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Vertex-Based Resolvability Parameters for Identification of Certain Chemical Structures

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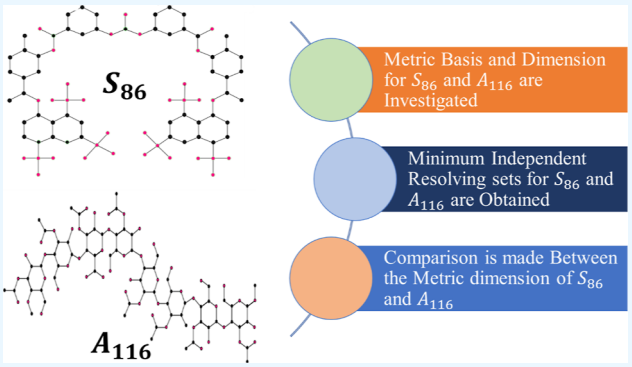
ABSTRACT: Chemical graph theory explores chemical phenomena and entities through the conceptual framework of graph theory. In chemical graph theory, molecular structures are represented by chemical graphs, where edges and vertices correspond to bonds and atoms, respectively. Chemical graphs serve as fundamental data types in cheminformatics for illustrating chemical structures. The computable properties of graphs form the basis for quantitative structure−property and structure−activity predictions, which are central to cheminformatics. These graphs capture the physical characteristics of molecules and can be further reduced to graph-theoretical indices or descriptors. One extensively studied distance-based graph descriptor is the resolving set Z, which enables the distinction of every pair of distinct vertices in a connected simple graph. Resolving sets were specifically employed 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 investigate minimum resolving sets for certain significant drug molecular structures, namely, suramin (S_{86}) and acemannan (A_{116})



1. INTRODUCTION

The field of graph theory, which falls under the realm of emerging mathematics, has found extensive application in various domains such as sociology, computer science, electrical engineering, chemical engineering, geography, transportation, and statistical mechanics. Presently, chemical structures have firmly established themselves as valuable entities within graph theory.[1] The methods rooted in the field of graph theory are employed in chemistry, as well as numerous other scientific disciplines, necessitating a diverse range of graph operations, including the transformation and determination of various graph invariants. A highly sophisticated approach is required to calculate a specific graph invariant if it holds any chemical significance.[2] One such graph invariant is the investigation of the metric dimension (and its versions) within the complex structures of chemical compounds.

The notion of a metric dimension in graphs was introduced by Slater[3] and subsequently explored by Harary and Melter.[4] Notably, Erdos et al.[5] had already studied the concept of dimension in graphs in 1965. To better grasp these notions, let us consider an example: any set of three noncollinear points can uniquely determine the location of every point within the Euclidean plane based on their respective distances.

Next, the concept described by Slater[3] was applied in various practical scenarios, such as facility location problems, sound navigation and ranging (SONAR), and coast guard long-range navigation (LORAN). Caceres et al.[6] explored the concept of metric basis and its corresponding dimension in mastermind games and coin-weighing problems. Chartrand et al.[7] showcased its applications in the field of chemistry, whereas Tomescu and Melter[8] utilized this concept in the context of pattern recognition and image processing. Additionally, Khuller et al.[9] documented the utilization of a metric dimension in robot navigation. Chemical structures can be easily studied by using chemical graph theory. Chemical graph theory serves as a valuable tool for the examination of diverse chemical networks, intricate structures, and topologies, presented in the form of a graph, which can be challenging to analyze in their inherent configuration. Medicinal drugs, fundamental chemical compounds employed to improve the physical or mental well-being of humans/animals through the treatment, cure, prevention, and diagnosis of various hazardous diseases, are the focus of this study. Within this research, we ascertain the metric basis and dimensions of noteworthy drugs, specifically suramin and acemannan.

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The chemists Oskar Dressel, Richard Kothe, and Bernhard Heymann developed suramin for the first time in 1916 at the Bayer AG laboratory in Elberfeld after studying a number of urea-like chemicals. The drug is still sold by Bayer under the brand name Germanin. The molecular formula of suramin is $C_{51}H_{40}N_6O_{23}S_6$, and the chemical structure of suramin is shown in Figure 1. Suramin is used to treat trypanosome-

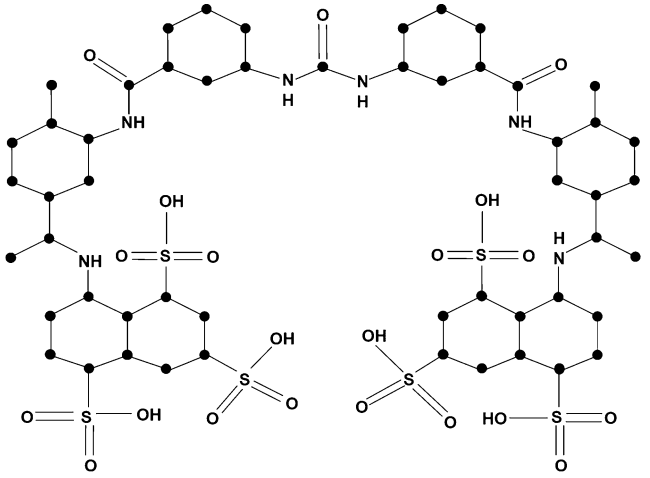

Figure 1. Chemical structure of suramin.

related human sleeping sickness. It is used to treat first-stage African trypanosomiasis without affecting the central nervous system, specifically caused by *Trypanosoma brucei* rhodesiense and *T. brucei* gambiense. It has been used in the treatment of river blindness (onchocerciasis). It is a symmetric molecule with a urea (NH−CO−NH) functional group in its center. Suramin has four amide functional groups (in addition to the urea) and six sulfonic acid groups, as well as six aromatic systems, including four benzene rings sandwiched between two naphthalene moieties. Because this formulation is water-soluble and does not degrade quickly in the air, it is commonly prescribed as sodium sulfonate salt when given as a medicine.

Polysaccharides are a type of carbohydrate with a high molecular weight, which represent a large class of bioactive molecules derived from microorganisms, plants, or animals.[10] Due to their great and remarkable bioactivities, such as their antimicrobial,[11] anticancer,[12] and antioxidant[13] properties, polysaccharides are widely employed in a variety of healthcare goods and medications. One of the most well-liked medical plants, aloe vera, is used extensively worldwide for the prevention or treatment of skin conditions, metabolic disorders, cardiovascular conditions, and cancers. One of aloe vera's primary bioactive polysaccharides, acemannan, a (1,4)-acetylated soluble polymannose, has a number of biological effects, including immunoregulation, anticancer, antioxidation, the promotion of bone proliferation and wound healing, neuroprotection, and intestinal health promotion.[14] The molecular formula of acemannan is $C_{66}H_{100}NO_{49}$, and the chemical structure of acemannan is shown in Figure 2. Acemannan typically has molecular weights between 1000 and 1600 kDa.[15,16] The majority of plant polysaccharides, including rhamnose (Rha), mannose (Man), fucose (Fuc), glucose (Glc), xylose (Xyl), arabinose (Ara), and galactose (Gal), are made up of two or more types of monosaccharides. In contrast, acemannan is primarily made up of mannose (84.9%), glucose (7.2%), and galactose (3.9%).[15] Next, we will provide an applicative review regarding these two aforementioned chemically significant drugs, i.e., S_{86} and A_{116}.

