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EDGE-BASED STUDY FOR MOLECULAR GRAPHS OF SURAMIN AND ACEMANNAN

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Abstract:

The most significant use of graph theory in chemistry is the modelling of molecules by graphs, where atoms and valence bonds between atoms are represented as the graphs' vertices and edges, respectively. Minimum resolving sets (edges or vertices) are now fundamental to combinatorial chemistry and molecular topology. Resolving sets for a given network include important information needed to uniquely identify every object on the network. In pharmaceutical research, resolving sets were especially used to identify patterns shared by several drugs. Medicinal drugs have been a major component of human society since very early times. In the present manuscript, minimum edge resolving sets for the molecular graph of some important drugs, namely Suramin (S_{86}) and Acemannan (A_{116}) have been taken into consideration.

MSC(2020): 05C10, 05C12, 68R10.

Keywords: Suramin, molecular graph, resolving set, acemannan, minimum edge resolving set.

1 Introduction

The area of graph theory that addresses both chemistry and mathematics is called Chemical graph theory. Chemical graph theory is the study of different chemical structures from a graph viewpoint. In their native condition, complex, large-scale chemical structures are challenging to study. To then make sense of these intricate chemical structures, chemical graph theory is applied. The atoms are the vertices and the bonds between the atoms are reflected in the edges of a graph representing a chemical structure, which is called a molecular graph. Using a special mathematical representation where each atom (vertex) has a unique identity or place inside the provided chemical structure, the physical characteristics of a chemical structure are explored. For the purpose of uniquely identifying the whole vertex set, a small number of atoms or vertices are chosen so that the atom set has a distinct position relative to the chosen vertices. In graph theory, this concept is called the metric basis [1], and in applied graph theory, it is called a resolving set (metric generator) [2]. Hernando et al. [3] proposed the idea of fault tolerance in metric generators to handle situations where a single component of the system malfunctions or crashes, potentially resulting in the whole system being shut down.

In order to address this, Kelenc et al. [4] proposed and started the study of a new variant of metric dimension in non-trivial connected graphs that focuses on uniquely identifying the graph's edges, called the edge metric dimension (EMD). One could then consider that, rather than obtaining a unique atomic position, bonds could be utilised to shape the given structure.

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Liu et al. [5] also developed the notion of fault tolerance in edge resolving sets, which is comparable to the concept of fault tolerance in resolving sets. The metric dimension has been thoroughly studied since it has many real-world applications, which serves as a source of motivation for academics. Numerous scientific domains, such as robotic navigation [6], geographic routing protocols [7], linked joints in chemistry and networks [8], telecommunications [9], combinatorial optimisation [10], network discovery and verification [11], etc., use metric dimension. Lewis et al. [12] and Hauptmann et al. [13] discuss NP-hardness and computational complexity for the resolvability parameters.

Chemical graph theory has contributed to the development of computational methods for molecular modeling, drug design, and chemical reaction prediction. It explores the mathematical properties and relationships of these graphs in order to gain insights into the structure, behavior, and properties of chemical substances. By applying graph algorithms and graph invariants, scientists can predict molecular properties, study molecular similarity, identify substructures with specific attributes, and explore reaction pathways. Chemical graph theory makes it simple to study chemical structures.

CGT is a useful tool for analysing various chemical networks, complex structures, and topologies that are presented as graphs that might be difficult to analyse in their natural format. The application of chemical graph theory extends beyond individual molecules. It also encompasses the study of larger chemical systems, such as polymers and complex networks of chemical reactions. This research focuses on medicinal drugs, which are basic chemical substances used to treat, cure, prevent, and diagnose a variety of dangerous diseases in humans and animals. We determine the edge metric basis and edge resolving number of two notable medications, acemannan and suramin, in the present study.

After researching many compounds that resembled urea, the chemists Bernhard Heymann, Oskar Dressel, and Richard Kothe created suramin for the very first time at the Bayer AG laboratory in Elberfeld in 1916. Germanin is the brand under which Bayer continues to sell the medicine. Suramin's molecular formula is $C_{51}H_{40}N_6O_{23}S_6$, and Figure 1 depicts its chemical structure. Human sleeping sickness caused by trypanosomes is treated with suramin. It is used to treat African trypanosomiasis, especially that caused by Trypanosoma brucei gambiense and Trypanosoma rhodesiense, at its earliest stage without harming the central nervous system. River blindness (onchocerciasis) has been treated with it. The urea group is located in the middle of this symmetric molecule. In addition to the urea, suramin has six sulfonic acid groups, four amide functional groups, and six aromatic systems, including two naphthalene moieties sandwiched between four benzene rings. This formulation is frequently recommended as the sodium sulfonate salt when administered as medication because it is soluble in water and does not break down rapidly in air.

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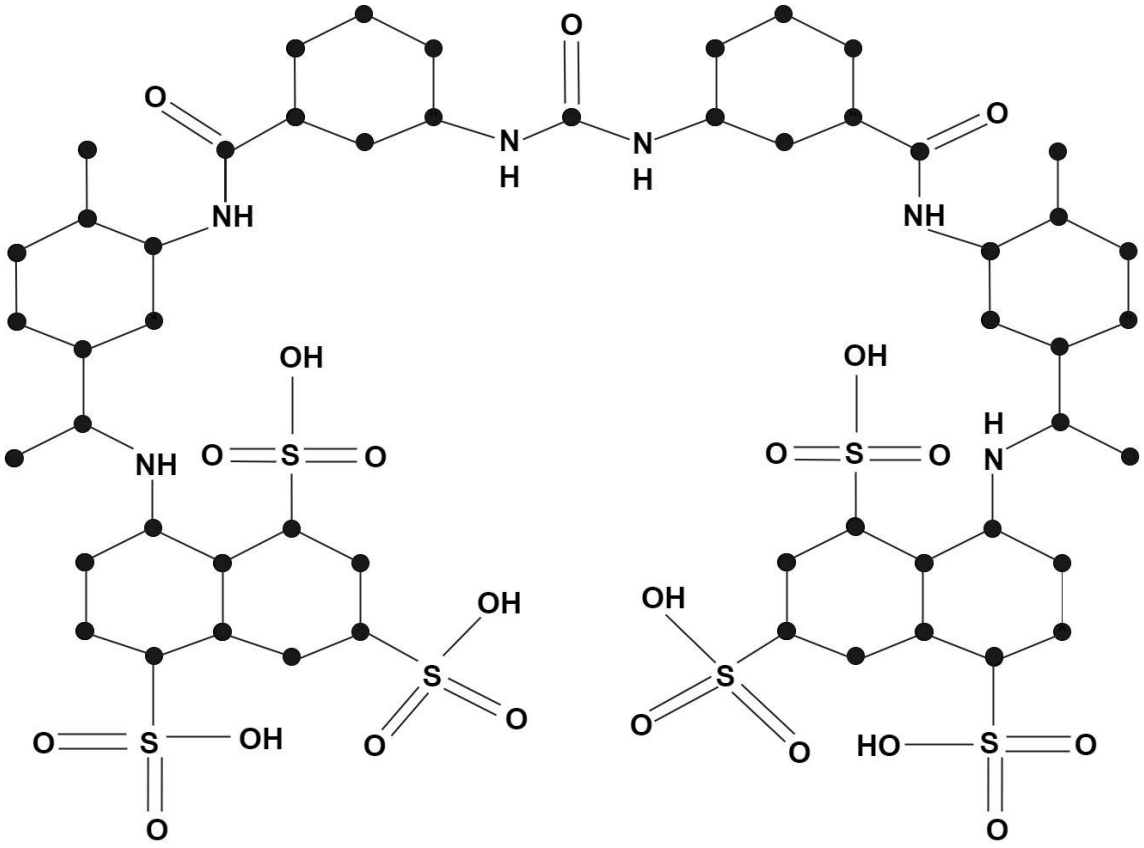

