7,16,16,2,9,9)
$\varsigma(c24c25\|Er)$	(13,9,5,4,13,13,4,13,13)	$\varsigma(c54c55\|Er)$	(13,9,5,6,15,15,2,10,10)
$\varsigma(c25c26\|Er)$	(12,8,4,12,12,5,14,14)	$\varsigma(c59c60\|Er)$	(16,12,8,9,18,18,1,8,8)
$\varsigma(c22c26\|Er)$	(11,7,3,3,12,12,4,13,13)	$\varsigma(c58c59\|Er)$	(17,13,9,10,19,19,2,7,7)
$\varsigma(c26c27\|Er)$	(12,8,4,2,11,11,5,14,14)	$\varsigma(c57c58\|Er)$	(16,12,8,9,18,18,3,7,7)
$\varsigma(c27c28\|Er)$	(13,9,5,1,11,11,6,15,15)	$\varsigma(c56c57\|Er)$	(15,11,7,8,17,17,2,8,8)
$\varsigma(c28c29\|Er)$	(14,10,6,1,11,11,1,16,16)	$\varsigma(c58c64\|Er)$	(17,13,9,10,19,19,3,6,6)
$\varsigma(c28c30\|Er)$	(14,10,6,0,10,10,7,16,16)	$\varsigma(c64c65\|Er)$	(18,14,10,11,20,20,4,6,6)

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$\varsigma(c30c31\|Er)$	(15,11,7,0,9,9,8,17,17)	$\varsigma(c65c66\|Er)$	(19,15,11,12,21,21,5,7,7)
$\varsigma(c31c32\|Er)$	(15,11,7,1,9,9,8,17,17)	$\varsigma(c66c67\|Er)$	(20,16,12,13,22,22,6,6,6)
$\varsigma(c32c33\|Er)$	(14,10,6,2,9,9,7,16,16)	$\varsigma(c67c68\|Er)$	(19,15,11,12,21,21,5,5,5)
$\varsigma(c26c33\|Er)$	(13,9,5,2,10,10,6,15,15)	$\varsigma(c64c68\|Er)$	(18,14,10,11,20,20,4,5,5)
$\varsigma(c32c34\|Er)$	(15,11,7,2,8,8,8,17,17)	$\varsigma(c68c69\|Er)$	(19,15,11,12,21,21,5,4,4)
$\varsigma(c34c35\|Er)$	(16,12,8,3,7,7,9,18,18)	$\varsigma(c69c70\|Er)$	(20,16,12,13,22,22,6,4,4)
$\varsigma(c35c36\|Er)$	(17,13,9,2,7,7,10,19,19)	$\varsigma(c69c71\|Er)$	(20,16,12,13,22,22,6,3,3)
$\varsigma(c71c72\|Er)$	21,17,13,14,23,23,7,2,3)	$\varsigma(c72c73\|Er)$	(22,18,14,15,24,24,8,2,4)
$\varsigma(c72c74\|Er)$	(22,18,14,15,24,24,8,1,4)	$\varsigma(c74c75\|Er)$	(23,19,15,16,25,25,9,0,5)
$\varsigma(c71c76\|Er)$	(21,17,13,14,23,23,7,3,2)	$\varsigma(c76c77\|Er)$	(22,18,14,15,24,24,8,4,1)
$\varsigma(c77c78\|Er)$	(23,19,15,16,25,25,9,5,0)	$\varsigma(c77c79\|Er)$	(23,19,15,16,25,25,9,5,1)
$\varsigma(c79c80\|Er)$	(24,20,16,17,26,26,10,6,2)		

From the Table 1, it is clear that the metric code respresentation for each edge of P_{80} is unique, so $edim(P_{80}) \leq 9$. Now, it only remains to show that $edim(P_{80}) \geq 9$.

If none of the vertices among $\{c_3,c_4,c_6,c_7\}$ is not involved in the edge resolving set, E_r then the edge metric codes for two different edges becomes identical. So, one among the vertices $\{c_3,c_4,c_6,c_7\}$ must be included in E_r. Similarly, one among the vertices $\{c_9,c_{10},c_{12},c_{13}\}$ must be included in E_r.