1.1. Applications of S_{86} and A_{116}. The first stage of acute human sleeping sickness, which is brought on by *T. brucei* rhodesiense, is still treated with suramin, a drug that has been around for 100 years.[17] However, because it cannot pass the blood−brain barrier, it is only used to treat the early (hemolymphatic) stage of sleeping sickness when the patient's central nervous system has not yet been infected with trypanosomes. An initial test dosage of 4 to 5 mg/kg of body weight is usually followed by five-week intravenously administered doses of 20 mg/kg (but not more than 1 g) of suramin.[18] In addition, suramin is used to treat camels suffering from surra (mal de caderas), which is brought on by *Trypanosoma* evansi.[19] Suramin also prevents the dengue

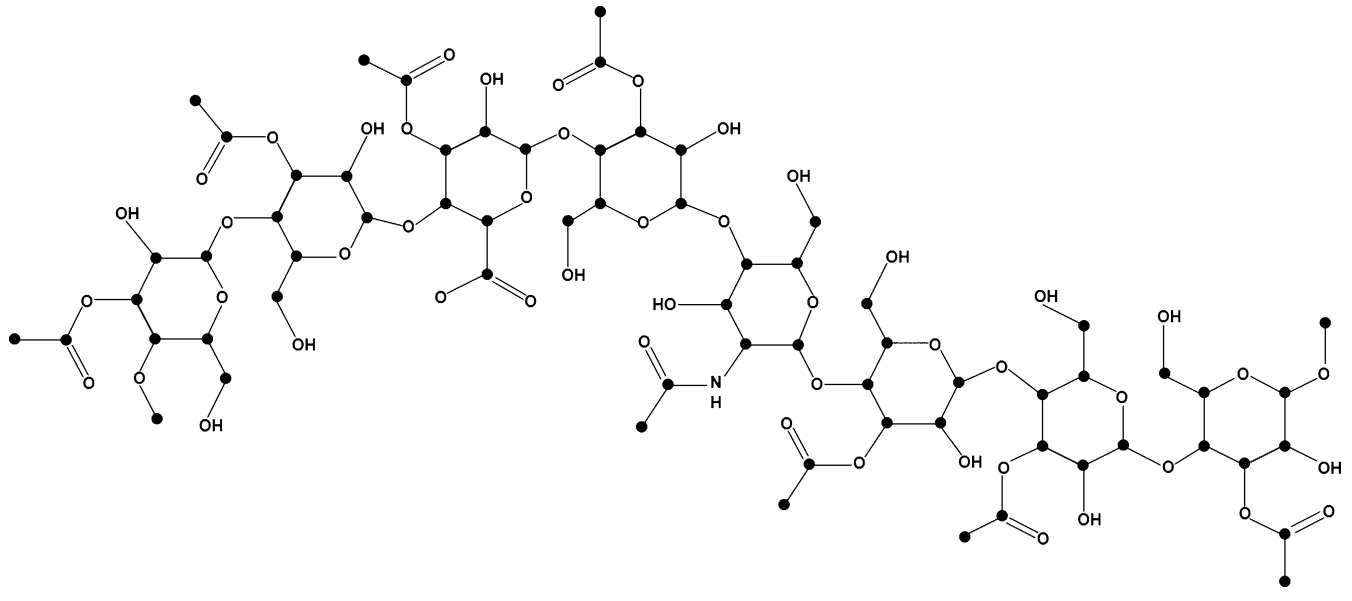

Figure 2. Chemical structure of acemannan.

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virus from attaching to host cells by directly affecting the viral envelope protein.[20] It was demonstrated that it prevented the chikungunya virus from producing RNA or replicating it.[21] When present at the time of infection, suramin offered protection in vitro, and this was attributed to a decrease in the viral host cell binding and uptake.[22]

Acemannan, which has been extracted and refined from aloe vera, is frequently employed in pharmaceuticals and functional foods because of its wide range of biological activities.[14] Acemannan has reportedly had numerous pharmacological and biological uses in the medical and industrial domains in recent years, including the treatment of tumor disorders,[23] metabolic diseases,[24] cardiovascular diseases, and oral diseases. Acemannan's potential applications frequently entail processing, which can include heating, drying, pasteurization, and dehydration.[15,25] It can also serve as a scaffold to facilitate the migration and attachment of cell growth factors. Acemannan significantly affects alveolar bone healing and further encourages bone formation. As a result, acemannan might be a biopolysaccharide substance that naturally regenerates bone.[26] Next, we discuss the most active research domains and topics known as the chemical graph theory, metric dimension, and edge metric dimension, respectively.

1.2. Molecular and Resolvability Parameters in Graph Theory. Chemical graph theory is a fascinating discipline that lies at the intersection of chemistry and mathematics. It involves the application of graph theory concepts and techniques to analyze and understand chemical compounds at the molecular level. Over the past few decades, this field has undergone significant growth, offering novel and innovative ideas for such studies. In essence, chemical graph theory encompasses all aspects of applying graph theory to chemistry. Chemical graph theory plays a critical role in various areas of chemistry including drug discovery, material science, and computational chemistry. It enables scientists to analyze and compare molecular structures, identify isomeric relationships, and explore the relationships between the structure and properties. By employing graph theoretical algorithms and techniques, researchers can unravel complex structural patterns, elucidate reaction mechanisms, and design novel molecules with the desired properties.

Moreover, chemical graph theory serves as a foundation for the development of computational methods used in chemoinformatics and molecular modeling. It provides a rigorous framework for the construction and manipulation of molecular graphs, facilitating the development of algorithms for molecular simulation, property prediction, and virtual screening of chemical compounds. Upon converting the molecular structure into a graph, a comprehensive examination of the structures can be conducted.[1] Detailed structural analysis becomes readily achievable by translating the molecular structure into a graph representation. Notably, two significant chemical compounds, suramin and acemannan, play crucial roles in medicinal drugs for treating life-threatening diseases. In graph theory, the metric dimension and its developed versions are extensively researched parameters. Similarly aligned with this theme, our research investigates the metric dimension of the molecular structures of S_{86} and A_{116}.

The term "locating set" was initially coined by Slater in 1975 to denote the issue of unambiguously determining or distinguishing the positions of intruders within a network, thereby introducing the concept of a metric dimension. In a separate development, Harary and Melter independently introduced a similar concept in 1976, referring to a specific set as a "resolving set". Following the publication of such pivotal works, a considerable amount of research has been conducted on the theoretical properties and specific applications of this graph invariant. Notably, Chvatal[27] and Erdos and Rényi[28] explored important links between graph-resolving sets and coin-weighing games. Melter and Tomescu,[8] as well as Chartrand et al.,[7] applied this concept to image processing, pattern recognition, and chemistry-related fields, respectively. The combinatorial optimization perspective of a metric dimension was investigated by Sebo and Tannier.[29] Additionally, Khuller et al.[9] came up with the utilization of a metric dimension in robot navigation, while Slater[3] examined its relevance to problems in SONAR, facility location, and LORAN for the coast guard.

In the realm of the metric dimension, the literature has introduced various iterations of resolving set variations. One such variation involves the resolution of two edges based not only on individual vertices but also on a specific set of selected vertices. Kelenc et al.[30] proposed the notion of an edge metric dimension (EMD) to encapsulate this concept. In a similar vein, Kelenc et al.[31] introduced mixed metric resolving sets, which combine both vertex resolvability and edge resolvability. In a mixed resolving set for a graph $G = G(V, E)$, each element of $V(G) \cup E(G)$ is uniquely determined with respect to an ordered subset of a set of vertices of G.

Researchers have conducted investigations on the resolvability parameters of various graph families, which have had a significant impact. For instance, Koam and Ahmad[32] examined the EMD of the barycentric subdivision of Cayley graphs. Ahsan et al.[33] and Sharma and Bhat[34] obtained metric dimension and EMD values for specific families of convex polytope graphs. Xing et al.[35] explored the mixed metric dimension (MMD) for selected graphs, including wheel graphs. Furthermore, recent research has focused on the conceptualizations of metric dimension, EMD, and MMD for various important molecular graphs. For example, Hussain et al.[36] investigated the metric dimension of 1-pentagonal carbon nanocone networks. Siddiqui and Imran[37] examined the metric dimension of H-naphthalenic and VC5C7 nanotubes. The concept of EMD for the same nanocone network was applied by Sharma and Bhat.[38] For networks such as the silicate star network, the metric dimension was determined by Simonraj and George.[39]

2. PRELIMINARIES

We will discuss some fundamental definitions related to metric dimensions in this particular section.