Figure 1: Structure of Suramin

One family of bioactive compounds originating from bacteria, plants, or animals are polysaccharides, a high molecular weight type of carbohydrate [14]. Polysaccharides are extensively used in a range of healthcare products and medications because of their great and exceptional bioactivities, such as their antimicrobial [15], anticancer [16], and antioxidant [17] characteristics. Aloe vera, one of the most popular medicinal plants, is widely used across the world to prevent or cure cancer, metabolic problems, skin issues, and cardiovascular conditions. Acemannan, a -(1,4)-acetylated soluble polymannose and one of the main bioactive polysaccharides found in aloe vera, has several biological effects, such as immunoregulation, anti-oxidation, anti-cancer, and the promotion of bone proliferation, wound healing, as well as intestinal health promotion, neuroprotection, etc [18]. Acemannan's molecular formula is $C_{66}H_{100}NO_{49}$, and Figure 2 depicts its chemical structure. Molecular weights of acemannan generally range from 1000 to 1600 kDa [19, 20]. Most plant polysaccharides consist of two or more forms of monosaccharides, such as rhamnose (Rha), fucose (Fuc), mannose (Man), glucose (Glc), xylose (Xyl), galactose (Gal), and arabinose (Ara). In contrast, the main constituents of acemannan are galactose, glucose, and mannose [19]. Subsequently, we are going to provide an applicable review for these two important medications, S_{86} and A_{116}.

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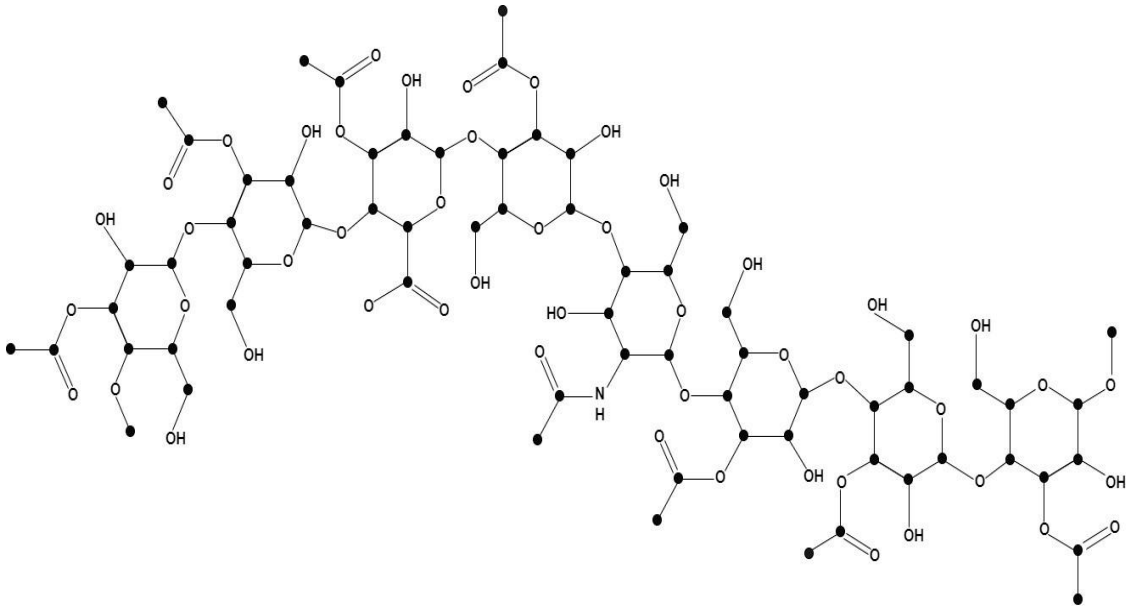

Figure 2: Structure of Acemannan

1.1 Applications of S_{86} and A_{116}

Suramin, a medication that has been used for a century, is still used to treat the initial stage of acute human sleeping sickness, which is caused by Trypanosoma brucei rhodesiense [21]. But it can only be used to treat the early (hemolymphatic) stage of sleeping sickness, when trypanosomes have not yet invaded the patient's central nervous system. This is because it can't cross the blood-brain barrier. Suramin is commonly supplied intravenously for five weeks at a dose of 20 mg/kg after an initial test dosage of 4 to 5 mg/kg of body weight [22]. Furthermore, suramin treats camels with surra (mal de caderas), a condition caused by Trypanosoma evansi [23]. Additionally, by its direct effect on the viral envelope protein, suramin stops the dengue virus from adhering to host cells [24]. It was shown that it stopped the Chikungunya virus from replicating or generating RNA [25]. Suramin provided protection in vitro when it was present during infection, and this was explained by a reduction in the binding and absorption of the virus by host cells [26].

Due to its broad spectrum of biological activity, acemannan, that has been isolated and purified from Aloe vera, is widely used in medicines and functional foods [18]. In the medical and industrial areas acemannan is said to have several pharmacological and biological applications. These include the treatment of tumour like diseases [27], metabolic illnesses [28], oral and cardiovascular diseases. Processing techniques such as heating, pasteurisation, drying, and dehydration are typical for acemannan's possible uses [29, 19]. Additionally, it can operate as a scaffold to help cell growth factors migrate and attach. Acemannan further promotes bone formation and has a strong impact on alveolar bone repair. Thus, acemannan may be a biopolysaccharide material that promotes bone growth naturally [30]. Next, we talk about metric dimension and edge metric dimension, which are the most active research domain and issue in chemical graph theory, respectively.

