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Exchange Property in the Resolvability Parameters of Quinine Anti-Malarial Drug and the Importance of Resolving Sets in Drug Delivery

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ABSTRACT

In the realm of chemical graph theory, the study of resolvability parameters such as metric and edge metric dimensions has opened new avenues in modeling and analyzing molecular structures. This paper explores the exchange property within the resolvability parameters of the quinine anti-malarial drug, represented as a molecular graph, to uncover deeper structural symmetries and redundancies. By examining the presence and implications of the exchange property in resolving sets, we highlight their essential role in optimizing molecular identification, network navigation, and targeted drug delivery systems. Our findings underscore the critical importance of graph-theoretical tools in the design, simulation, and deployment of effective drug delivery mechanisms, where precision and efficiency are paramount. Resolvability parameters, such as metric, edge metric, and mixed metric dimensions, of the quinine anti-malaria drug exhibit an exchange property in the molecular graph of quinine. We convert the molecular structures of quinine into molecular graphs and then find these resolvability parameters.

Keywords: Resolving set; metric dimension; edge metric dimension; mixed metric dimension; quinine; exchange property.

(MSC2020) Codes: 05C10, 05C50, 05C70, 05C90

1. Introduction

Chemical graph theory serves as a valuable framework for analyzing chemical arrangements and representing molecular structures mathematically. This approach facilitates the description of the structural

attributes of various substances, including crystals, processes, clusters, molecules, and polymers. By leveraging chemical graph theory, it becomes possible to examine chemical structures from multiple perspectives within the context of emerging mathematical chemistry. This field incorporates contemporary advancements and insights into mathematical models that depict chemical scenarios, along with the practical utilization of mathematical methods and principles in the realm of chemistry [1]. The application of chemical graph theory proves particularly useful in simplifying and constructing intricate chemical configurations that might be challenging to comprehend in their original, unabstracted forms.

The medication quinine used in the treatment and prevention of malaria is accurate and informative. These medications play a vital role in combating malaria, a disease that affects millions of people worldwide. It's important for individuals taking these drugs to use them under the guidance of healthcare professionals to ensure proper dosing and to monitor for any potential side effects. Additionally, it's crucial to consider regional recommendations and drug resistance patterns when selecting the appropriate medication for malaria treatment. A locating set for a graph was first presented by Slater in 1975 [2]. The identical concept was later presented by Harary in 1976 with the title "metric dimension of a graph"[3]. Blumenthal first introduced the concepts of *RS* and metric dimensions in his monograph[4], which covered metric spaces and applications of distance geometry in a wider context.

Several scholars have been attracted by the idea of metric dimension. For instance, Hernando et al. explored this idea by investigating the fault-tolerant resolution set of tree graphs, demonstrating that P_n for $n \geq 2$ in the case of path graphs with $n > 2$ vertices[5,6]. Voronov estimated the king's graph's fault-tolerant metric dimension in their work [7]. Double resolving set and exchange property in a nanotube discussed in [8]. The study of homogeneous caterpillar graphs with fault-tolerant partition size was carried out in the context of [9]. Hussain et al. delved into the fault-tolerance of lattices of boron nanotubes [10], while Guo discussed certain types of line graphs' fault-tolerant resolvability [11]. The fault-tolerant metric dimension of graphs was explored in detail in [6], and chemical graph fault-tolerant partition resolvability was discussed in [12]. Extremal structures and the fault-tolerant resolvability of graphs were subjects of study in [13]. In contrast, the fault-tolerant metric dimension and edge fault-tolerant metric dimension of hollow coronoid structures were addressed in [14]. Finally, the investigation into fault-tolerant *RSs* for certain families of ladder networks was carried out in [15].

In our daily lives, the concept of metric dimension finds a multitude of practical applications that serve as a source of inspiration for researchers and have been widely explored. One noteworthy example is the application of metric dimension in discerning analogous patterns among a diverse range of medications [16]. The versatility of metric dimensions extends to various fields: Combinatorial Optimization: Metric dimension proves valuable in solving combinatorial optimization problems [17,18]. Robot Navigation: Metric dimension plays a pivotal role in robot navigation [19] and optimizing emergency response services discussed in [20]. Pharmaceutical Chemistry: The practical implications of metric dimension are evident in the realm of pharmaceutical chemistry [21]. Computer Networks: The metric dimension contributes to understanding and optimizing computer networks [22]. Graph Labeling: The concept of metric dimension is harnessed for canonically labeling graphs [23]. Location Problems: The metric dimension plays a role in addressing location

problems, including navigation systems like sonar and Loran [2,24]. Mastermind Game: Metric dimension is applied to the coding and decoding of the Mastermind game [25].

In the realm of chemistry, the concept of double-*RSs* finds numerous applications, with its exploration spanning various articles. The investigation into the double-*RS* of distinct chemical structures has been the subject of several studies. The double-*RS* of the Cocktail Party and Jellyfish graphs was examined in the work by [26]. The computation of minimum double-*RSs* of graphs was explored in the research by [27]. Further contributions include the determination of the metric dimension of nanotubes of VC_4C_7 and H-Naphtalenic nanotubes, as discussed in the study by [28], and fault-tolerant topological indices of graphs are discussed in [29]. Heptagonal snake graph using distance formulas studied in [30] and recent advancements in graph resolvability have introduced innovative parameters like the cycle-super magic labeling for polyomino chains [31] and the local edge partition dimension for complex networks [32]. In particular, the face metric dimension and the mixed partition dimension have been explored to strengthen face-based and mixed resolvability in planar and general graphs, respectively [33,34]. The *RS* of silicate stars was examined by [35]. Upper bounds on the metric dimension of cellulose networks were established in the research by [36]. Discussions about the Convex polytopes graph were presented in the work by [37]. The versatility of the concept of metric dimension is demonstrated by its application to solve various intricate problems across different domains. For insights into the resolvability parameters of diverse chemical structures, additional references can be found in sources such as [38–40].