Definition 1. Resolving set:[3] Let $\Gamma = (V, E)$ be a simple connected graph and let $R = \{r_1, r_2, r_3, ..., r_k\}$ be an ordered

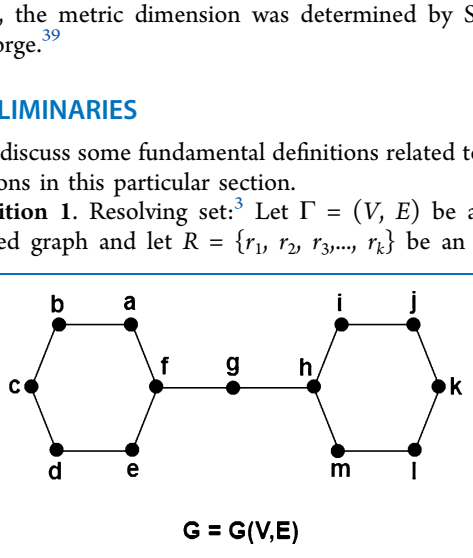

Figure 3. Graph G.

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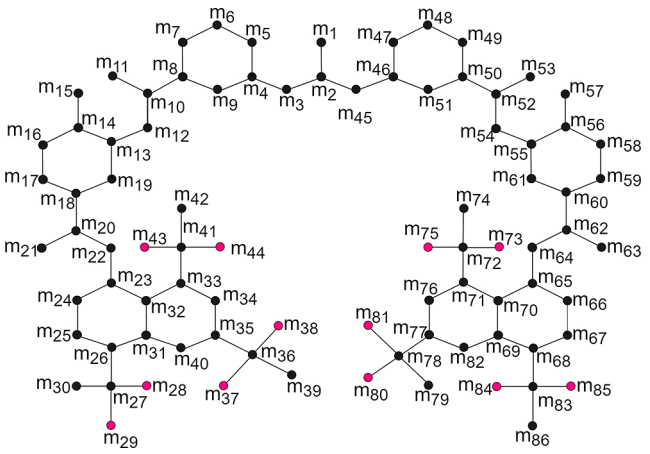

Figure 4. Molecular graph of S_{86}.

subset of the set of vertices $V(\Gamma)$ of Γ. The distance $d(p, q)$ between two vertices of Γ is the length of the shortest path between p and q. The representation of a vertex s of Γ with respect to R is the k-vector $(d(s, r_1), d(s, r_2),..., d(s, r_k))$ and it is denoted as $\varsigma(s|R)$. If the representation for different vertices in Γ is distinct, then the set R is called a resolving set for Γ.

Definition 2. Metric dimension:[3] A resolving set with a minimum number of elements is referred to as the metric basis for Γ, and the cardinality of the minimum resolving set is called the metric dimension of the graph Γ and is represented by $\dim(\Gamma)$.

Definition 3. Independent set:[40] A subset of vertices in a graph in which there is no pair of vertices that are adjacent is called an independent set.

Example 1. Consider a graph $G = G(V, E)$ with 13 vertices and 14 edges as shown in Figure 3.

The set $H_1 = \{a, b, m\}$ is a resolving set for the graph $G = G(V, E)$. Since the metric codes for the vertices of $G = G(V, E)$ with respect to H_1 are $\varsigma(a|H_1) = (0, 1, 4)$, $\varsigma(b|H_1) = (1, 0, 5)$, $\varsigma(c|H_1) = (2, 1, 6)$, $\varsigma(d|H_1) = (3, 2, 5)$, $\varsigma(e|H_1) = (2, 3, 4)$, $\varsigma(f|H_1) = (1, 2, 3)$, $\varsigma(g|H_1) = (2, 3, 2)$, $\varsigma(h|H_1) = (3, 4, 1)$, $\varsigma(i|H_1)$