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1.2 Chemical Graph Theory

Chemical graph theory is an interdisciplinary field that focuses on applying graph theory to understand and model chemical compounds. In chemical graph theory, graphs are used to represent chemical structures, with atoms being depicted as vertices and chemical bonds as edges. The analysis of these graphs provides insights into the properties and behavior of chemical compounds. Through the application of graph theoretical concepts, researchers can investigate molecular symmetry, connectivity, isomerism, and the prediction of chemical reactivity. One of the primary objectives of chemical graph theory is to develop graph-based models that accurately capture the structural and chemical properties of molecules. These models aid in predicting and understanding various phenomena, such as molecular stability, aromaticity, and the conformational analysis of molecules.

Moreover, chemical graph theory plays a crucial role in the design and study of molecular structures, especially in the field of drug discovery and materials science. By leveraging graph theoretical approaches, researchers can analyze molecular descriptors, study structure-activity relationships, and predict the bioactivity of compounds, which is fundamental in drug design and discovery processes. Furthermore, the application of chemical graph theory extends to the development of algorithms and computational techniques for solving chemical problems. Graph theoretical algorithms are employed in tasks such as molecular similarity analysis, chemical database mining, and the elucidation of molecular properties, facilitating advancements in computational chemistry and chemoinformatics. Interestingly, two important chemical substances called acemannan and suramin are used in medications that cure serious illnesses. The metric dimension and its extended variants are wellstudied parameters in graph theory. In keeping with this theme, we also look at the edge metric basis and edge resolving number of S_{86} and A_{116} molecular structures.

2 Preliminaries

In this section, we will go through some basic definitions pertaining to minimal edge resolving sets.

Definition 1. Resolving Set: [1] Let $\pi = (V,E)$ be a simple, connected graph and consider an ordered subset $T = \{s_1,s_2,s_3,...,s_m\}$ of vertices of π. For any two vertices g, h in the graph π, the distance between these two vertices is denoted by $d(g,h)$ and is the length of smallest path between g and h. The metric code of a vertex x of π with respect to T is the m-vector

$(d(x,s_1),d(x,s_2),...,d(x,s_m))$ and it is represented by $\varsigma(x|T)$. If this code is unique for each vertex in π, then T is referred as resolving set for π.

Definition 2. Edge Resolving Set: [4] Let $T = \{s_1,s_2,s_3,...,s_m\}$ of vertices of a simple and connected graph $\pi = (V,E)$ and an edge $e = xy$, where x and y are end vertices of the edge e in the graph π. The distance between the edge e and a vertex k in the graph π is denoted by $d(e,k)$ and is defined as $d(e,k) = min\{\mathrm{d(x,k)},d(y,k)\}$ The edge metric code for an edge e with respect to the set T is the m-vector $(d(e,s_1),d(e,s_2),...,d(e,s_m))$ and it is represented by $\eta(e|T)$. If this representation is unique for each edge in π, then T is referred as edge resolving set for π.

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Definition 3. Metric Dimension: [1] Metric dimension of a graph π is defined as the number of elements of in smallest resolving set for π and is denoted by $dim(\pi)$ and the smallest resolving set serves as metric basis for π.

Definition 4. Edge Metric Dimension: [4] Edge metric dimension of a graph π is defined as the number of elements of in smallest edge resolving set for π and we denoted it by $edim(\pi)$ and the smallest edge resolving set serves as edge metric basis for π.

Definition 5. Independent Set: [31] An independent set is a subset of nodes (vertices) in a graph where there is not a pair of adjacent vertices.

We specifically concentrate on two medications in this study: acemannan (A_{116}) and suramin (S_{86}).

3 Edge Metric Basis and Edge Resolving Number of S_{86}

In this section, we discuss the structure of S_{86}. We explore some of its basic characteristics and find the edge metric dimension of S_{86}.

The Chemical Graph of S_{86}:

S_{86} has 86 vertices and 93 edges in its molecular graph, as shown in Figure 3. There are eight 6-cycles in it. In the molecular graph of S_{86}, the total number of nodes or vertices to the left of m_2 equals the number of nodes or vertices to the right of m_2. The symmetry assist in determining the structure's metric codes. The coloured vertices in Figure 3 represent the set of S_{86} that are present in minimum edge resolving set.

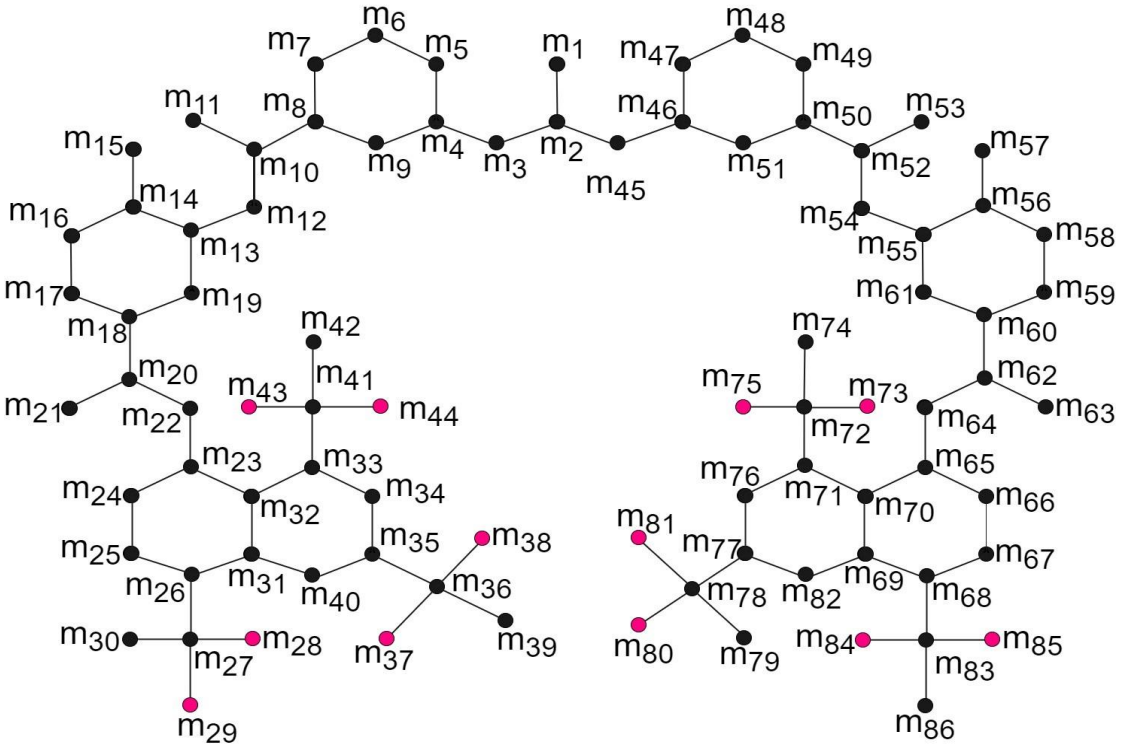

Figure 3: Chemical graph of S_{86}

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Theorem 1. *The edge metric dimension of* S_{86} *is* 12 *i.e.,* $edim(S_{86}) = 12$.