To explore additional physical and chemical attributes of octagonal grids, further insights can be found in references such as [41–43]. To facilitate a clearer understanding of the concepts used in this article, here are some fundamental mathematical definitions: Distance: Distance refers to the measure of separation between two points or objects in a space. It is the distance in a network that the shortest path takes between any two vertices. *RS* In a graph, a *RS* is a subset of vertices that, based on their distances from one another, uniquely determines the positions of all other vertices. The lowest cardinality of a *RS* that can definitively identify the locations of every other graph vertex is known as the metric dimension of a graph. These definitions serve as foundational concepts that play a pivotal role in the discussions presented in this article.

Definition 1. The shortest path length between vertices β_1 and β_2 in graph G is referred to as the distance, often termed as a geodesic, between these two vertices $\beta_1, \beta_2 \in V(G)$. In the context of the simple, undirected graph G, where the sets of vertices and edges are denoted by V(G) and E(G) respectively, the distance between vertices is represented as $\eta(\beta_1, \beta_2)$.

This article relies on several fundamental theorems. In the work by [44], the author establishes that $dim(G) = 1$ if and only if G is the path graph P_n. Additionally, in the study conducted by [45], it is demonstrated that $dim(C_n) = 2$ for cycles C_n where $n \geq 3$.

Lemma 2. *Let G be any graph. Then* $\beta(G) < \beta'(G)$.

Lemma 3. [46] *For all G,* $\beta'(G) \geq 3$ *if* $G \neq P_n$.

In this article, we use *RS* for resolving set and *ERS* for edge resolving set.

2. Main Results

We compute the resolvability parameter just like the double *RS*, double *ERS*, and double mixed *RS* of Quinine.

2.1. Metric Dimension of various malaria drugs

In this section, we compute the resolvability parameter just like the double *RS* and exchange property of the molecular graph of Quinine.

2.1.1. Quinine

Quinine is a historically significant alkaloid that was first discovered in the cinchona tree. Here are some details regarding quinine: *Inherent Natural Source:* The source of quinine was the bark of the Andean cinchona tree, which grows throughout South America. Native Americans have been treating fevers with the bark for ages.

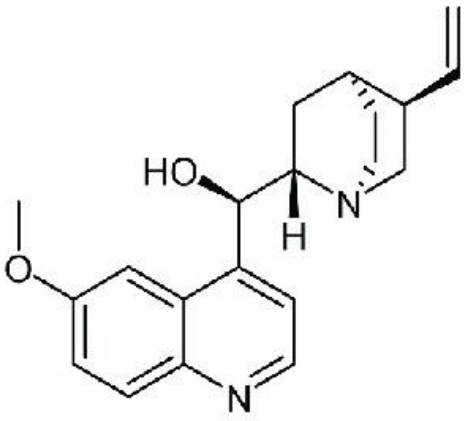

Figure 1. Quinine Molecular graph

Antimalarial Characteristics: The most well-known use of quinine is for antimalarial purposes. For generations, it has been a vital malaria remedy. It works well against the malaria-causing Plasmodium parasites. Quinine interferes with the parasites' capacity to utilize and get hemoglobin, which is necessary for their life cycle. *Classical Usage:* During the colonial era, cinchona bark and later refined quinine were widely used to cure malaria. Quinine had a crucial role in the creation of anti-malarial medications, particularly in the years when the disease was common in tropical and subtropical areas. *Plantations Cinchona:* To guarantee a more consistent supply of quinine, cinchona plantations were built outside of South America, namely in Java and India, in response to the growing demand for the drug.*Artificial Quinine:* Although quinine was first taken from natural sources, in the 20th century, synthetic techniques for generating quinine were discovered. This made it possible to produce the medication more dependably and economically. *Treatment Options for Leg Cramps:*

Quinine has also been used to relieve leg cramps that occur at night, though this use has generated debate because of possible negative consequences. *Warnings and Adverse Reactions:* One of the possible adverse effects of quinine is cinchonism, which can result in headache, nausea, and tinnitus. Using quinine under medical supervision is crucial, particularly when treating malaria. Regulating and Making Available: Quinine may have negative consequences; thus, some nations only allow prescriptions for it because of this and the advancement of alternative antimalarial medications. It's vital to remember that other, more recent antimalarial drugs are frequently chosen over quinine because of their effectiveness and decreased likelihood of negative effects. Furthermore, the availability and regulatory status of quinine may vary by region. *Derivatives:* Numerous artificial quinine derivatives, including mefloquine and chloroquine, have been created and are currently being utilized as antimalarial medications. Given quinine's history and contemporary uses in the treatment of malaria and other illnesses, it is imperative to speak with medical professionals when using quinine. Furthermore, quinine availability and regulatory status may differ by location.

Construction of Quinine Molecular graph. The color scheme is used for vertex labeling. The green color vertices are the members of the RS, and the remaining vertices are back-colored, and Figure 1 is the molecular graph of Quinine, but we convert it into a mathematical graph in Figure 2.

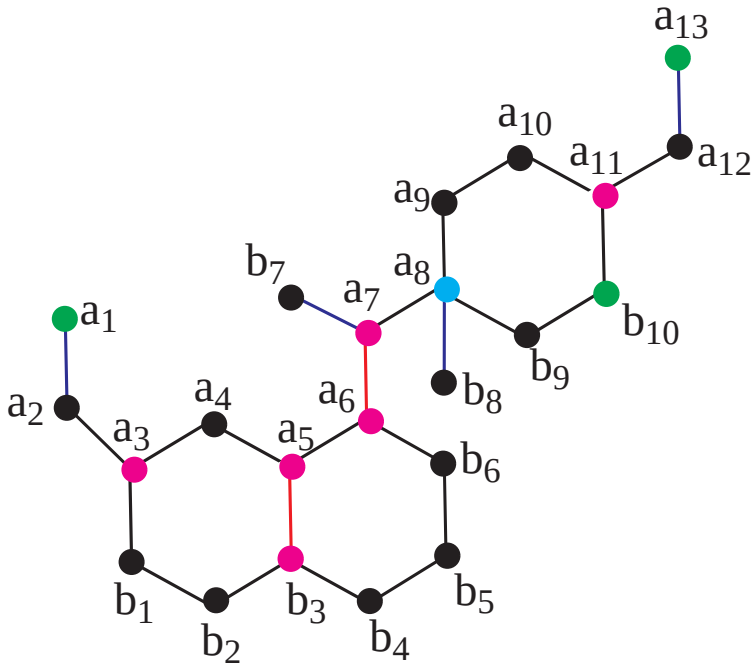

Figure 2. Quinine Molecular structures

The total number of vertices is 23, the total number of edges is 25, and the vertex and edge set is defined as