In the same way, if at least one vertex from each of the sets $\{c_{15},c_{17},c_{19},c_{20}\}$, $\{c_{47},c_{48},c_{50},c_{51}\}$, $\{c_{74},c_{75},c_{77},c_{78}\}$, $\{c_{51},c_{52}\}$, $\{c_{79},c_{78}\}$, $\{c_{30},c_{32}\}$ and $\{c_{56},c_{61}\}$ are not taken in E_r then metric codes for two different edges becomes identical. So, one vertex from each of these sets must be included in E_r. From the above discussion, it follows that $edim(P_{80}) \geq 9$. This completes the proof of the theorem. □

Corollary 1. *The independent edge resolving number of P_{80} is 9.*

4. Edge Basis and Edge Metric Dimension of V_{101}

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

The Chemical Graph of Graph of 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 chemical graph of V_{101}, as shown in Figure 4, consists of 101 vertices ad 110 edges. It contains seven 6 cycles. The red coloured vertices in Figure 4 represent those vertices which are present in minimal edge resolving set of V_{101}.

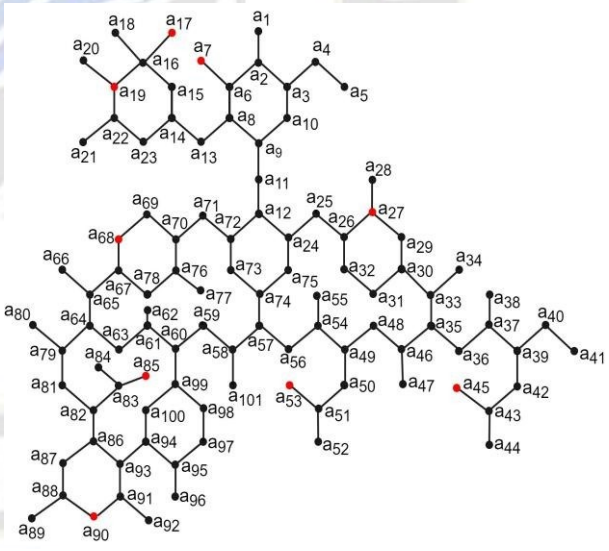

Figure 4. Chemical graph of V_{101}

Theorem 1. *The edge metric dimension of V_{101} is 9 i.e., $edim(V_{101}) = 9$.*

Proof. Let $E_r = \{a_7,a_{17},a_{19},a_{27},a_{45},a_{53},a_{68},a_{85},a_{90}\}$ be a subset of vertices of V_{101}. We will prove that E_r is edge resolving set with smallest number of vertices i.e., E_r serves as edge metric basis for V_{101}. The edge metric codes for the edges in V_{101} are given in Table 2 and Table 3.

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Table 2. Edge Metric codes for the edges of V_{101}