Proof. Let $W_r = \{m_{28},m_{29},m_{37},m_{38},m_{43},m_{44},m_{73},m_{75},m_{80},m_{81},m_{84},m_{85}\}$ be an ordered subset of vertices of S_{86}. We shall prove that W_r is a smallest edge resolving for S_{86} i.e., W_r is an edge metric basis for S_{86}.

The edge metric codes for the edges in S_{86} are presented in Table 1:

It can be easily seen from table 1 that the edge metric code for each edge of S_{86} is unique i.e., for distinct edges of S_{86} the respective edge metric codes are distinct and thus W_r is an edge resolving set. It follows that $edim(S_{86}) \leq 12$. Now, we shall show that W_r is smallest edge resolving set i.e., $edim(S_{86}) \geq 12$.

If we do not involve any of the vertex from the set $\{m_{28},m_{29}\}$ in the set W_r then the edge metric codes are found to be equal for two distinct edges of S_{86} and so the set $H = W_r - \{x\}$; $x \in \{m_{28},m_{29}\}$ will not serve as an edge resolving set. Thus at least one element from the set $\{m_{28},m_{29}\}$ must be involved in an edge resolving set. Also, If we do not involve any of the vertex from the set $\{m_{29},m_{30}\}$ in the set W_r then the edge metric codes are found to be equal for two distinct edges of S_{86}. So, two vertices from the set $\{m_{28},m_{29},m_{30}\}$ must be added in W_r.

Similarly, two vertices from the set $\{m_{37},m_{38},m_{39}\}$ must be contained in the set W_r. Proceeding in the same way, two elements from the set $\{m_{42},m_{43},m_{44}\}$, two vertices from the set $\{m_{73},m_{74},m_{75}\}$,

Table 1: Unique representations for edges in S_{86}

Edge metric codes	Corresponding values	Edge metric codes	Corresponding values
$\eta(m_1m_2\|W_r)$	(17,17,18,18,16,16,16,16,18,18,17,17)	$\eta(m2m45\|Wr)$	(17,17,18,18,16,16,15,15,17,17,16,16)
$\eta(m_2m_3\|W_r)$	(16,16,17,17,15,15,16,16,18,18,17,17)	$\eta(m45m46\|Wr)$	(18,18,19,19,17,17,14,14,16,16,15,15)
$\eta(m_3m_4\|W_r)$	(15,15,16,16,14,14,17,17,19,19,18,18)	$\eta(m46m47\|Wr)$	(19,19,20,20,18,18,14,14,16,16,15,15)

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$\eta(m_4m_5\|W_r)$	(15,15,16,16,14,14,18,18,20,20,19,19)	$\eta(m47m48\|Wr)$	(20,20,21,21,19,19,14,14,16,16,15,15)
$\eta(m_5m_6\|W_r)$	(15,15,16,16,14,14,19,19,21,21,20,20)	$\eta(m48m49\|Wr)$	(21,21,22,22,20,20,13,13,15,15,14,14)
$\eta(m_6m_7\|W_r)$	(14,14,15,15,13,13,20,20,22,22,21,21)	$\eta(m49m50\|Wr)$	(21,21,22,22,20,20,12,12,14,14,13,13)
$\eta(m_7m_8\|W_r)$	(13,13,14,14,12,12,20,20,22,22,21,21)	$\eta(m50m51\|Wr)$	(20,20,21,21,19,19,12,12,14,14,13,13)
$\eta(m_8m_9\|W_r)$	(13,13,14,14,12,12,19,19,21,21,20,20)	$\eta(m46m51\|Wr)$	(19,19,20,20,18,18,13,13,15,15,14,14)
$\eta(m_4m_9\|W_r)$	(14,14,15,15,13,13,18,18,20,20,19,19)	$\eta(m50m52\|Wr)$	(21,21,22,22,20,20,11,11,13,13,,12,12)
$\eta(m8m10\|Wr)$	(12,12,13,13,11,11,20,20,22,22,21,21)	$\eta(m52m53\|Wr)$	(22,22,23,23,21,21,11,11,13,13,12,12)
$\eta(m10m11\|Wr)$	(12,12,13,13,11,11,21,21,23,23,22,22)	$\eta(m52m54\|Wr)$	(22,22,23,23,21,1,10,10,12,12,11,11)
$\eta(m10m12\|Wr)$	(11,11,12,12,10,10,21,21,23,23,22,22)	$\eta(m54m55\|Wr)$	(23,23,24,24,22,22,9,9,11,11,10,10)
$\eta(m12m13\|Wr)$	(10,10,11,11,9,9,22,22,24,24,23,23)	$\eta(m55m56\|Wr)$	(24,24,25,25,23,23,9,9,11,11,10,10)

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$\eta(m13m14\|Wr)$	(10,10,11,11,9,9,23,23,25,25,24,24)	$\eta(m56m57\|Wr)$	(25,25,26,26,24,24,10,10,12,12,11,11)
$\eta(m14m15\|Wr)$	(11,11,12,12,10,10,24,24,26,26,25,25)	$\eta(m56m58\|Wr)$	(25,25,26,26,24,24,9,9,11,11,10,10)
$\eta(m14m16\|Wr)$	(10,10,11,11,9,9,24,24,26,26,25,25)	$\eta(m58m59\|Wr)$	(26,26,27,27,25,25,8,8,10,10,9,9)
$\eta(m16m17\|Wr)$	(9,9,10,10,8,8,25,25,27,27,26,26)	$\eta(m59m60\|Wr)$	(26,26,27,27,25,25,7,7,9,9,8,8)
$\eta(m17m18\|Wr)$	(8,8,9,9,7,7,25,25,27,27,26,26)	$\eta(m60m61\|Wr)$	(25,25,26,26,24,24,7,7,9,9,8,8)
$\eta(m18m19\|Wr)$	(8,8,9,9,7,7,8,8,24,24,26,26,25,25)	$\eta(m55m61\|Wr)$	(24,24,25,25,23,23,8,8,10,10,9,9)
$\eta(m13m19\|Wr)$	(9,9,10,10,8,8,23,23,25,25,24,24)	$\eta(m60m62\|Wr)$	(26,26,27,27,25,25,6,6,8,8,7,7)
$\eta(m18m20\|Wr)$	(7,7,8,8,6,6,26,26,28,28,27,27)	$\eta(m62m63\|Wr)$	(27,27,28,28,26,26,6,6,8,8,7,7)
$\eta(m20m21\|Wr)$	(7,7,8,8,6,6,7,7,26,26,28,28,27,27)	$\eta(m62m64\|Wr)$	(27,27,28,28,26,26,5,5,7,7,6,6)
$\eta(m20m22\|Wr)$	(6,6,7,7,5,5,26,26,28,28,27,27)	$\eta(m64m65\|Wr)$	(28,28,29,29,27,27,4,4,6,6,5,5)