$$V(QN) = \{a_i, b_j; 1 \leq i \leq 13, 1 \leq j \leq 10\},$$
$$E(QN) = \{a_i a_{i+1}, b_j b_{j+1}, a_i b_i; 1 \leq i \leq 13, 1 \leq j \leq 10\}.$$

In Figure 2, the green color vertices are members of the RS and pink color vertices are of degree 3, the sky blue color vertex has degree 4, and the remaining vertices are black. The blue color is assigned to pendant edges, and the red color edges have end points of degree 3, and the remaining edges are black.

Theorem 4. *If QN is a molecular graph of a Quinine malaria drug. Then exchange property held in double RSs of cardinality* 3.

Proof. Let R_1 and R_2 be two sets of vertices of a Quinine molecular graph. We wish to display the unique representation of both sets to substantiate this assertion. The representation of R_1 is present in Theorem 5 and the representation of R_2 is shown in Theorem 6. □

Theorem 5. *If QN is a molecular graph of a Quinine malaria drug. Then R_1 be a RS of cardinality* 3.

Proof. Let R_1 be a set of vertices of a quinine molecular graph. We wish to display the unique representation of R_1 to substantiate this assertion. Let's proceed to prove this by demonstrating that the set R_1 has a unique representation with all the vertices of the quinine molecular graph QN. Let $R = \{a_1, b_{10}, a_{13}\}$. We now aim to show that R_1 has a unique representation with all the vertices of QN.

Table 2. Representation of the vertices of quinine

The representation of $R = \{a_1, b_{10}, a_{13}\}$ present in Table 1, 2

$r(. \mid R_1)$	(a_1, b_{10}, a_{13})
a_1	(0, 9, 12)
a_2	(1, 8, 11)
a_3	(2, 7, 10)
a_4	(3, 6, 9)
a_5	(4, 5, 8)
a_6	(5, 4, 7)
a_7	(6, 3, 6)
a_8	(7, 2, 5)
a_9	(8, 3, 4)
a_{10}	(9, 2, 3)
a_{11}	(10, 1, 2)
a_{12}	(11, 2, 1)
a_{13}	(12, 3, 0)

$r(. \mid R_1)$	(a_1, b_{10}, a_{11})
b_1	(3, 8, 11)
b_2	(4, 7, 10)
b_3	(5, 6, 9)
b_4	(6, 7, 10)
b_5	(7, 6, 9)
b_6	(6, 5, 8)
b_7	(7, 4, 7)
b_8	(8, 3, 6)
b_9	(8, 1, 4)
b_{10}	(9, 0, 3)

From Table 1 and 2 it is clear that the R_1 has unique Representation with all vertices of QN so R_1 is RS of cardinality 3. The minimum cardinality of R_1 is the metric dimension, so the metric dimension of quinine is 3. From all the above discussion, it is clear that the cardinality of RS of QN is less than or equal to 3. Now we are going to prove that the cardinality of RS of QN is not less than 3. The cardinality of RS of QN is possible only in the case of a path graph. The cardinality 2 of RS of QN is not possible because when we take any set of cardinality two, the representation is the same as the same vertices of quinine. Hence the cardinality of RS of quinine is 3. □

Theorem 6. *If QN is a molecular graph of a Quinine malaria drug. Then R_2 is also a RS of cardinality* 3.

Proof. Let R_2 be a set of vertices of a Quinine molecular graph. We wish to display the unique representation of R_2 to substantiate this assertion. Let's proceed to prove this by demonstrating that the set R_2 has a unique representation with all the vertices of the Quinine molecular graph QN. Let $R_2 = \{a_1, a_{10}, a_{13}\}$. We now aim to show that R_2 has a unique representation with all the vertices of QN.

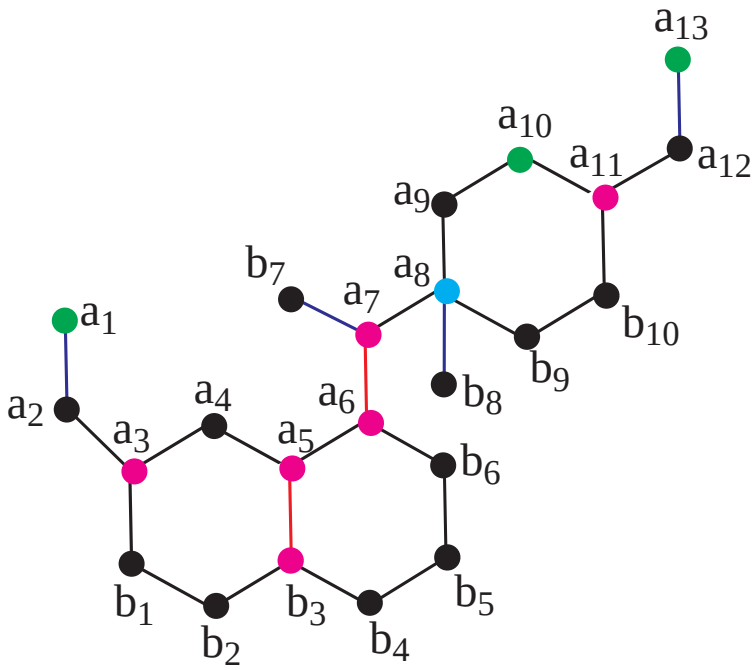

Figure 3. Quinine Molecular graph

Table 4. Representation of the vertices of quinine

The representation of $R = \{a_1, a_{10}, a_{13}\}$ present in Table 3, 4

$r(. \mid R_1)$	(a_1, a_{10}, a_{13})
a_1	(0, 9, 12)
a_2	(1, 8, 11)
a_3	(2, 7, 10)
a_4	(3, 6, 9)
a_5	(4, 5, 8)
a_6	(5, 4, 7)
a_7	(6, 3, 6)
a_8	(7, 2, 5)
a_9	(8, 1, 4)
a_{10}	(9, 0, 3)
a_{11}	(10, 1, 2)
a_{12}	(11, 2, 1)
a_{13}	(12, 3, 0)