Table 1. Metric Coordinates for the Vertices of S_{86}

metric codes	corresponding values	metric codes	corresponding values
$\varsigma(m_1\|H_r)$	(18, 18, 19, 19, 17, 17, 17, 17, 19, 19, 18, 18)	$\varsigma(m_{44}\|H_r)$	(7, 7, 6, 6, 2, 0, 32, 32, 34, 34, 33, 33)
$\varsigma(m_2\|H_r)$	(17, 17, 18, 18, 16, 16, 16, 16, 18.18.17, 17)	$\varsigma(m_{45}\|H_r)$	(18, 18, 19, 19, 17, 17, 15, 15, 17, 17, 16, 16)
$\varsigma(m_3\|H_r)$	(16, 16, 17, 17, 15, 15, 17, 17, 19, 19, 18, 18)	$\varsigma(m_{46}\|H_r)$	(19, 19, 20, 20, 18, 18, 14, 14, 16, 16, 15, 15)
$\varsigma(m_4\|H_r)$	(15, 15, 16, 16, 14, 14, 18, 18, 20, 20, 19, 19)	$\varsigma(m_{47}\|H_r)$	(20, 20, 21, 21, 19, 19, 15, 15, 17, 17, 16, 16)
$\varsigma(m_5\|H_r)$	(16, 16, 17, 17, 15, 15, 19, 19, 21, 21, 20, 20)	$\varsigma(m_{48}\|H_r)$	(21, 21, 22, 22, 20, 20, 14, 14, 16, 16, 15, 15)
$\varsigma(m_6\|H_r)$	(15, 15, 16, 16, 14, 14, 20, 20, 22, 22, 21, 21)	$\varsigma(m_{49}\|H_r)$	(22, 22, 23, 23, 21, 21, 13, 13, 15, 15, 14, 14)
$\varsigma(m_7\|H_r)$	(14, 14, 15, 15, 13, 13, 21, 21, 23, 23, 22, 22)	$\varsigma(m_{50}\|H_r)$	(21, 21, 22, 22, 20, 20, 12, 12, 14, 14, 13, 13)
$\varsigma(m_8\|H_r)$	(13, 13, 14, 14, 12, 12, 20, 20, 22, 22, 21, 21)	$\varsigma(m_{51}\|H_r)$	(20, 20, 21, 21, 19, 19, 13, 13, 15, 15, 14, 14)
$\varsigma(m_9\|H_r)$	(14, 14, 15, 15, 13, 13, 19, 19, 21, 21, 20, 20)	$\varsigma(m_{52}\|H_r)$	(22, 22, 23, 23, 21, 21, 11, 11, 13, 13, 12, 12)
$\varsigma(m_{10}\|H_r)$	(12, 12, 13, 13, 11, 11, 21, 21, 23, 23, 22, 22)	$\varsigma(m_{53}\|H_r)$	(23, 23, 24, 24, 22, 22, 12, 12, 14, 14, 13, 13)
$\varsigma(m_{11}\|H_r)$	(13, 13, 14, 14, 12, 12, 22, 22, 24, 24, 23, 23)	$\varsigma(m_{54}\|H_r)$	(23, 23, 24, 24, 22, 10, 10, 12, 12, 11, 11)
$\varsigma(m_{12}\|H_r)$	(11, 11, 12, 12, 10, 10, 22, 22, 24, 24, 23, 23)	$\varsigma(m_{55}\|H_r)$	(24, 24, 25, 25, 23, 23, 9, 9, 11, 11, 10, 10)
$\varsigma(m_{13}\|H_r)$	(10, 10, 11, 11, 9, 9, 23, 23, 25, 25, 24, 24)	$\varsigma(m_{56}\|H_r)$	(25, 25, 26, 26, 24, 24, 10, 10, 12, 12, 11, 11)
$\varsigma(m_{14}\|H_r)$	(11, 11, 12, 12, 10, 10, 24, 24, 26, 26, 25, 25)	$\varsigma(m_{57}\|H_r)$	(26, 26, 27, 27, 25, 25, 11, 11, 13, 13, 12, 12)
$\varsigma(m_{15}\|H_r)$	(12, 12, 13, 13, 11, 11, 25, 25, 27, 27, 26, 26)	$\varsigma(m_{58}\|H_r)$	(26, 26, 27, 27, 25, 25, 9, 9, 11, 11, 10, 10)
$\varsigma(m_{16}\|H_r)$	(10, 10, 11, 11, 9, 9, 25, 25, 27, 27, 26, 26)	$\varsigma(m_{59}\|H_r)$	(27, 27, 28, 28, 26, 26, 8, 8, 10, 10, 9, 9)
$\varsigma(m_{17}\|H_r)$	(9, 9, 10, 10, 8, 8, 26, 26, 28, 28, 27, 27)	$\varsigma(m_{60}\|H_r)$	(26, 26, 27, 27, 25, 25, 7, 7, 9, 9, 8, 8)
$\varsigma(m_{18}\|H_r)$	(8, 8, 9, 9, 7, 7, 25, 25, 27, 27, 26, 26)	$\varsigma(m_{61}\|H_r)$	(25, 25, 26, 26, 24, 24, 8, 8, 10, 10, 9, 9)
$\varsigma(m_{19}\|H_r)$	(9, 9, 10, 10, 8, 8, 24, 24, 26, 26, 25, 25)	$\varsigma(m_{62}\|H_r)$	(27, 27, 28, 28, 26, 26, 6, 6, 8, 8, 7, 7)
$\varsigma(m_{20}\|H_r)$	(7, 7, 8, 8, 6, 6, 26, 26, 28, 28, 27, 27)	$\varsigma(m_{63}\|H_r)$	(28, 28, 29, 29, 27, 27, 7, 7, 9, 9, 8, 8)
$\varsigma(m_{21}\|H_r)$	(8, 8, 9, 9, 7, 7, 27, 27, 29, 29, 28, 28)	$\varsigma(m_{64}\|H_r)$	(28, 28, 29, 29, 27, 27, 5, 5, 7, 7, 6, 6)
$\varsigma(m_{22}\|H_r)$	(6, 6, 7, 7, 5, 5, 27, 27, 29, 29, 28, 28)	$\varsigma(m_{65}\|H_r)$	(29, 29, 30, 30, 28, 28, 4, 4, 6, 6, 5, 5)
$\varsigma(m_{23}\|H_r)$	(5, 5, 6, 6, 4, 4, 28, 28, 30, 30, 29, 29)	$\varsigma(m_{66}\|H_r)$	(30, 30, 31, 31, 29, 29, 5, 5, 7, 7, 4, 4)
$\varsigma(m_{24}\|H_r)$	(4, 4, 7, 7, 5, 5, 29, 29, 31, 31, 30, 30)	$\varsigma(m_{67}\|H_r)$	(31, 31, 32, 32, 30, 30, 6, 6, 6, 6, 3, 3)
$\varsigma(m_{25}\|H_r)$	(3, 3, 6, 6, 6, 6, 30, 30, 32, 32, 31, 31)	$\varsigma(m_{68}\|H_r)$	(32, 32, 33, 33, 31, 31, 5, 5, 5, 5, 2, 2)
$\varsigma(m_{26}\|H_r)$	(2, 2, 5, 5, 5, 5, 31, 31, 33, 33, 32, 32)	$\varsigma(m_{69}\|H_r)$	(31, 31, 32, 32, 30, 30, 4, 4, 4, 4, 3, 3)
$\varsigma(m_{27}\|H_r)$	(1, 1, 6, 6, 6, 6, 32, 32, 34, 34, 33, 33)	$\varsigma(m_{70}\|H_r)$	(30, 30, 31, 31, 29, 29, 3, 3, 5, 5, 4, 4)
$\varsigma(m_{28}\|H_r)$	(0, 2, 7, 7, 7, 7, 33, 33, 35, 35, 34, 34)	$\varsigma(m_{71}\|H_r)$	(31, 31, 32, 32, 30, 30, 2, 2, 4, 4, 5, 5)
$\varsigma(m_{29}\|H_r)$	(2, 0, 7, 7, 7, 7, 33, 33, 35, 35, 34, 34)	$\varsigma(m_{72}\|H_r)$	(32, 32, 33, 33, 31, 31, 1, 1, 5, 5, 6, 6)
$\varsigma(m_{30}\|H_r)$	(2, 2, 7, 7, 7, 7, 33, 33, 35, 35, 34, 34)	$\varsigma(m_{73}\|H_r)$	(33, 33, 34, 34, 32, 32, 0, 2, 6, 6, 7, 7)
$\varsigma(m_{31}\|H_r)$	(3, 3, 4, 4, 4, 4, 30, 30, 32, 32, 31, 31)	$\varsigma(m_{74}\|H_r)$	(33, 33, 34, 34, 32, 32, 2, 2, 6, 6, 7, 7)
$\varsigma(m_{32}\|H_r)$	(4, 4, 5, 5, 3, 3, 29, 29, 31, 31, 30, 30)	$\varsigma(m_{75}\|H_r)$	(33, 33, 34, 34, 32, 32, 2, 0, 6, 6, 7, 7)
$\varsigma(m_{33}\|H_r)$	(5, 5, 4, 4, 2, 2, 30, 30, 32, 32, 31, 31)	$\varsigma(m_{76}\|H_r)$	(32, 32, 33, 33, 31, 31, 3, 3, 3, 3, 6, 6)
$\varsigma(m_{34}\|H_r)$	(6, 6, 3, 3, 3, 3, 31, 31, 33, 33, 32, 32)	$\varsigma(m_{77}\|H_r)$	(33, 33, 34, 34, 32, 32, 4, 4, 2, 2, 5, 5)
$\varsigma(m_{35}\|H_r)$	(5, 5, 2, 2, 4, 4, 32, 32, 34, 34, 33, 33)	$\varsigma(m_{78}\|H_r)$	(34, 34, 35, 35, 33, 33, 5, 5, 1, 1, 6, 6)
$\varsigma(m_{36}\|H_r)$	(6, 6, 1, 1, 5, 5, 33, 33, 35, 35, 34, 34)	$\varsigma(m_{79}\|H_r)$	(35, 35, 36, 36, 34, 34, 6, 6, 2, 2, 7, 7)
$\varsigma(m_{37}\|H_r)$	(7, 7, 0, 2, 6, 6, 34, 34, 36, 36, 35, 35)	$\varsigma(m_{80}\|H_r)$	(35, 35, 36, 36, 34, 34, 6, 6, 0, 2, 7, 7)
$\varsigma(m_{38}\|H_r)$	(7, 7, 2, 0, 6, 6, 34, 34, 36, 36, 35, 35)	$\varsigma(m_{81}\|H_r)$	(35, 35, 36, 36, 34, 34, 6, 6, 2, 0, 7, 7)
$\varsigma(m_{39}\|H_r)$	(7, 7, 2, 2, 6, 6, 34, 34, 36, 36, 35, 35)	$\varsigma(m_{82}\|H_r)$	(32, 32, 33, 33, 31, 31, 5, 5, 3, 3, 4, 4)
$\varsigma(m_{40}\|H_r)$	(4, 4, 3, 3, 5, 5, 31, 31, 33, 33, 32, 32)	$\varsigma(m_{83}\|H_r)$	(33, 33, 34, 34, 32, 32, 6, 6, 6, 6, 1, 1)
$\varsigma(m_{41}\|H_r)$	(6, 6, 5, 5, 1, 1, 31, 31, 33, 33, 32, 32)	$\varsigma(m_{84}\|H_r)$	(34, 34, 35, 35, 33, 33, 7, 7, 7, 7, 0, 2)
$\varsigma(m_{42}\|H_r)$	(7, 7, 6, 6, 2, 2, 32, 32, 34, 34, 33, 33)	$\varsigma(m_{85}\|H_r)$	(34, 34, 35, 35, 33, 33, 7, 7, 7, 7, 2, 0)
$\varsigma(m_{43}\|H_r)$	(7, 7, 6, 6, 0, 2, 32, 32, 34, 34, 33, 33)	$\varsigma(m_{86}\|H_r)$	(34, 34, 35, 35, 33, 33, 7, 7, 7, 7, 2, 2)