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$\eta(m22m23\|Wr)$	(5,5,6,6,4,4,27,27,29,29,28,28)	$\eta(m65m66\|Wr)$	(29,29,30,30,28,28,4,4,6,6,4,4)
$\eta(m23m24\|Wr)$	(4,4,6,6,4,4,28,28,30,30,29,29)	$\eta(m66m67\|Wr)$	(30,30,31,31,29,29,5,5,6,6,3,3)
$\eta(m24m25\|Wr)$	(3,3,6,6,5,5,29,29,31,31,30,30)	$\eta(m67m68\|Wr)$	(31,31,32,32,30,30,5,5,5,5,2,2)
$\eta(m25m26\|Wr)$	(2,2,5,5,5,5,30,30,32,32,31,31)	$\eta(m68m83\|Wr)$	(32,32,33,33,31,31,5,5,5,5,1,1)
$\eta(m26m31\|Wr)$	(2,2,4,4,4,4,30,30,32,32,31,31)	$\eta(m83m85\|Wr)$	(33,33,34,34,32,32,6,6,6,6,1,0)
$\eta(m31m32\|Wr)$	(3,3,4,4,3,3,29,29,31,31,30,30)	$\eta(m83m86\|Wr)$	(33,33,34,34,32,32,6,6,6,6,1,1)
$\eta(m23m32\|Wr)$	(4,4,5,5,3,3,28,28,30,30,29,29)	$\eta(m83m84\|Wr)$	(33,33,34,34,32,32,6,6,6,6,0,1)
$\eta(m32m33\|Wr)$	(4,4,4,4,2,2,29,29,31,31,30,30)	$\eta(m68m69\|Wr)$	(31,31,32,32,30,30,4,4,4,4,2,2)
$\eta(m33m41\|Wr)$	(5,5,4,4,1,1,30,30,32,32,31,31)	$\eta(m69m70\|Wr)$	(30,30,31,31,29,29,3,3,4,4,3,3)
$\eta(m41m43\|Wr)$	(6,6,5,5,0,1,31,31,33,33,32,32)	$\eta(m65m70\|Wr)$	(29,29,30,30,28,28,3,3,5,5,4,4)

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$\eta(m41m42\|Wr)$	(6,6,5,5,1,1,31,31,33,33,32,32)	$\eta(m70m71\|Wr)$	(30,30,31,31,29,29,2,2,4,4,4,4)
$\eta(m41m44\|Wr)$	(6,6,5,5,1,0,31,31,33,33,32,32)	$\eta(m71m72\|Wr)$	(31,31,32,32,30,30,1,1,4,4,5,5)
$\eta(m33m34\|Wr)$	(5,5,3,3,2,2,30,30,32,32,31,31)	$\eta(m72m75\|Wr)$	(32,32,33,33,31,31,1,0,5,5,6,6)
$\eta(m34m35\|Wr)$	(5,5,2,2,3,3,31,31,33,33,32,32)	$\eta(m72m74\|Wr)$	(32,32,33,33,31,31,1,1,5,5,6,6)
$\eta(m35m40\|Wr)$	(4,4,2,2,4,4,31,31,33,33,32,32)	$\eta(m72m73\|Wr)$	(32,32,33,33,31,31,0,1,5,5,6,6)
$\eta(m31m40\|Wr)$	(3,3,3,3,4,4,30,30,32,32,31,31)	$\eta(m71m76\|Wr)$	(31,31,32,32,30,30,2,2,3,3,5,5)
$\eta(m35m36\|Wr)$	(5,5,1,1,4,4,32,32,34,34,33,33)	$\eta(m76m77\|Wr)$	(32,32,33,33,31,31,3,3,2,2,5,5)
$\eta(m36m38\|Wr)$	(6,6,1,0,5,5,33,33,35,35,34,34)	$\eta(m77m78\|Wr)$	(33,33,34,34,32,32,4,4,1,1,5,5)
$\eta(m36m39\|Wr)$	(6,6,1,1,5,5,33,33,35,35,34,34)	$\eta(m78m81\|Wr)$	(34,34,35,35,33,33,5,5,1,1,6,6)
$\eta(m36m37\|Wr)$	(6,6,1,0,5,5,33,33,35,35,34,34)	$\eta(m78m80\|Wr)$	(34,34,35,35,33,33,5,5,0,1,6,6)

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$\eta(m26m27\|Wr)$	(1,1,5,5,5,5,31,31,33,33,32,32)	$\eta(m78m79\|Wr)$	(34,34,35,35,33,33,5,5,1,1,6,6)
$\eta(m27m30\|Wr)$	(1,1,6,6,6,6,32,32,34,34,33,33)	$\eta(m77m82\|Wr)$	(32,32,33,33,31,31,4,4,2,2,4,4)
$\eta(m27m28\|Wr)$	(0,1,6,6,6,6,32,32,34,34,33,33)	$\eta(m69m82\|Wr)$	(31,31,32,32,30,30,4,4,3,3,3,3)
$\eta(m27m29\|Wr)$	(1,0,6,6,6,6,32,32,34,34,33,33)		

two elements from $\{m_{79},m_{80},m_{81}\}$, and two from $\{m_{84},m_{85},m_{86}\}$ must be added in set W_r in order to serves as an edge resolving set. From this, it follows that $edim(S_{86}) \geq 12$ and W_r is an edge metric basis for S_{86} implying that $edim(S_{86}) = 12$.

□**Corollary 2.** *The independent edge resolving number of* S_{86} *is 12.*

4 Metric Basis and Metric Dimension of A_{116}

We begin this section by discussing the structure of A_{116}. We look into a few of its basic characteristics and figure out its edge metric dimension.