$r(. \mid R_1)$	(a_1, b_{10}, a_{11})
b_1	(3, 8, 11)
b_2	(4, 7, 10)
b_3	(5, 6, 9)
b_4	(6, 7, 10)
b_5	(7, 6, 9)
b_6	(6, 5, 8)
b_7	(7, 4, 7)
b_8	(8, 3, 6)
b_9	(8, 3, 4)
b_{10}	(9, 2, 3)

From Table 3 and 4 it is clear that the R_2 has unique Representation with all vertices of QN so R_2 is RS of cardinality 3. Hence prove that the cardinality of R_2 is also 3. □

2.1.2. Exchange Property in Resolving sets

As we've seen, a subset W of the vertices of graph G is a RS if every vertex in graph G can be uniquely recognised by its distances to the vertices of subset W. RSs work similarly to bases in a vector space, because every vertex in the graph may be uniquely recognised among the vertices of these sets. While RSs have several properties similar to bases in a vector space, they may not always have the exchange feature from linear algebra. The exchange property in this case is that if S and R_1 are minimum RSs for G and $r \in R$, then there exists $s \in S$ such that $(S\backslash\{s\}) \cup \{r\}$ is a minimal RS for G.All of a graph G's minimal RSs have the same size when it satisfies the exchange property; this makes algorithmic methods more useful for figuring out $G's$ metric dimension. Therefore, to show that the exchange property does not hold in a given graph, one only needs to show two minimal RSs of different sizes. Note that the contrary is not true: the lack of the exchange condition does not entail the presence of minimal RSs of different sizes. The following deductions about the exchange property for RSs were made in [5].

Theorem 7. *According to [5], in a tree graph for resolving sets, the exchange property is valid.*

Theorem 8. *In wheels W_n for $n \geq 8$ [5], resolving sets do not have the exchange property.*

The exchange property for solving sets of necklace graphs Ne_n does not hold, as has recently been demonstrated.

Theorem 9. *The exchange property is absent from RSs of the necklace graph Ne_n for $n \geq 4$ [47]*

Theorem 10. *For $n \geq 4$ [48], the quasi-flower snarks do not satisfy the exchange property for minimum RSs.*

Theorem 11. *For $h, v \geq 1$ [49], the exchange property for minimal resolving sets holds in a nanosheet derived from the octagonal grid.*

We prove that the exchange property holds for RSs of Quinine molecular graphs in the following theorem.

Theorem 12. *The exchange property is valid for RSs of Quinine molecular graphs.*

Proof. In Quinine molecular graph we have two RSs let $R_1 = \{a_1, b_{10}, a_{13}\}$ and $R_2 = \{a_1, a_{10}, a_{13}\}$. According to the definition of exchange property $b_{10} \in R_1$ and $a_{10} \in R_2$ such that $(R_1\backslash\{b_{10}\} \cup \{a_{10}\})$ is also a resoling set. In these RSs, we change $\{b_{10}\}$ and $\{a_{10}\}$. Let $v = \{b_{10}\}$, $u = \{a_{10}\}$ and $v \in R_1$, $u \in R_2$ such that $(R_1\backslash\{v\} \cup \{u\}) = R_2$. R_2 is also a RS proved in theorem 2.3 □

2.2. Edge Metric Dimension of Anti-Malaria Drugs

In this section, the resolvability parameter is computed in the same way as the exchange property and double-ERS of the Quinine molecular graph.

2.2.1. Quinine

Theorem 13. *If QN is a molecular graph of a Quinine malaria drug. Then exchange property held in double ERSs of cardinality* 3.

Proof. Let R_1 and R_2 be two sets of vertices of a Quinine molecular graph. We wish to display the unique representation of both sets with all edges of quinine to substantiate this assertion. The representation of R_1 is in theorem 2.11, and the representation of R_2 is in theorem 2.12. □

Theorem 14. *If QN is a molecular graph of a Quinine malaria drug. Then R_1 be an edge resolving a set of cardinality* 3.

Proof. Let R_1 be a set of vertices of a quinine molecular graph. We wish to display the unique representation of R_1 to substantiate this assertion. Let's proceed to prove this by demonstrating that the set R_1 has a unique representation with all the edges of the quinine molecular graph QN. Let $R_1 = \{a_1, b_{10}, a_{13}\}$. We now aim to show that R_1 has a unique representation with all the edges of QN.