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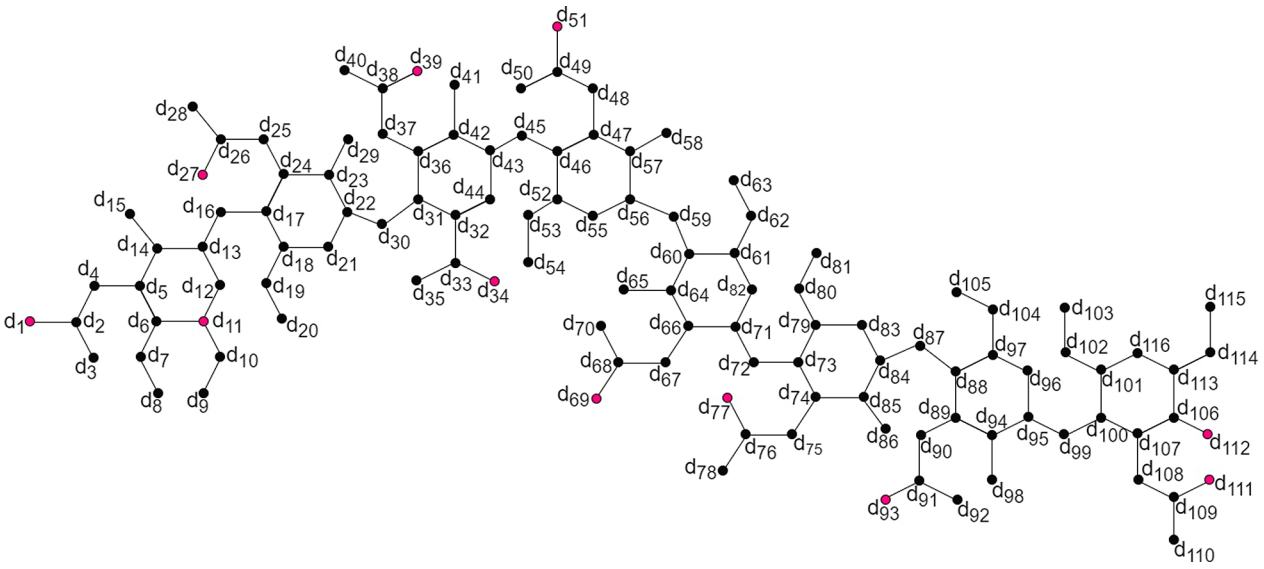

Figure 5. Molecular graph of A_{116}.

Table 2. Metric Coordinates for the Vertices of A_{116}

metric codes	corresponding values	metric codes	corresponding values
$\varsigma(d_1\|H_r)$	(0, 5, 11, 15, 16, 21, 27, 31, 36, 41, 40)	$\varsigma(d_{21}\|H_r)$	(9, 6, 6, 6, 7, 12, 18, 22, 27, 32, 31)
$\varsigma(d_2\|H_r)$	(1, 4, 10, 14, 15, 20, 26, 30, 35, 40, 39)	$\varsigma(d_{22}\|H_r)$	(10, 7, 5, 5, 6, 11, 17, 21, 26, 31, 30)
$\varsigma(d_3\|H_r)$	(2, 5, 11, 15, 16, 21, 27, 31, 36, 41, 40)	$\varsigma(d_{23}\|H_r)$	(9, 6, 4, 6, 7, 12, 18, 22, 27, 32, 31)
$\varsigma(d_4\|H_r)$	(2, 3, 9, 13, 14, 19, 25, 29, 34, 39, 38)	$\varsigma(d_{24}\|H_r)$	(8, 5, 3, 7, 8, 13, 19, 23, 28, 33, 32)
$\varsigma(d_5\|H_r)$	(3, 2, 8, 12, 13, 18, 24, 28, 33, 38, 37)	$\varsigma(d_{25}\|H_r)$	(9, 6, 2, 8, 9, 14, 20, 24, 29, 34, 33)
$\varsigma(d_6\|H_r)$	(4, 1, 9, 13, 14, 19, 25, 29, 34, 39, 38)	$\varsigma(d_{26}\|H_r)$	(10, 7, 1, 9, 10, 15, 21, 25, 30, 35, 34)
$\varsigma(d_7\|H_r)$	(5, 2, 10, 14, 15, 20, 26, 30, 35, 40, 39)	$\varsigma(d_{27}\|H_r)$	(11, 8, 0, 10, 11, 16, 22, 26, 31, 36, 35)
$\varsigma(d_8\|H_r)$	(6, 3, 11, 15, 16, 21, 27, 31, 36, 41, 40)	$\varsigma(d_{28}\|H_r)$	(11, 8, 2, 10, 11, 16, 22, 26, 31, 36, 35)
$\varsigma(d_9\|H_r)$	(7, 2, 10, 14, 15, 20, 26, 30, 35, 40, 39)	$\varsigma(d_{29}\|H_r)$	(10, 7, 5, 7, 8, 13, 19, 23, 28, 33, 32)
$\varsigma(d_{10}\|H_r)$	(6, 1, 9, 13, 14, 19, 25, 29, 34, 39, 38)	$\varsigma(d_{30}\|H_r)$	(11, 8, 6, 4, 5, 10, 16, 20, 25, 30, 29)
$\varsigma(d_{11}\|H_r)$	(5, 0, 8, 12, 13, 18, 24, 28, 33, 38, 37)	$\varsigma(d_{31}\|H_r)$	(12, 9, 7, 3, 4, 9, 15, 19, 24, 29, 28)
$\varsigma(d_{12}\|H_r)$	(6, 1, 7, 11, 12, 17, 23, 27, 32, 37, 36)	$\varsigma(d_{32}\|H_r)$	(13, 10, 8, 2, 5, 8, 14, 18, 23, 28, 27)
$\varsigma(d_{13}\|H_r)$	(5, 2, 6, 10, 11, 16, 22, 26, 31, 36, 35)	$\varsigma(d_{33}\|H_r)$	(14, 11, 9, 1, 6, 9, 15, 19, 24, 29, 28)
$\varsigma(d_{14}\|H_r)$	(4, 3, 7, 11, 12, 17, 23, 27, 32, 37, 36)	$\varsigma(d_{34}\|H_r)$	(15, 12, 10, 0, 7, 10, 16, 20, 25, 30, 29)
$\varsigma(d_{15}\|H_r)$	(5, 4, 8, 12, 13, 18, 24, 28, 33, 38, 37)	$\varsigma(d_{35}\|H_r)$	(15, 12, 10, 2, 7, 10, 16, 20, 25, 30, 29)
$\varsigma(d_{16}\|H_r)$	(6, 3, 5, 9, 10, 15, 21, 25, 30, 35, 34)	$\varsigma(d_{36}\|H_r)$	(13, 10, 8, 4, 3, 8, 14, 18, 23, 28, 27)

= (4, 5, 2), $\varsigma(j|H_1)$ = (5, 6, 3), $\varsigma(k|H_1)$ = (6, 7, 2), $\varsigma(l|H_1)$ = (5, 6, 1), $\varsigma(m|H_1)$ = (4, 5, 0).