The Chemical Graph of Graph of A_{116}

Since it has 116 atoms other than hydrogen atoms and 123 bonds other than those connecting hydrogen to other atoms, A_{116} has a very complicated structure. As observed in Figure 4, the molecular graph of A_{116} has 116 vertices and 123 edges. There are eight 6 cycles in it. The nodes in Figure 4 that are involved in minimal edge resolving set W_r of A_{116} are indicated by pink colouring.

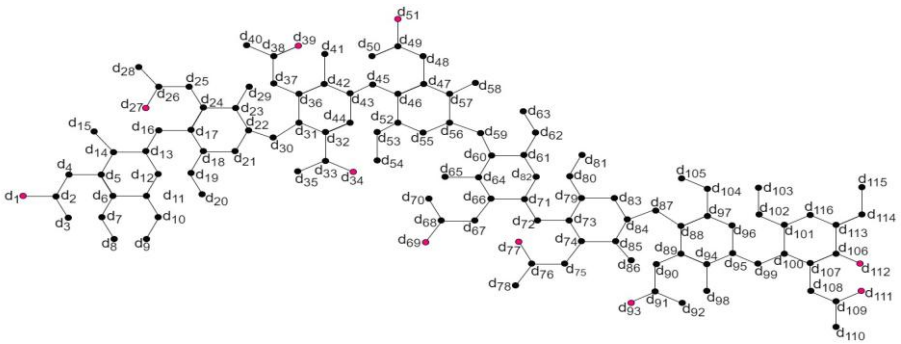

Figure 4: Chemical graph of A_{116}

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Theorem 1. *The edge metric dimension of* A_{116} *is* 10 *i.e.,* $edim(A_{116}) = 10$.

Proof. Let $W_r = \{d_1, d_{27}, d_{34}, d_{39}, d_{51}, d_{69}, d_{77}, d_{93}, d_{111}, d_{112}\}$ be an ordered subset of vertices of A_{116}. We shall prove that E_r is an edge resolving set for A_{116} and is of minimal cardinality i.e., W_r is an edge metric basis for A_{116}.

The edge metric codes for each edge in A_{116} are listed in Table 2 and Table 3:

Table 2: Unique representations for edges in A_{116}

Edge Metric codes	Corresponding values	Edge Metric codes	Corresponding values
$\eta(d_1d_2\|W_r)$	(0,10,14,15,20,26,30,35,40,39)	$\eta(d59d60\|Wr)$	(21,16,10,11,6,5,9,14,19,18)
$\eta(d_2d_3\|W_r)$	(1,10,14,15,20,26,30,35,40,39)	$\eta(d60d61\|Wr)$	(22,17,11,12,7,5,8,13,18,17)
$\eta(d_2d_4\|W_r)$	(1,9,13,14,19,25,29,34,39,38)	$\eta(d61d62\|Wr)$	(23,18,12,13,8,6,8,13,18,17)
$\eta(d_4d_5\|W_r)$	(2,8,12,13,18,24,28,33,38,37)	$\eta(d62d63\|Wr)$	(24,19,13,14,9,7,9,14,19,18)
$\eta(d_5d_6\|W_r)$	(3,8,12,13,18,24,28,33,38,37)	$\eta(d61d82\|Wr)$	(23,18,12,13,8,5,7,12,17,16)
$\eta(d_6d_7\|W_r)$	(4,9,13,14,19,25,29,34,39,38)	$\eta(d71d82\|Wr)$	(22,17,11,12,7,4,8,13,18,17)
$\eta(d_7d_8\|W_r)$	(5,10,14,15,20,26,30,35,40,39)	$\eta(d66d71\|Wr)$	(23,18,12,13,8,3,7,12,17,16)
$\eta(d6d11\|Wr)$	(4,8,12,13,18,24,28,33,38,37)	$\eta(d64d66\|Wr)$	(24,19,13,14,9,3,6,11,16,15)
$\eta(d10d11\|Wr)$	(5,8,12,13,18,24,28,33,38,37)	$\eta(d64d65\|Wr)$	(24,19,13,14,9,4,6,11,16,15)
$\eta(d9d10\|Wr)$	(6,9,13,14,19,25,29,34,39,38)	$\eta(d60d64\|Wr)$	(23,18,12,13,8,4,8,13,18,17)
$\eta(d11d12\|Wr)$	(5,7,11,12,17,23,27,32,37,36)	$\eta(d66d67\|Wr)$	(24,19,13,14,9,2,7,12,17,16)
$\eta(d12d13\|Wr)$	(5,6,10,11,16,22,26,31,36,35)	$\eta(d67d68\|Wr)$	(25,20,14,15,10,1,8,13,18,17)

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$\eta(d13d14\|Wr)$	(4,6,10,11,16,22,26,31,36,35)	$\eta(d68d70\|Wr)$	(26,21,15,16,11,1,9,14,19,18)
$\eta(d5d14\|Wr)$	(3,7,11,12,17,23,27,32,37,36)	$\eta(d68d69\|Wr)$	(26,21,15,16,11,0,9,14,19,18)
$\eta(d14d15\|Wr)$	(4,7,11,12,17,23,27,32,37,36)	$\eta(d71d72\|Wr)$	(25,20,14,15,10,4,5,10,15,14)
$\eta(d13d16\|Wr)$	(5,5,9,10,15,21,25,30,35,34)	$\eta(d72d73\|Wr)$	(26,21,15,16,11,5,4,9,14,13)
$\eta(d16d17\|Wr)$	(6,4,8,9,14,20,24,29,34,33)	$\eta(d73d74\|Wr)$	(27,22,16,17,12,6,3,8,13,12)
$\eta(d17d18\|Wr)$	(7,4,7,8,13,19,23,28,33,32)	$\eta(d74d75\|Wr)$	(28,23,17,18,13,7,2,8,13,12)
$\eta(d18d21\|Wr)$	(8,5,6,7,12,18,22,27,32,31)	$\eta(d75d76\|Wr)$	(29,24,18,19,14,8,1,9,14,13)
$\eta(d21d22\|Wr)$	(9,5,5,6,11,17,21,26,31,30)	$\eta(d76d78\|Wr)$	(30,25,19,20,15,9,1,10,15,14)
$\eta(d22d23\|Wr)$	(9,4,5,6,11,17,21,26,31,30)	$\eta(d76d77\|Wr)$	(30,25,19,20,15,9,0,10,15,14)
$\eta(d23d24\|Wr)$	(8,3,6,7,12,18,22,27,32,31)	$\eta(d73d79\|Wr)$	(27,22,16,17,12,6,4,8,13,12)
$\eta(d17d24\|Wr)$	(7,3,7,8,13,19,23,28,33,32)	$\eta(d79d80\|Wr)$	(28,23,17,18,13,7,5,8,13,12)
$\eta(d24d25\|Wr)$	(8,2,7,8,13,19,23,28,33,32)	$\eta(d80d81\|Wr)$	(29,24,18,19,14,8,6,9,14,13)
$\eta(d25d26\|Wr)$	(9,1,8,9,14,20,24,29,34,33)	$\eta(d79d83\|Wr)$	(28,23,17,18,13,7,5,7,12,11)
$\eta(d26d27\|Wr)$	(10,0,9,10,15,21,25,30,35,34)	$\eta(d83d84\|Wr)$	(29,24,18,19,14,8,5,6,11,10)
$\eta(d26d28\|Wr)$	(10,1,9,10,15,21,25,30,35,34)	$\eta(d84d85\|Wr)$	(29,24,18,19,14,8,4,6,11,10)
$\eta(d18d19\|Wr)$	(8,5,7,8,13,19,23,28,33,32)	$\eta(d74d85\|Wr)$	(28,23,17,18,13,7,3,7,12,11)