Edge Metric codes	Corresponding values	Edge Metric codes	Corresponding values
$\varsigma(a_1a_2\|E_r)$	(2,7,7,9,19,15,10,18,18)	$\varsigma(a19a22\|Er)$	(6,2,0,11,21,17,12,20,20)
$\varsigma(a_2a_3\|E_r)$	(2,7,7,8,18,14,9,17,17,)	$\varsigma(a21a22\|Er)$	(6,3,1,11,21,17,12,20,20)
$\varsigma(a_3a_4\|E_r)$	(3,8,8,8,18,14,9,17,17)	$\varsigma(a22a23\|Er)$	(5,3,1,10,20,16,11,19,19)
$\varsigma(a_4a_5\|E_r)$	(4,9,9,9,19,15,10,18,18)	$\varsigma(a14a23\|Er)$	(4,3,2,9,19,15,10,18,18)
$\varsigma(a_2a_6\|E_r)$	(1,6,6,8,18,14,9,17,17)	$\varsigma(a12a24\|Er)$	(5,8,8,3,13,9,5,13,12)
$\varsigma(a_6a_7\|E_r)$	(0,6,6,8,18,14,9,17,17)	$\varsigma(a24a25\|Er)$	(6,9,9,2,12,9,6,14,12)
$\varsigma(a_6a_8\|E_r)$	(1,5,5,7,17,13,8,16,16)	$\varsigma(a25a26\|Er)$	(7,10,10,1,11,10,7,15,13)
$\varsigma(a_8a_9\|E_r)$	(2,5,5,6,16,12,7,15,15)	$\varsigma(a26a27\|Er)$	(8,11,11,0,10,10,8,16,14)
$\varsigma(a9a10\|Er)$	(3,6,6,6,16,12,7,15,15)	$\varsigma(a27a28\|Er)$	(9,12,12,0,10,10,9,17,15)
$\varsigma(a3a10\|Er)$	(3,7,7,7,17,13,8,16,16)	$\varsigma(a27a29\|Er)$	(9,12,12,0,9,9,9,17,15)
$\varsigma(a9a11\|Er)$	(3,6,6,5,15,11,6,14,14)	$\varsigma(a29a30\|Er)$	(10,13,13,1,8,8,10,18,16)
$\varsigma(a11a12\|Er)$	(4,7,7,4,14,10,5,13,13)	$\varsigma(a30a31\|Er)$	(10,13,13,2,8,8,10,18,16)
$\varsigma(a8a13\|Er)$	(2,4,4,7,17,13,8,16,16)	$\varsigma(a31a32\|Er)$	(9,12,12,2,9,9,9,17,15)
$\varsigma(a13a14\|Er)$	(3,3,3,8,18,14,9,17,17)	$\varsigma(a26a32\|Er)$	(8,11,11,1,10,10,8,16,14)
$\varsigma(a14a15\|Er)$	(4,2,2,9,19,15,10,18,18)	$\varsigma(a30a33\|Er)$	(11,14,14,2,7,7,11,18,16)
$\varsigma(a15a16\|Er)$	(5,1,1,10,20,16,11,19,19)	$\varsigma(a33a34\|Er)$	(12,15,15,3,7,7,12,18,16)
$\varsigma(a16a17\|Er)$	(6,0,1,11,21,17,12,20,20)	$\varsigma(a33a35\|Er)$	(12,15,15,3,6,6,12,17,15)
$\varsigma(a16a18\|Er)$	(6,1,1,11,21,17,12,20,20)	$\varsigma(a35a36\|Er)$	(13,16,16,4,5,6,13,17,15)
$\varsigma(a16a19\|Er)$	(6,1,0,11,21,17,12,20,20)	$\varsigma(a36a37\|Er)$	(14,17,17,5,4,7,14,18,16)
$\varsigma(a19a20\|Er)$	(7,2,0,12,22,18,13,21,21)	$\varsigma(a37a38\|Er)$	(15,18,18,6,4,8,15,19,17)
$\varsigma(a37a39\|Er)$	(15,18,18,6,3,8,15,19,17)	$\varsigma(a69a70\|Er)$	(8,11,11,7,17,11,1,9,11)
$\varsigma(a39a40\|Er)$	(16,19,19,7,3,9,16,20,18)	$\varsigma(a70a71\|Er)$	(7,10,10,6,16,10,2,10,12)
$\varsigma(a40a41\|Er)$	(17,20,20,8,4,10,17,21,19)	$\varsigma(a71a72\|Er)$	(6,9,9,5,15,9,3,11,12)
$\varsigma(a39a42\|Er)$	(16,19,19,7,2,9,16,20,18)	$\varsigma(a12a72\|Er)$	(5,8,8,4,14,9,4,12,12)
$\varsigma(a42a43\|Er)$	(17,20,20,8,1,10,17,21,19)	$\varsigma(a72a73\|Er)$	(6,9,9,5,14,8,4,12,11)
$\varsigma(a43a45\|Er)$	(18,21,21,9,0,11,18,22,20)	$\varsigma(a73a74\|Er)$	(7,10,10,5,13,7,5,12,10)
$\varsigma(a43a44\|Er)$	(18,21,21,9,1,11,18,22,20)	$\varsigma(a74a75\|Er)$	(7,10,10,4,13,7,6,12,10)
$\varsigma(a35a46\|Er)$	(13,16,16,4,6,5,12,16,14)	$\varsigma(a24a75\|Er)$	(6,9,9,3,13,8,6,13,11)
$\varsigma(a46a47\|Er)$	(14,17,17,5,7,5,12,16,14)	$\varsigma(a57a74\|Er)$	(8,11,11,5,12,6,6,11,9)
$\varsigma(a46a48\|Er)$	(13,17,17,5,7,4,11,15,13)	$\varsigma(a76a77\|Er)$	(9,12,12,8,18,12,3,9,11)