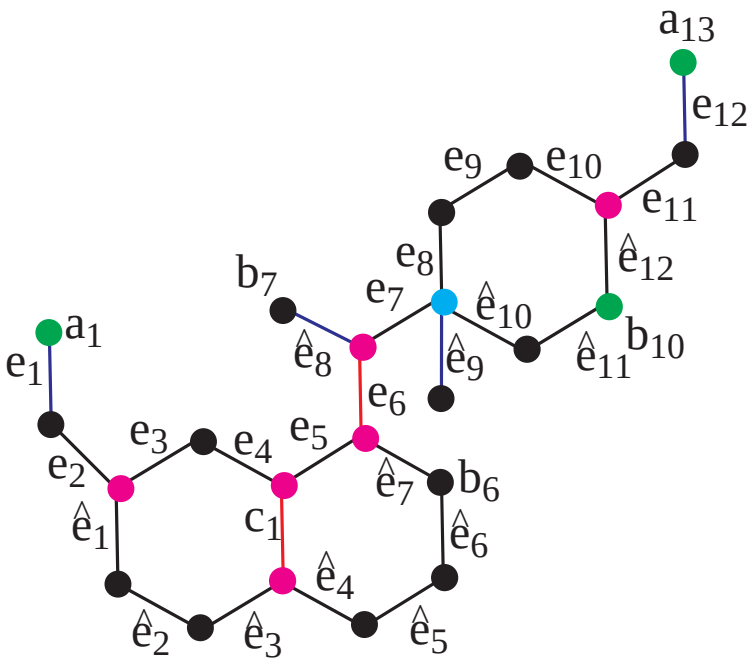

Figure 4. quinine Molecular graph

From Table 5 and 6 it is clear that the R_1 has unique Representation with all edges of QN so R_1 is ERS of cardinality 3. From all the above discussion, it is clear that the cardinality of ERS of QN is less than or equal to 3. Now we are going to prove that the cardinality of RS of QN is not less than 3. The cardinality of RS of QN is possible only in the case of a path graph. The cardinality 2 of RS of QN is not possible because when we take any set of cardinality two, the representation is the same as the same vertices of quinine. Hence the cardinality of RS of quinine is 3. □

Table 6. Representation of edges of quinine

The representation of $R = \{a_1, b_{10}, a_{13}\}$ present in Table 5, 6

$r(. \mid R_1)$	(a_1, b_{10}, a_{13})
e_1	(0, 8, 11)
e_2	(1, 7, 10)
e_3	(2, 6, 9)
e_4	(3, 5, 8)
e_5	(4, 4, 7)
e_6	(5, 3, 6)
e_7	(6, 2, 5)
e_8	(7, 2, 4)
e_9	(8, 2, 3)
e_{10}	(9, 1, 2)
e_{11}	(10, 1, 1)
e_{12}	(11, 2, 0)

$r(. \mid R_1)$	(a_1, b_{10}, a_{13})
$\hat{e}_1$	(2, 7, 10)
$\hat{e}_2$	(3, 7, 10)
$\hat{e}_3$	(4, 6, 9)
$\hat{e}_4$	(5, 6, 9)
$\hat{e}_5$	(6, 6, 9)
$\hat{e}_6$	(6, 5, 8)
$\hat{e}_7$	(5, 4, 7)
$\hat{e}_8$	(4, 3, 8)
$\hat{e}_9$	(7, 2, 6)
$\hat{e}_{10}$	(8, 1, 5)
$\hat{e}_{11}$	(8, 0, 4)
$\hat{e}_{12}$	(9, 0, 3)
c_1	(4, 5, 8)

Theorem 15. *If QN is a molecular graph of a Quinine malaria drug. Then R_2 is also be a ERS of cardinality* 3.

Proof. Let R_2 be a set of vertices of a Quinine molecular graph. We wish to display the unique representation of R_2 with all edges of Quinine to substantiate this assertion. Let's proceed to prove this by demonstrating that the set R_2 has a unique representation with all the edges of the Quinine molecular graph QN. Let $R_1 = \{a_1, b_2, b_4\}$. We now aim to show that R_2 has a unique representation with all the edges of QN.

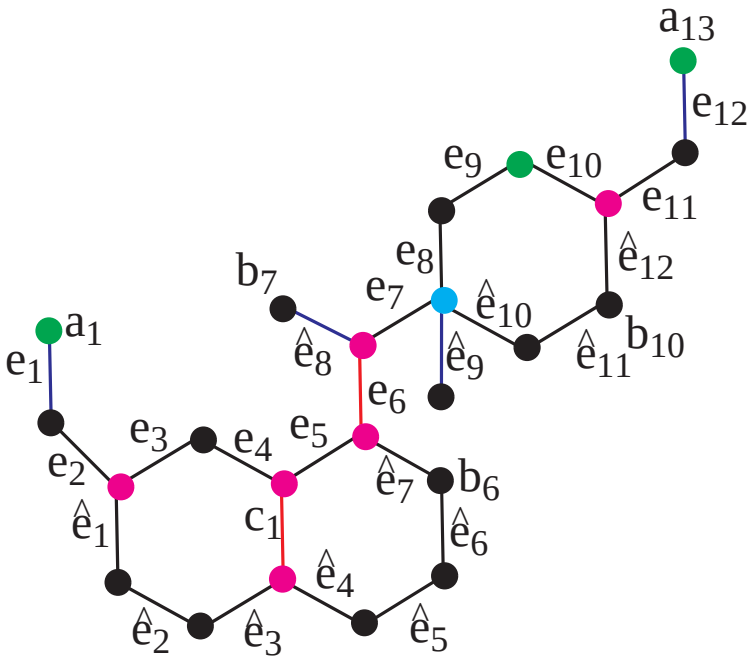

Figure 5. Quinine Molecular graph

From Table 7 and 8 it is clear that the R_2 has unique Representation with all edges of QN so R_2 is ERS of cardinality 3. The minimum cardinality of R_2 is the edge metric dimension, so the edge metric dimension of

Table 8. Representation of edges of quinine

The representation of $R = \{a_1, b_{10}, a_{13}\}$ present in Table 7, 8

$r(. \mid R_1)$	(a_1, a_{10}, a_{13})
e_1	(0, 8, 11)
e_2	(1, 7, 10)
e_3	(2, 6, 9)
e_4	(3, 5, 8)
e_5	(4, 4, 7)
e_6	(5, 3, 6)
e_7	(6, 2, 5)
e_8	(7, 1, 4)
e_9	(8, 0, 3)
e_{10}	(9, 0, 2)
e_{11}	(10, 1, 1)
e_{12}	(11, 2, 0)