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Table 3: Unique representations for edges in A_{116}

Edge Metric codes	Corresponding values	Edge Metric codes	Corresponding values
$\eta(d19d20\|Wr)$	(9,6,8,9,14,20,24,29,34,33)	$\eta(d84d87\|Wr)$	(30,25,19,20,15,9,5,5,10,9)
$\eta(d22d30\|Wr)$	(10,5,4,5,10,16,20,25,30,29)	$\eta(d87d88\|Wr)$	(31,26,20,21,16,10,6,4,9,8)
$\eta(d23d29\|Wr)$	(9,4,6,7,12,18,22,27,32,31)	$\eta(d88d89\|Wr)$	(32,27,21,22,17,11,7,3,8,7)
$\eta(d30d31\|Wr)$	(11,6,3,4,9,15,19,24,29,28)	$\eta(d89d90\|Wr)$	(33,28,22,23,18,12,8,2,8,7)
$\eta(d33d35\|Wr)$	(14,9,1,6,9,15,19,24,29,28)	$\eta(d90d91\|Wr)$	(34,29,23,24,19,13,9,1,9,8)
$\eta(d33d34\|Er)$	(14,9,0,6,9,15,19,24,29,28)	$\eta(d91d92\|Er)$	(35,30,24,25,20,14,10,1,10,9)
$\eta(d32d33\|Wr)$	(13,8,1,5,8,14,18,23,28,27)	$\eta(d91d93\|Wr)$	(35,30,24,25,20,04,10,1,10,9)
$\eta(d31d32\|Wr)$	(12,7,2,4,8,14,18,23,28,27)	$\eta(d85d86\|Wr)$	(29,24,18,19,14,8,4,7,12,11)
$\eta(d31d36\|Wr)$	(12,7,3,3,8,14,18,23,28,27)	$\eta(d89d94\|Wr)$	(33,28,22,23,18,12,8,3,7,6)
$\eta(d36d42\|Er)$	(13,8,4,3,7,13,17,22,27,26)	$\eta(d94d98\|Er)$	(34,29,23,24,19,13,9,4,7,6)
$\eta(d42d43\|Wr)$	(14,9,4,4,6,12,16,21,26,25)	$\eta(d94d95\|Wr)$	(34,29,23,24,19,13,9,4,6,5)
$\eta(d43d44\|Wr)$	(14,9,3,5,6,12,16,21,26,25)	$\eta(d95d96\|Wr)$	(34,29,23,24,19,13,9,5,6,5)
$\eta(d32d44\|Wr)$	(13,8,2,5,7,13,17,22,27,26)	$\eta(d96d97\|Wr)$	(33,28,22,23,18,12,8,5,7,6)
$\eta(d41d42\|Er)$	(14,9,5,4,7,13,17,22,27,26)	$\eta(d88d97\|Er)$	32,27,21,22,17,11,7,4,8,7)
$\eta(d36d37\|Wr)$	(13,8,4,2,8,14,18,23,28,27)	$\eta(d97d104\|Wr)$	(33,28,22,23,18,12,8,5,8,7)

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$\eta(d37d38\|Wr)$	(14,9,5,1,9,15,19,24,29,28)	$\eta(d104d105\|Wr)$	(34,29,23,24,19,13,9,6,9,8)
$\eta(d38d40\|Wr)$	(15,10,6,1,10,16,20,25,30, 29)	$\eta(d95d99\|Wr)$	(35,30,24,25,20,14,10,5,5,4)
$\eta(d38d39\|Wr)$	(15,10,6,0,10,16,20,25,30, 29)	$\eta(d99d100\|Wr)$	(36,31,25,26,21,15,11,16,4,3)
$\eta(d43d45\|Wr)$	(15,10,4,5,5,11,15,20,25,2 4)	$\eta(d100d101\|Wr)$	(37,32,26,27,22,16,12,17,4,3)
$\eta(d45d46\|Wr)$	(16,11,5,6,4,10,14,19,24,2 3)	$\eta(d101d102\|Wr)$	(38,33,27,28,23,17,13,18,5,4)
$\eta(d46d47\|Wr)$	(17,12,6,7,3,9,13,18,23,22)	$\eta(d102d103\|Wr)$	(39,34,28,29,24,18,14,19,6,5)
$\eta(d47d48\|Wr)$	(18,13,7,8,2,9,13,18,23,22)	$\eta(d101d116\|Wr)$	(38,33,27,28,23,17,18,13,5,3)
$\eta(d48d49\|Wr)$	(19,14,8,9,1,1,14,19,24,23)	$\eta(d113d116\|Wr)$	(39,34,28,29,24,18,14,19,5,2)
$\eta(d49d50\|Wr)$	(20,15,9,10,1,11,15,20,25, 24)	$\eta(d106d113\|Wr)$	(39,34,28,29,24,18,14,19,4,1)
$\eta(d49d51\|Wr)$	(20,15,9,10,0,11,15,20,25, 24)	$\eta(d106d107\|Wr)$	(38,33,27,28,23,17,13,18,3,1)
$\eta(d46d52\|Wr)$	(17,12,6,7,4,9,14,19,24,23)	$\eta(d100d107\|Wr)$	(37,32,26,27,22,22,18,14,19, 3,2)
$\eta(d52d53\|Wr)$	(18,13,7,8,5,9,14,19,24,23)	$\eta(d113d114\|Wr)$	(40,35,29,30,15,19,15,20,5,2)
$\eta(d53d54\|Wr)$	(19,14,8,9,6,10,14,19,24,2 3)	$\eta(d114d115\|Wr)$	(41,36,30,31,26,20,16,21,6,3)
$\eta(d52d55\|Wr)$	(18,13,7,8,5,8,12,17,22,21)	$\eta(d106d112\|Wr)$	(39,34,28,29,24,18,14,19,4,0)
$\eta(d55d56\|Wr)$	(19,14,8,9,5,7,11,16,21,20)	$\eta(d107d108\|Wr)$	(38,33,27,28,23,,17,13,18,2,2)
$\eta(d56d57\|Wr)$	(19,14,8,9,4,7,11,16,21,20)	$\eta(d108d109\|Wr)$	(39,34,28,29,24,18,14,19,1,3)