$\varsigma(a48a49\|Er)$	(12,15,15,6,8,3,10,14,12)	$\varsigma(a70a76\|Er)$	(8,11,11,7,17,11,2,9,11)
$\varsigma(a49a50\|Er)$	(12,15,15,7,9,2,10,14,12)	$\varsigma(a76a78\|Er)$	(9,12,12,8,18,12,2,8,10)
$\varsigma(a50a51\|Er)$	(13,16,16,8,10,1,11,15,13)	$\varsigma(a67a78\|Er)$	(10,13,13,9,19,13,1,7,9)
$\varsigma(a51a53\|Er)$	(14,17,17,9,11,0,12,16,14)	$\varsigma(a64a79\|Er)$	(13,16,16,12,18,12,3,4,6)
$\varsigma(a51a52\|Er)$	(14,17,17,9,11,1,12,16,14)	$\varsigma(a79a80\|Er)$	(14,17,17,13,19,13,4,4,6)
$\varsigma(a49a54\|Er)$	(11,14,14,7,9,3,9,13,11)	$\varsigma(a79a81\|Er)$	(14,17,17,13,19,13,4,3,5)
$\varsigma(a54a55\|Er)$	(11,14,14,8,10,4,9,13,11)	$\varsigma(a81a82\|Er)$	(15,18,18,14,20,14,5,2,4)
$\varsigma(a54a56\|Er)$	(10,13,13,7,10,4,8,12,10)	$\varsigma(a82a83\|Er)$	(16,19,19,15,21,15,6,1,4)
$\varsigma(a56a57\|Er)$	(9,12,12,6,11,5,7,11,9)	$\varsigma(a83a84\|Er)$	(17,20,20,16,22,16,7,1,5)
$\varsigma(a57a58\|Er)$	(9,12,12,6,12,6,7,10,8)	$\varsigma(a83a85\|Er)$	(17,20,20,16,22,16,7,0,5)
$\varsigma(a58a59\|Er)$	(10,13,13,7,13,7,7,9,7)	$\varsigma(a82a86\|Er)$	(16,19,19,14,20,14,6,2,3)
$\varsigma(a59a60\|Er)$	(11,14,14,8,14,8,6,8,6)	$\varsigma(a86a87\|Er)$	(17,20,20,14,20,14,7,3,2)
$\varsigma(a60a61\|Er)$	(12,15,15,9,15,9,5,7,6)	$\varsigma(a87a88\|Er)$	(18,21,21,15,21,15,8,4,1)
$\varsigma(a61a62\|Er)$	(13,16,16,10,16,10,5,7,7)	$\varsigma(a88a89\|Er)$	(19,22,22,16,22,16,9,5,1)
$\varsigma(a61a63\|Er)$	(13,16,16,10,16,10,4,6,7)	$\varsigma(a88a90\|Er)$	(18,21,21,15,21,15,9,5,0)
$\varsigma(a63a64\|Er)$	(13,16,16,11,17,11,3,5,7)	$\varsigma(a90a91\|Er)$	(17,20,20,14,20,14,9,5,0)
$\varsigma(a64a65\|Er)$	(12,15,15,11,18,12,2,5,7)	$\varsigma(a91a92\|Er)$	(17,20,20,14,20,14,9,5,1)
$\varsigma(a65a66\|Er)$	(12,15,15,11,19,13,2,6,8)	$\varsigma(a91a93\|Er)$	(16,19,19,13,19,13,8,4,1)
$\varsigma(a65a67\|Er)$	(11,14,14,10,19,13,1,6,8)	$\varsigma(a86a93\|Er)$	(16,19,19,13,19,13,7,3,2)
$\varsigma(a67a68\|Er)$	(10,13,13,9,19,13,0,7,9)	$\varsigma(a93a94\|Er)$	(15,18,18,12,18,12,8,4,2)

Table 3. Edge Metric co-ordinates for the edges of V_{101}

Edge Metric codes	Corresponding values	Edge Metric codes	Corresponding values
$\varsigma(a68a69\|Er)$	(9,12,12,8,18,12,0,8,10)	$\varsigma(a58a101\|Er)$	(10,3,13,7,13,7,8,10,8)
$\varsigma(a94a95\|Er)$	(15,18,18,12,18,12,9,5,3)	$\varsigma(a95a96\|Er)$	(16,19,19,13,19,13,10,6,4)
$\varsigma(a95a97\|Er)$	(15,18,18,12,18,12,9,6,4)	$\varsigma(a97a98\|Er)$	(14,17,17,11,17,11,8,7,5)
$\varsigma(a98a99\|Er)$	(13,16,16,10,16,10,7,7,5)	$\varsigma(a99a100\|Er)$	(13,16,16,10,16,10,7,6,4)
$\varsigma(a94a100\|Er)$	(14,17,17,11,17,11,8,5,3)	$\varsigma(a60a99\|Er)$	(12,15,15,9,15,9,6,7,5)

From the above Table 2 and Table 3, it is clear that each edge of V_{101} has unique metric code representation, so $edim(V_{101}) \leq 9$. Now, it only remains to show that $edim(V_{101}) \geq 9$.