$r(. \mid R_1)$	(a_1, a_{10}, a_{13})
$\hat{e}_1$	(2, 7, 10)
$\hat{e}_2$	(3, 7, 10)
$\hat{e}_3$	(4, 6, 9)
$\hat{e}_4$	(5, 6, 9)
$\hat{e}_5$	(6, 6, 9)
$\hat{e}_6$	(6, 5, 8)
$\hat{e}_7$	(5, 4, 7)
$\hat{e}_8$	(4, 3, 3)
$\hat{e}_9$	(7, 2, 2)
$\hat{e}_{10}$	(7, 1, 2)
$\hat{e}_{11}$	(8, 0, 2)
$\hat{e}_{12}$	(9, 0, 1)
c_1	(4, 5, 8)

Quinine is 3. From all the above discussion, it is clear that the metric dimension of QN is less than or equal to 3. Now we are going to prove that the cardinality of the ERS of QN is not less than 3. The cardinality of the ERS is one, possible only in the case of a path graph. The cardinality of the ERS is 2, which is not possible because when we take any set of cardinality two, the representation remains the same for some edges of Quinine. Hence, the cardinality of the edge-RS of Quinine is 3. □

2.2.2. Exchange Property in Edge Resolving Sets

We demonstrate that the exchange property is valid for $ERSs$ of Quinine molecular graphs in the following theorem.

Theorem 16. *The exchange property is valid for ERSs of Quinine molecular graphs.*

Proof. In quinine molecular graph we have two $ERSs$ let $R_1 = \{a_1, b_{10}, a_{13}\}$ and $R_2 = \{a_1, a_{10}, a_{13}\}$. According to the definition of exchange property $b_{10} \in R_1$ and $a_{10} \in R_2$ such that $(R_1 \backslash \{b_{10}\} \cup \{a_{10}\})$ is also a edge resoling set. In these $ERSs$, we change $\{b_{10}\}$ and $\{a_{10}\}$. Let $v = \{b_{10}\}$, $u = \{a_{10}\}$ and $v \in R_1$, $u \in R_2$ such that $(R_1 \backslash \{v\} \cup \{u\}) = R_2$. R_2 is also a ERS proved in theorem 2.3 □

2.3. Mixed Metric Dimension of Anti-Malaria Drugs

In this section, the resolvability parameter is computed in the same way as the exchange property and double-MRS of the Quinine molecular graph.

2.3.1. Quinine

Theorem 17. *If QN is a molecular graph of a Quinine malaria drug. Then exchange property held in double mixed RSs of cardinality* 3.

Proof. Let R_1 and R_2 be two sets of vertices of a Quinine molecular graph. We wish to display the unique representation of both sets to substantiate this assertion. The representation of R_1 is in theorem 2.15, and the representation of R_2 is in theorem 2.16. □

Theorem 18. *If QN is a molecular graph of a Quinine malaria drug. Then R_1 be a mixed RS of cardinality* 3.

Proof. Let R_1 be a set of vertices of a Quinine molecular graph. We wish to display the unique representation of R_1 with all vertices and edges of QN to substantiate this assertion. Let's proceed to prove this by demonstrating that the set R_1 has a unique representation with all the vertices and edges of the Quinine molecular graph QN. Let $R_1 = \{a_1, b_1, a_8\}$. We now aim to show that R_1 has a unique representation with all the vertices of QN.

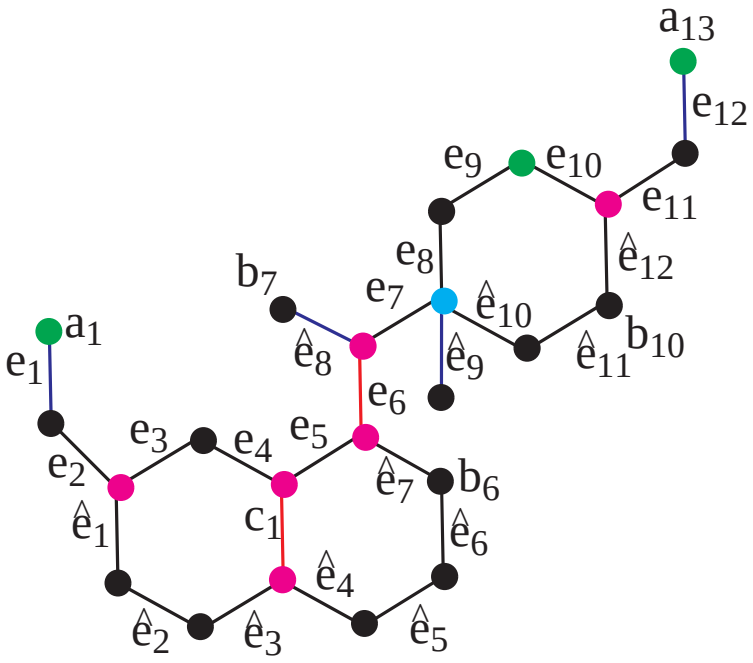

Figure 6. quinine Molecular graph

Table 10. Representation of edges of quinine

The representation of $R = \{a_1, a_{10}, a_{13}\}$ present in Table 9, 10

$r(. \mid R_1)$	(a_1, a_{10}, a_{13})
a_1	(0, 9, 12)
a_2	(1, 8, 11)
a_3	(2, 7, 10)
a_4	(3, 6, 9)
a_5	(4, 5, 8)
a_6	(5, 4, 7)
a_7	(6, 3, 6)
a_8	(7, 2, 5)
a_9	(8, 1, 4)
a_{10}	(9, 0, 3)
a_{11}	(10, 1, 2)
a_{12}	(11, 2, 1)
a_{13}	(12, 3, 0)
b_1	(3, 8, 11)
b_2	(4, 7, 10)
b_3	(5, 6, 9)
b_4	(6, 7, 10)
b_5	(7, 6, 9)
b_6	(6, 5, 8)
b_7	(7, 4, 7)
b_8	(8, 3, 6)
b_9	(8, 3, 4)
b_{10}	(9, 2, 3)