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$\eta(d57d58\|Wr)$	(19,14,8,9,4,8,12,17,22,21)	$\eta(d109d110\|Wr)$	(40,35,29,30,25,19,15,20,1,4)
$\eta(d47d57\|Wr)$	(18,13,7,8,3,8,12,17,22,21)	$\eta(d109d111\|Wr)$	(40,35,29,30,25,19,15,20,0,4)
$\eta(d56d59\|Wr)$	(20,15,9,10,5,6,10,15,20,19)		

It can be easily seen from the Table 2 and Table 3 that each edge of A_{116} has unique edge representation with respect to the set W_r. Thus W_r is an edge resolving set and $edim(A_{116}) \leq 10$. Now, we shall prove that W_r is a smallest edge resolving set for A_{116} i.e., $dim(A_{116}) \geq 10$.

If we do not involve any of the vertex from the set $\{d_1,d_3\}$ in the set W_r then the edge metric codes are found to be equal for two distinct edges of A_{116} and so the set $H = W_r - \{x\}; x \in \{d_1,d_3\}$ will not serve as an edge resolving set. Thus at least one element from the set $\{d_1,d_3\}$ must be involved in an edge resolving set. In the similar way, at least one element from each set: $\{d_{34},d_{35}\}$,

$\{d_{50},d_{51}\}$, $\{d_{69},d_{70}\}$, $\{d_{77},d_{78}\}$, $\{d_{92},d_{93}\}$, $\{d_{110},d_{111}\}$, and $\{d_{112},d_{113}\}$ must be included in the set W_r in order to serve as an edge resolving set. From this discussion it is clear that $edim(A_{116}) \geq 10$ and so w_r is an edge metric basis for A_{116} implying that $edim(A_{116}) = 10$. □

Corollary 2. The independent edge resolving number of A_{116} is 10.

5 Comparison Between Minimum Edge Resolving Sets of S_{86} and A_{116}

Metric basis for $S86$ and $A116$ are $K1 = \{m28,m29,m37,m38,m43,m44,m73,m75,m80,m81,m84,m85\}$ and $K2 = \{d1,d27,d34,d39,d51,d69,d77,d93,d111,d112\}$ respectively. The nodes m_{28}, m_{29}, m_{37}, m_{38}, m_{43}, m_{44}, m_{73}, m_{75}, m_{80}, m_{81}, m_{84}, m_{85}, in K_1 represents the oxygen atoms in the chemical structure of S_{86}. The nodes $d_{27},d_{34},d_{39},d_{77},d_{92},d_{112}$ in K_2 also represents the oxygen atoms in the structure of A_{116}. There are few functional groups that are common in the chemical structures of S_{86} and A_{116}. Edge metric dimension of S_{86} and A_{116} is 12 and 10 respectively but instead of having distinct edge metric dimensions, six elements in the both smallest edge resolving sets K_1 and K_2 represents oxygen atoms. Also, there are other possible smallest edge resolving sets of S_{86}, but in every smallest edge resolving set for S_{86}, every element will be representing oxygen atom in the chemical structure of S_{86}.

Also, there are other possible smallest edge resolving sets for A_{116} as shown in Table 4.

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The sets Table 4: Minimum edge resolving sets for A_{116}

Minimal Edge Resolving set	Total nodes that represent carbon atoms	Total nodes that represent oxygen atoms
$A1$ = {$d1$,$d28$,$d35$,$d40$,$d51$,$d69$,$d78$,$d93$,$d110$,$d113$}	9	1
$A2$ = {$d3$,$d28$,$d35$,$d40$,$d51$,$d69$,$d78$,$d93$,$d110$,$d113$}	8	2
$A3$ = {$d3$,$d27$,$d35$,$d40$,$d51$,$d69$,$d78$,$d93$,$d110$,$d113$}	7	3
$A4$ = {$d3$,$d27$,$d35$,$d39$,$d51$,$d69$,$d78$,$d93$,$d110$,$d113$}	6	4
$A5$ = {$d3$,$d27$,$d35$,$d39$,$d50$,$d69$,$d78$,$d93$,$d110$,$d113$}	5	5
$A6$ = {$d3$,$d27$,$d35$,$d39$,$d50$,$d70$,$d78$,$d93$,$d110$,$d113$}	4	6
$A7$ = {$d3$,$d27$,$d35$,$d39$,$d50$,$d70$,$d77$,$d93$,$d110$,$d113$}	3	7
$A8$ = {$d3$,$d27$,$d35$,$d39$,$d50$,$d70$,$d77$,$d92$,$d110$,$d113$}	2	8
$A9$ = {$d3$,$d27$,$d35$,$d39$,$d50$,$d70$,$d77$,$d92$,$d111$,$d113$}	1	9
$A10$ = {$d3$,$d27$,$d35$,$d39$,$d50$,$d70$,$d77$,$d92$,$d111$,$d112$}	0	10

A_1,A_2,A_3,A_4,A_5,A_6,A_7,A_8,A_9,A_{10} in Table 4 are the different smallest edge resolving sets for A_{116} possessing different number of elements that represents carbon atoms and oxygen atoms in the structure of A_{116}.

6 Conclusion

A medication, often known as medicine, is a substance used to treat or reduce the symptoms of a disease or other medical condition. In every period of human history, the development of a therapeutic medicine has been essential. In this paper, we examine some of the molecular properties of two important medications. This study investigates the edge metric basis and the corresponding dimensions of two well-known medications, S_{86} and A_{116}. For these two medications, we have demonstrated that $edim(S_{86}) = 12$ and $edim(A_{116}) = 10$. This article also

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demonstrates the independence of the minimal edge resolving set for each of the two structures. It could be useful for chemists to identify common patterns among various pharmaceuticals so they can use them to their medical study. We will be discussing about additional newly introduced metric dimension variants (such mixed metric dimension, partition dimension, square metric dimension, etc.) for these important medications, A_{116} and S_{86}, in the future.

7 Declarations

Ethical Approval Not applicable.

Availability of data and materials

The conclusions of this study were not supported by the use of any data or software, and no new data or software have been created.

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