However, H_1 is not a resolving set of the smallest cardinality because the set $H_2 = \{a, m\}$ is also a resolving set. Again, the set $H_3 = \{a\}$ is not a resolving set because $\varsigma(m|H_3) = \varsigma(i|H_3) = 4$. Since the graph $G = G(V, E)$ is not a path graph, no singleton vertex forms a resolving set for G and hence $\dim(G) = 2$.

In this study, we particularly focus on two drugs, namely, suramin (S_{86}) and acemannan (A_{116}).

3. METRIC BASIS AND METRIC DIMENSION OF S_{86}

The structure of S_{86} is discussed in this section. We examine some of its fundamental attributes and determine its metric dimension.

3.1. Molecular Graph of S_{86}. The molecular graph of S_{86}, as can be seen in Figure 4, consists of 86 vertices and 93 edges. It contains eight 6-cycles. The number of vertices to the left of m_2 is equal to the number of vertices to the right of m_2 in the molecular graph of S_{86}. This symmetry helps in finding metric codes for the structure. The colored vertices in Figure 4 are those that are involved in the resolving set of S_{86}.

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

Proof: Let $H_r = \{m_{28}, m_{29}, m_{37}, m_{38}, m_{43}, m_{44}, m_{73}, m_{75}, m_{80}, m_{81}, m_{84}$, and $m_{85}\}$ be a subset of vertices of S_{86}. We will show that H_r serves as a resolving set for S_{86} and has the smallest number of elements, i.e., H_r serves as a metric basis for S_{86}.

The metric code representations for each vertex in S_{86} are given in Table 1:

From Table 1, we can see that all the metric codes for distinct vertices are distinct and it follows that $\dim(S_{86}) \leq 12$. Now, it only remains to show that $\dim(S_{86}) \geq 12$.

If none of the vertices among $\{m_{28}, m_{29}\}$ is not involved in the resolving set, H_r, then the metric codes for two different vertices become identical. Also, if none of the vertices among $\{m_{29}, m_{30}\}$ is not involved in the resolving set, H_r, then the metric codes for two different vertices become identical. So, two vertices from the set $\{m_{28}, m_{29}$, and $m_{30}\}$ must be included in the resolving set, H_r.

If none of the vertices among $\{m_{37}, m_{38}\}$ is not involved in the resolving set, H_r, then the metric codes for two different vertices become identical. Also, if none of the vertices among $\{m_{38}, m_{39}\}$ is not involved in the resolving set, H_r, then the metric codes for two different vertices become identical. So, two vertices from the set $\{m_{37}, m_{38}$, and $m_{39}\}$ must be included in the resolving set, H_r. In the same way, two vertices from the set $\{m_{42}, m_{43}$, and $m_{44}\}$ must be included in H_r.

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Table 3. Metric Coordinates for the Vertices of A_{116}