$r(. \mid R_1)$	(a_1, b_{10}, a_{11})
e_1	(0, 8, 11)
e_2	(1, 7, 10)
e_3	(2, 6, 9)
e_4	(3, 5, 8)
e_5	(4, 4, 7)
e_6	(5, 3, 6)
e_7	(6, 2, 5)
e_8	(7, 2, 4)
e_9	(8, 2, 3)
e_{10}	(9, 1, 2)
e_{11}	(10, 1, 1)
e_{12}	(11, 2, 0)
$\hat{e}_1$	(2, 7, 10)
$\hat{e}_2$	(3, 7, 10)
$\hat{e}_3$	(4, 6, 9)
$\hat{e}_4$	(5, 6, 9)
$\hat{e}_5$	(6, 6, 9)
$\hat{e}_6$	(6, 5, 8)
$\hat{e}_7$	(5, 4, 7)
$\hat{e}_8$	(4, 3, 8)
$\hat{e}_9$	(7, 2, 6)
$\hat{e}_{10}$	(8, 1, 5)
$\hat{e}_{11}$	(8, 0, 4)
$\hat{e}_{12}$	(9, 0, 3)
c_1	(4, 5, 8)

From Table 9 and 10 it is clear that the ${}_1R$ has unique Representation with all vertices and edges of QN so R_1 is mixed RS of cardinality 3. The minimum cardinality of R_1 is a mixed metric dimension, so the mixed metric dimension of Quinine is 3. From all the above discussion, it is clear that the cardinality of a mixed RS of QN is less than or equal to 3. Now we are going to prove that it is not less than 3. The mixed RS of cardinality 1 is possible only in the case of a path graph. The mixed RS of cardinality 2 is not possible because when we take any set of cardinality two, the representation remains the same for some vertices of Quinine. Hence R_1 is the mixed RS of cardinality 3. □

Theorem 19. *If QN is a molecular graph of a Quinine malaria drug. Then R_2 is also a mixed RS of cardinality* 3.

Proof. Let R_2 be a set of vertices of a Quinine molecular graph. We wish to display the unique representation of R_2 with all vertices and edges of QN to substantiate this assertion. Let's proceed to prove this by demonstrating that the set R_2 has a unique representation with all the vertices and edges of the Quinine molecular graph QN. Let $R_2 = \{a_1, b_2, b_4\}$. We now aim to show that R_2 has a unique representation with all the vertices and edges of QN.

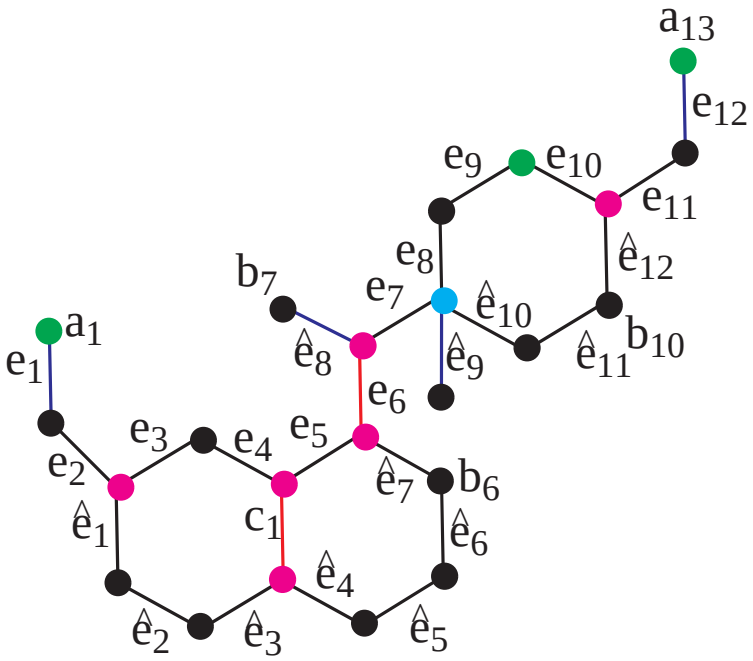

Figure 7. Molecular graph

Table 12. Representation of edges of quinine

The representation of $R = \{a_1, a_{10}, a_{13}\}$ present in Table 11, 12

$r(. \mid R_1)$	(a_1, a_{10}, a_{13})
a_1	(0, 9, 12)
a_2	(1, 8, 11)
a_3	(2, 7, 10)
a_4	(3, 6, 9)
a_5	(4, 5, 8)
a_6	(5, 4, 7)
a_7	(6, 3, 6)
a_8	(7, 2, 5)
a_9	(8, 1, 4)
a_{10}	(9, 0, 3)
a_{11}	(10, 1, 2)
a_{12}	(11, 2, 1)
a_{13}	(12, 3, 0)
b_1	(3, 8, 11)
b_2	(4, 7, 10)
b_3	(5, 6, 9)
b_4	(6, 7, 10)
b_5	(7, 6, 9)
b_6	(6, 5, 8)
b_7	(7, 4, 7)
b_8	(8, 3, 6)
b_9	(8, 3, 4)
b_{10}	(9, 2, 3)

$r(. \mid R_1)$	(a_1, a_{10}, a_{13})
e_1	(0, 8, 11)
e_2	(1, 7, 10)
e_3	(2, 6, 9)
e_4	(3, 5, 8)
e_5	(4, 4, 7)
e_6	(5, 3, 6)
e_7	(6, 2, 5)
e_8	(7, 1, 4)
e_9	(8, 0, 3)
e_{10}	(9, 0, 2)
e_{11}	(10, 1, 1)
e_{12}	(11, 2, 0)
$\hat{e}_1$	(2, 7, 10)
$\hat{e}_2$	(3, 7, 10)
$\hat{e}_3$	(4, 6, 9)
$\hat{e}_4$	(5, 6, 9)
$\hat{e}_5$	(6, 6, 9)
$\hat{e}_6$	(6, 5, 8)
$\hat{e}_7$	(5, 4, 7)
$\hat{e}_8$	(4, 3, 3)
$\hat{e}_9$	(7, 2, 2)
$\hat{e}_{10}$	(7, 1, 2)
$\hat{e}_{11}$	(8, 0, 2)
$\hat{e}_{12}$	(9, 0, 1)
c_1	(4, 5, 8)

From Table 11 and 12 it is clear that the R_2 has unique Representation with all vertices and edges of QN so R_2 is mixed RS of cardinality 3. The minimum cardinality of R_2 is mixed metric dimension, so the mixed metric dimension of Quinine is 3. □

2.3.2. Exchange Property in Mixed *RSs*

In the next theorem, we show that the exchange property holds for mixed *RSs* of the Quinine molecular graph.