If none of the vertices among $\{a_1,a_2,a_6,a_7\}$ is not involved in the edge resolving set E_r then the edge metric codes for two different edges becomes identical. So, one among the vertices $\{a_1,a_2,a_6,a_7\}$ must be included in E_r.

In the similar way, if no vertices among $\{a_{18},a_{19},a_{21}\}$ is not included in the edge resolving set E_r then the edge metric codes for two different edges have been found to be equal. So, one among the vertices

$\{a_{18},a_{19},a_{21}\}$ must be included in E_r.

Similarly, if at least one vertex from each of the sets $\{a_{17},a_{18}\}$, $\{a_{27},a_{29},a_{31},a_{32}\}$, $\{a_{98},a_{99},a_{76},a_{78}\}$, $\{a_{44},a_{45}\}$, $\{a_{52},a_{53}\}$ and $\{a_{90},a_{92}\}$ are not present in E_r then the edge metric codes for two different edges becomes equal. So, one vertex from each of these sets must be included in the edge resolving set

E_r.

From the above discussion, it follows that $edim(V_{101}) \geq 9$. This completes the proof of the theorem. □

Corollary 2. *The independent edge resolving number of* V_{101} *is* 9.

5. Conclusion

In this article, the edge metric basis as well as on the respective dimensions of the two famous drugs viz., P_{80} and V_{101} are studied. We have shown for these two drugs that $edim(P_{80}) = 9 = edim(V_{101})$. We also proved that the edge resolving set for both of the structures are independent. In this study, the focus is only on assigning unique position to each edges of the chemical graphs in terms of distances. However this method is not applicable if unique position to each edge and each vertex of chemical graph is taken into consideration.

One may consider resolving sets for these two drugs which will identify each vertex and each edge of the chemical graphs uniquely. This study may help the chemists in research related to medicines for discovering patterns common to a variety of drugs. In future, we will discuss various other recently introduced variations of the metric dimension (such as, local metric dimension, partition dimension, etc.) for the these two globally important significant drugs viz., P_{80} and V_{101}.

6. Declarations

Ethical Approval

There is no need for an ethical investigation.

Competing interests

The authors affirm that they do not have any competing interests.

Availability of data and materials

The results of this study were not supported by any data or software, nor were any data or software created.

References

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

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

3 P. Manuel, R. Bharati, and I. Rajasingh, *On minimum metric dimension of honeycomb networks*, J. Discrete Algorithms **6(1)** (2008) 20-27.

4 S. S¨oderberg and H. S. Shapiro, *A combinatory detection problem*, The American Mathematical Monthly **70(10)** (1963) 1066-1070.

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

6 R.A. Melter and I. Tomescu, *Metric bases in digital geometry*, Comput. Gr. Image Process. **25** (1984)113–121. 4-189X(84)90051-3.

7 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.

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

9 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.

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

11 J. Ca´ceres, C. Hernando, M. Mora, I. M. Pelayo, M. L. Puertas, C. Seara, et al., ”On the metric dimension of Cartesian products of graphs”, SIAM J. Discrete Math., **21(2)** (2007) 423-441.

12 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/S0166-218X(00)00198-0.

13 A. Sebo˜ and E. Tannier, *On metric generators of graphs*, Math. Oper. Res., **29(2)** (2004) 383–393.

14 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.

15 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

16 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.

17 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.

18 Sharma, S. K., & Bhat, V. K. (2020, December). Location Number of Edges and Vertices of Two-Fold Hepta-Pentagonal Circular Ladder. In International Conference on" Applied Nonlinear Analysis and Soft Computing" (pp. 131-145). Singapore: Springer Nature Singapore.

19 Liu, J. B., Aslam, M. K., & Javaid, M. (2020). Local fractional metric dimensions of rotationally symmetric and planar networks. IEEE Access, 8, 82404-82420.

20 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.

21 Raj, F. S., & George, A. (2015, March). Network embedding on planar octahedron networks. In 2015 IEEE international conference on electrical, computer and communication technologies (ICECCT) (pp. 1-6). IEEE.

22 B. Yang, M. Rafullah, H.M.A. Siddiqui and S. Ahmad, *On resolvability parameters of some wheel-related graphs*, J. Chem. 9259032 (2019). https://doi.org/10.1155/2019/9259032

23 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.

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

25 Sivagami, P., & Rajasingh, I. (2016). T-coloring of certain networks. Mathematics in Computer Science, 10(2), 239-248.

26 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.

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