metric codes	corresponding values	metric codes	corresponding values
$\varsigma(d_{17}\|H_r)$	(7, 4, 4, 8, 9, 14, 20, 24, 29, 34, 33)	$\varsigma(d_{37}\|H_r)$	(14, 11, 9, 5, 2, 9, 15, 19, 24, 29, 28)
$\varsigma(d_{18}\|H_r)$	(8, 5, 5, 7, 8, 13, 19, 23, 28, 33, 32)	$\varsigma(d_{38}\|H_r)$	(15, 12, 10, 6, 1, 10, 16, 20, 25, 30, 29)
$\varsigma(d_{19}\|H_r)$	(9, 6, 6, 8, 9, 14, 20, 24, 29, 34, 33)	$\varsigma(d_{39}\|H_r)$	(16, 13, 11, 7, 0, 11, 17, 21, 26, 31, 30)
$\varsigma(d_{20}\|H_r)$	(10, 7, 7, 9, 10, 15, 21, 25, 30, 35, 34)	$\varsigma(d_{40}\|H_r)$	(16, 13, 11, 7, 2, 11, 17, 21, 26, 31, 30)
$\varsigma(d_{41}\|H_r)$	(15, 12, 10, 6, 5, 8, 14, 18, 23, 28, 27)	$\varsigma(d_{79}\|H_r)$	(28, 25, 23, 17, 18, 13, 7, 5, 8, 13, 12)
$\varsigma(d_{42}\|H_r)$	(14, 11, 9, 5, 4, 7, 13, 17, 22, 27, 26)	$\varsigma(d_{80}\|H_r)$	(29, 26, 24, 18, 19, 14, 8, 6, 9, 14, 13)
$\varsigma(d_{43}\|H_r)$	(15, 12, 10, 4, 5, 6, 12, 16, 21, 26, 25)	$\varsigma(d_{81}\|H_r)$	(30, 27, 25, 19, 20, 15, 9, 7, 10, 15, 14)
$\varsigma(d_{44}\|H_r)$	(14, 11, 9, 3, 6, 7, 13, 17, 22, 27, 26)	$\varsigma(d_{82}\|H_r)$	(24, 21, 19, 13, 14, 9, 5, 7, 12, 17, 16)
$\varsigma(d_{45}\|H_r)$	(16, 13, 11, 5, 6, 5, 11, 15, 20, 25, 24)	$\varsigma(d_{83}\|H_r)$	(29, 26, 24, 18, 19, 14, 8, 6, 7, 12, 11)
$\varsigma(d_{46}\|H_r)$	(17, 14, 12, 6, 7, 4, 10, 14, 19, 24, 23)	$\varsigma(d_{84}\|H_r)$	(30, 27, 25, 19, 20, 15, 9, 5, 6, 11, 10)
$\varsigma(d_{47}\|H_r)$	(18, 15, 13, 7, 8, 3, 9, 13, 18, 23, 22)	$\varsigma(d_{85}\|H_r)$	(29, 26, 24, 18, 19, 14, 8, 4, 7, 12, 11)
$\varsigma(d_{48}\|H_r)$	(19, 16, 14, 8, 9, 2, 10, 14, 19, 24, 23)	$\varsigma(d_{86}\|H_r)$	(30, 27, 25, 19, 20, 15, 9, 5, 8, 13, 12)
$\varsigma(d_{49}\|H_r)$	(20, 17, 15, 9, 10, 1, 11, 15, 20, 25, 24)	$\varsigma(d_{87}\|H_r)$	(31, 28, 26, 20, 21, 16, 10, 6, 5, 10, 9)
$\varsigma(d_{50}\|H_r)$	(21, 18, 16, 10, 11, 2, 12, 16, 21, 26, 25)	$\varsigma(d_{88}\|H_r)$	(32, 29, 27, 21, 22, 17, 11, 7, 4, 9, 8)
$\varsigma(d_{51}\|H_r)$	(21, 18, 16, 10, 11, 0, 12, 16, 21, 26, 25)	$\varsigma(d_{89}\|H_r)$	(33, 30, 28, 22, 23, 18, 12, 8, 3, 8, 7)
$\varsigma(d_{52}\|H_r)$	(18, 15, 13, 7, 8, 5, 9, 13, 18, 23, 22)	$\varsigma(d_{90}\|H_r)$	(34, 31, 29, 23, 24, 19, 13, 9, 2, 9, 8)
$\varsigma(d_{53}\|H_r)$	(19, 16, 14, 8, 9, 6, 10, 14, 19, 24, 23)	$\varsigma(d_{91}\|H_r)$	(35, 32, 30, 24, 25, 20, 14, 10, 1, 10, 9)
$\varsigma(d_{54}\|H_r)$	(20, 17, 15, 9, 10, 7, 11, 15, 20, 25, 24)	$\varsigma(d_{92}\|H_r)$	(36, 33, 31, 25, 26, 21, 15, 11, 2, 11, 10)
$\varsigma(d_{55}\|H_r)$	(19, 16, 14, 8, 9, 6, 8, 12, 17, 22, 21)	$\varsigma(d_{93}\|H_r)$	(36, 33, 31, 25, 26, 21, 15, 11, 0, 11, 10)
$\varsigma(d_{56}\|H_r)$	(20, 17, 15, 9, 10, 5, 7, 11, 16, 21, 20)	$\varsigma(d_{94}\|H_r)$	(34, 31, 29, 23, 24, 19, 13, 9, 4, 7, 6)
$\varsigma(d_{57}\|H_r)$	(19, 16, 14, 8, 9, 4, 8, 12, 17, 22, 21)	$\varsigma(d_{95}\|H_r)$	(35, 32, 30, 24, 25, 20, 14, 10, 5, 6, 5)
$\varsigma(d_{58}\|H_r)$	(20, 17, 15, 9, 10, 5, 9, 13, 18, 23, 22)	$\varsigma(d_{96}\|H_r)$	(34, 31, 29, 23, 24, 19, 13, 9, 6, 7, 6)
$\varsigma(d_{59}\|H_r)$	(21, 18, 16, 10, 11, 6, 6, 10, 15, 20, 19)	$\varsigma(d_{97}\|H_r)$	(33, 30, 28, 22, 23, 18, 12, 8, 5, 8, 7)
$\varsigma(d_{60}\|H_r)$	(22, 19, 17, 11, 12, 7, 5, 9, 14, 19, 18)	$\varsigma(d_{98}\|H_r)$	(35, 32, 30, 24, 25, 20, 14, 10, 5, 8, 7)
$\varsigma(d_{61}\|H_r)$	(23, 20, 18, 12, 13, 8, 6, 8, 13, 18, 17)	$\varsigma(d_{99}\|H_r)$	(36, 33, 31, 25, 26, 21, 15, 11, 6, 5, 4)
$\varsigma(d_{62}\|H_r)$	(24, 21, 19, 13, 14, 9, 7, 9, 14, 19, 18)	$\varsigma(d_{100}\|H_r)$	(37, 34, 32, 26, 27, 22, 16, 12, 7, 4, 3)
$\varsigma(d_{63}\|H_r)$	(25, 22, 20, 14, 15, 10, 8, 10, 15, 20, 19)	$\varsigma(d_{101}\|H_r)$	(38, 35, 33, 27, 28, 23, 17, 13, 8, 5, 4)
$\varsigma(d_{64}\|H_r)$	(23, 20, 18, 12, 13, 8, 4, 8, 13, 18, 17)	$\varsigma(d_{102}\|H_r)$	(39, 36, 34, 28, 29, 24, 18, 14, 9, 6, 5)
$\varsigma(d_{65}\|H_r)$	(24, 21, 19, 13, 14, 9, 5, 9, 14, 19, 18)	$\varsigma(d_{103}\|H_r)$	(40, 37, 35, 29, 30, 25, 19, 15, 10, 7, 6)
$\varsigma(d_{66}\|H_r)$	(24, 21, 19, 13, 14, 9, 3, 7, 12, 17, 16)	$\varsigma(d_{104}\|H_r)$	(34, 31, 29, 23, 24, 19, 13, 9, 6, 9, 8)
$\varsigma(d_{67}\|H_r)$	(25, 22, 20, 14, 15, 10, 2, 8, 13, 18, 17)	$\varsigma(d_{105}\|H_r)$	(35, 32, 30, 24, 25, 20, 14, 10, 7, 10, 9)
$\varsigma(d_{68}\|H_r)$	(26, 23, 21, 15, 16, 11, 1, 9, 14, 19, 18)	$\varsigma(d_{106}\|H_r)$	(39, 36, 34, 28, 29, 24, 18, 14, 9, 4, 1)
$\varsigma(d_{69}\|H_r)$	(27, 24, 22, 16, 17, 12, 0, 10, 15, 20, 19)	$\varsigma(d_{107}\|H_r)$	(38, 35, 33, 27, 28, 23, 17, 13, 8, 3, 2)
$\varsigma(d_{70}\|H_r)$	(27, 24, 22, 16, 17, 12, 4, 10, 15, 20, 19)	$\varsigma(d_{108}\|H_r)$	(39, 36, 34, 28, 29, 24, 18, 14, 9, 2, 3)
$\varsigma(d_{71}\|H_r)$	(25, 22, 20, 14, 15, 10, 4, 6, 11, 16, 15)	$\varsigma(d_{109}\|H_r)$	(40, 37, 35, 29, 30, 25, 19, 15, 10, 1, 4)
$\varsigma(d_{72}\|H_r)$	(26, 23, 21, 15, 16, 11, 5, 5, 10, 15, 14)	$\varsigma(d_{110}\|H_r)$	(41, 38, 36, 30, 31, 26, 20, 16, 11, 2, 5)
$\varsigma(d_{73}\|H_r)$	(27, 24, 22, 16, 17, 12, 6, 4, 9, 14, 13)	$\varsigma(d_{111}\|H_r)$	(41, 38, 36, 30, 31, 26, 20, 16, 11, 0, 5)
$\varsigma(d_{74}\|H_r)$	(28, 25, 23, 17, 18, 13, 7, 3, 8, 13, 12)	$\varsigma(d_{112}\|H_r)$	(40, 37, 35, 29, 30, 25, 19, 15, 10, 5, 0)
$\varsigma(d_{75}\|H_r)$	(29, 26, 24, 18, 19, 14, 8, 2, 9, 14, 13)	$\varsigma(d_{113}\|H_r)$	(40, 37, 35, 29, 30, 25, 19, 15, 10, 5, 2)
$\varsigma(d_{76}\|H_r)$	(30, 27, 25, 19, 20, 15, 9, 1, 10, 15, 14)	$\varsigma(d_{114}\|H_r)$	(41, 38, 36, 30, 31, 26, 20, 16, 11, 6, 3)
$\varsigma(d_{77}\|H_r)$	(31, 28, 26, 20, 21, 16, 10, 0, 11, 16, 15)	$\varsigma(d_{115}\|H_r)$	(42, 39, 37, 31, 32, 27, 21, 17, 12, 7, 4)
$\varsigma(d_{78}\|H_r)$	(31, 28, 26, 20, 21, 16, 10, 2, 11, 16, 15)	$\varsigma(d_{116}\|H_r)$	(39, 36, 34, 28, 29, 24, 18, 14, 9, 6, 3)

In a similar way, two vertices from the set $\{m_{73}, m_{74}, m_{75}\}$, two from the set $\{m_{79}, m_{80}, m_{81}\}$, and two from $\{m_{84}, m_{85}, m_{86}\}$ must be included in the set H_r. From the above discussion, it follows that $\dim(S_{86}) \geq 12$. Thus, H_r is a metric basis for S_{86}.

This completes the proof of the theorem.

Corollary 1. The independent resolving number of S_{86} is 12.

4. METRIC BASIS AND METRIC DIMENSION OF A_{116}

In this section, we start by discussing the structure of A_{116}. We investigate some of its fundamental properties and determine its metric dimension.

4.1. Molecular Graph of Graph of A_{116}. The structure of A_{116} is very complex as it consists of 116 atoms except hydrogen atoms and 123 bonds except the bonds between hydrogen and other atoms. The molecular graph of A_{116} consists of 116 vertices and 123 edges, as shown in Figure 5. It contains eight 6-cycles. The pink-colored vertices in Figure 5 represent those vertices that are involved in the resolving set of A_{116}.

Theorem 2. The metric dimension of A_{116} is 11, i.e., $\dim(A_{116}) = 11$.

Proof: Let $H_r = \{d_1, d_{11}, d_{27}, d_{34}, d_{39}, d_{51}, d_{69}, d_{77}, d_{93}, d_{111}$, and $d_{112}\}$ be a subset of vertices of A_{116}. We will show that H_r is a resolving set for A_{116} and has the smallest cardinality, i.e., H_r serves as a metric basis for A_{116}.

The metric codes for each vertex in A_{116} are given in Tables 2 and 3

From Tables 2 and 3, it is clear that H_r is a resolving set and it follows that $\dim(A_{116}) \leq 11$. Now, it only remains to show that $\dim(A_{116}) \geq 11$.

If none of the vertices among $\{d_1, d_3\}$ is not involved in the resolving set, H_r, then the metric codes for two different vertices become identical. So, one among the vertices in the set $\{d_1, d_3\}$ must be included in H_r. Similarly, one among the vertices $\{d_{11}, d_{15}\}$ must be included in H_r. Similarly, one vertex from the set $\{d_{27}, d_{28}\}$ must be included in H_r.

If none of the vertices among $\{d_{34}, d_{35}\}$ is not involved in the resolving set, H_r, then the metric codes for two different vertices become identical. So, one among the vertices $\{d_{34}, d_{35}\}$ must be included in H_r. Similarly, one among the vertices $\{d_{39}, d_{40}\}$ must be included in H_r.

In a similar way, one vertex from each of the sets, $\{d_{50}, d_{51}\}$, $\{d_{69}, d_{70}\}$, $\{d_{77}, d_{78}\}$, $\{d_{92}, d_{93}\}$, $\{d_{110}, d_{111}\}$, and $\{d_{112}, d_{113}\}$

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Table 4. Minimum Resolving Sets for A_{116}

resolving set	no. of vertices representing carbon atoms	no. of vertices representing oxygen atoms
$A_1 = \{d_1, d_{11}, d_{28}, d_{35}, d_{40}, d_{51}, d_{69}, d_{78}, d_{93}, d_{110}, d_{113}\}$	10	1
$A_2 = \{d_3, d_{11}, d_{28}, d_{35}, d_{40}, d_{51}, d_{69}, d_{78}, d_{93}, d_{110}, d_{113}\}$	9	2
$A_3 = \{d_3, d_{15}, d_{28}, d_{35}, d_{40}, d_{51}, d_{69}, d_{78}, d_{93}, d_{110}, d_{113}\}$	8	3
$A_4 = \{d_3, d_{15}, d_{27}, d_{35}, d_{40}, d_{51}, d_{69}, d_{78}, d_{93}, d_{110}, d_{113}\}$	7	4
$A_5 = \{d_3, d_{15}, d_{27}, d_{35}, d_{39}, d_{51}, d_{69}, d_{78}, d_{93}, d_{110}, d_{113}\}$	6	5
$A_6 = \{d_3, d_{15}, d_{27}, d_{35}, d_{39}, d_{50}, d_{69}, d_{78}, d_{93}, d_{110}, d_{113}\}$	5	6
$A_7 = \{d_3, d_{15}, d_{27}, d_{35}, d_{39}, d_{50}, d_{70}, d_{78}, d_{93}, d_{110}, d_{113}\}$	4	7
$A_8 = \{d_3, d_{15}, d_{27}, d_{35}, d_{39}, d_{50}, d_{70}, d_{77}, d_{93}, d_{110}, d_{113}\}$	3	8
$A_9 = \{d_3, d_{15}, d_{27}, d_{35}, d_{39}, d_{50}, d_{70}, d_{77}, d_{92}, d_{110}, d_{113}\}$	2	9
$A_{10} = \{d_3, d_{15}, d_{27}, d_{35}, d_{39}, d_{50}, d_{70}, d_{77}, d_{92}, d_{111}, d_{113}\}$	1	10
$A_{11} = \{d_3, d_{15}, d_{27}, d_{35}, d_{39}, d_{50}, d_{70}, d_{77}, d_{92}, d_{111}, d_{112}\}$	0	11

must be included in the set H_r. From the above discussion, it follows that $\dim(A_{116}) \geq 11$. Thus, H_r is a metric basis for A_{116} and $\dim(A_{116}) = 11$. This completes the proof of the theorem.

Corollary 2. The independent resolving number of A_{116} is 11.

5. COMPARISON BETWEEN MINIMUM RESOLVING SETS OF S_{86} AND A_{116}

The minimal resolving sets for S_{86} and A_{116} are $R_1 = \{m_{28}, m_{29}, m_{37}, m_{38}, m_{43}, m_{44}, m_{73}, m_{75}, m_{80}, m_{81}, m_{84}, m_{85}\}$ and $R_2 = \{d_3, d_{15}, d_{27}, d_{35}, d_{39}, d_{50}, d_{70}, d_{77}, d_{92}, d_{111}, d_{112}\}$, respectively. The vertices m_{28}, m_{29}, m_{37}, m_{38}, m_{43}, m_{44}, m_{73}, m_{75}, m_{80}, m_{81}, m_{84}, and m_{85} in R_1 represent the oxygen atoms in the chemical structure of S_{86}. The vertices d_3, d_{15}, d_{27}, d_{35}, d_{39}, d_{50}, d_{70}, d_{77}, d_{92}, d_{111}, and d_{112} in R_2 represent the oxygen atoms in the chemical structure of A_{116}. There are some common functional groups in the chemical structures of suramin and acemannan. The metric dimension of S_{86} is 12 and that of A_{116} is 11, but despite bearing different metric dimensions, there are 11 vertices in each of the minimum resolving sets R_1 and R_2, which represent the oxygen atom. There are other resolving sets for S_{86}, but in each minimum resolving set for S_{86}, each vertex will represent an oxygen atom in the chemical structure of suramin.

Also, there are other minimum resolving sets for A_{116} in which each vertex represents either a carbon atom or an oxygen atom, as shown in Table 4.

The sets A_1, A_2, A_3, A_4, A_5, A_6, A_7, A_8, A_9, A_{10}, and A_{11} in Table 4 are the different minimum resolving sets for A_{116}, each having a different number of vertices representing carbon atoms and oxygen atoms in the chemical structure of A_{116}. From Table 4, it can be seen that the minimum resolving set R_2 has 11 vertices, which represent 11 oxygen atoms. So, the minimum resolving sets R_1 and R_2 for S_{86} and A_{116}, respectively, have 11 vertices, which represent oxygen atoms in their chemical structures. This common pattern in S_{86} and A_{116} may help in pharmaceutical research for the formation of a new drug, which may be used instead of using S_{86} and A_{116} separately.

6. CONCLUSIONS

Medicine or medication is a drug taken to cure or alleviate any symptoms of an illness or medical condition. The need for advancement of any medicinal drug has always been a key component in human history. In this work, we consider two essential drugs and investigate some of their molecular characteristics. This investigation examines the metric basis as well as the respective dimensions of the two famous drugs, viz., S_{86} and A_{116}. We have shown for these two drugs that $\dim(S_{86}) = 12$ and $\dim(A_{116}) = 11$. The resolving set for both of the structures is independent and has also been shown in this article. It may help the chemists find a common pattern shared by different drugs and utilize it in research related to medicines. In the future, we will discuss various other recently introduced variations of metric dimensions (such as edge-metric dimension, local metric dimension, partition dimension, MMD, etc.) for these two globally significant drugs, viz., S_{86} and A_{116}.

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Author Contributions

The inception and proposal of the concept were attributed to Malkesh Singh, who undertook a thorough examination of the validity of the results, as verified by V.K. Bhat and S.K. Sharma. A comprehensive survey of the existing literature has been conducted by Malkesh Singh and S.K. Sharma. The figures, tables, alignment, data adjustment, and all calculations were executed by Malkesh Singh and S.K. Sharma, under the guidance of V.K. Bhat. The final version of the draft was subjected to a comprehensive process of review and editing, involving the active participation of all the authors.

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