Theorem 20. *The exchange property is valid for mixed RSs of Quinine molecular graphs.*

Proof. In quinine molecular graph we have two mixed *RSs* let $R_1 = \{a_1, b_{10}, a_{13}\}$ and $R_2 = \{a_1, a_{10}, a_{13}\}$. According to the definition of exchange property $b_{10} \in R_1$ and $a_{10} \in R_2$ such that $(R_1 \backslash \{b_{10}\} \cup \{a_{10}\})$ is also a mixed resoling set. In these mixed *RSs*, we change $\{b_{10}\}$ and $\{a_{10}\}$. Let $v = \{b_{10}\}$, $u = \{a_{10}\}$ and $v \in R_1$, $u \in R_2$ such that $(R_1 \backslash \{v\} \cup \{u\}) = R_2$. R_2 is also a mixed RS proved in theorem 2.3 □

Importance of Resolving Sets in Drug Delivery

- **Identifying Critical Positions:** A resolving set can help identify the most important positions in a drug molecule that determine its functionality. By using a resolving set, we can focus on these positions to optimize drug delivery. These positions are essentially the *critical functional groups* or atoms that interact with biological systems (e.g., enzymes, receptors).
- **Comparing Drug Molecules:** Once a resolving set is established for a given molecule, we can *compare different drugs* to see if their resolving sets (critical positions) overlap. If two drugs have *similar positions* in their resolving sets, they might share similar *biological activities* or interact with the same *biological target*. Conversely, if the positions differ, it may lead to *differentiating the therapeutic effects* or side effects between drugs.
- **Enhanced Drug Targeting:** Drug delivery systems, such as nanoparticles or liposomes, often need to target specific cells or tissues. By using a *resolving set* approach, the critical parts of the drug molecule (those that define how it interacts with its target) can be used to design drugs with higher specificity for their target, improving the *efficiency* and *precision* of drug delivery.
- **Functional Group Matching:** Functional groups in molecules (such as hydroxyl, amino, or carboxyl groups) are often key to determining how the drug behaves in the body. A resolving set can help identify which functional groups in the drug molecules *correspond to specific biological activities*, allowing researchers to optimize drug designs based on their desired effects.
- **Predicting Drug Interactions:** Resolving sets can also help in predicting potential *drug-drug interactions* by comparing the resolving sets of different molecules. If two drugs share similar resolving set positions, there might be a risk of interference or interaction when used together.

3. Conclusion

In this article, we talk about the Quinine anti-malaria drug. Based on the graph's distance, we determine some resolvability parameters: double RS and exchange property, double ERS and exchange property, and double mixed RS and exchange property for Quinine. The double RS, double ERS, and double mixed RS for Quinine have a cardinality of 3. The exchange property in this article used for two elements means we can change to elements of R_1 and R_2, then both remain show resolvability. Our results show that if two resolving sets R_1 and R_2 possess this property, then exchanging one element from each still preserves their resolvability. This highlights the structural symmetry and redundancy present in the molecular graph, offering insights into reliable identification and mapping strategies. Such properties are not only theoretically interesting but also carry potential applications in the optimization of drug delivery systems, where precise molecular recognition and adaptability are critical.

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References

[1] M. F. Nadeem, M. Hassan, M. Azeem, S. U. D. Khan, M. R. Shaik, M. A. F. Sharaf, A. Abdelgawad, E. M. Awwad. Application of Resolvability Technique to Investigate the Different Polyphenyl Structures for Polymer Industry, *Journal of Chemistry*, 2021(2021), 8. doi: 10.1155/2021/6633227.

[2] P. J. Slater. Leaves of trees, *Congressus Numerantium*, 14(1975) 549–559.

[3] F. Harary, R. A. Melter. On the metric dimension of graphs, *Ars Combinatoria*, 2(1976) 191–195.

[4] L. M. Blumenthal. Theory and Applications of Distance Geometry, *Clarendon Press, Oxford*, (1953).

[5] D. L. Boutin. Determining sets, Resolving sets, and the exchange property, *Graphs and Combinatorics*, 25(2009) 789–806. doi: 10.1007/s00373-010-0880-6.

[6] C. Hernando, M. Mora, P. J. Slater, D. R. Wood. Fault-tolerant metric dimension of graphs, *Convexity in Discrete Structures*, 5(2008) 81–85.

[7] R. V. Voronov. The fault-tolerant metric dimension of the king's graph, *Vestnik of Saint Petersburg University: Applied Mathematics, Computer Science, Control Processes*, 13(2017) 241–249.

[8] Ali N. A. Koam, Sikander Ali, Ali Ahmad, Muhammad Azeem, Muhammad Kamran Jamil. Double resolving set and exchange property in nanotube, *AIMS Mathematics*, 8(9)(2023) 20305–20323. doi: 10.3934/math 20231035.

[9] K. Azhar, S. Zafar, A. Kashif. On Fault-Tolerant Partition Dimension of Homogeneous Caterpillar Graphs, *Mathematical Problems in Engineering*, 2021(2021) 241–249. doi: 10.1155/2021/7282245.

[10] Z. Hussain, M. M. Munir. Fault-tolerance in the metric dimension of boron nanotube lattices, *Frontiers in Computational Neuroscience*, (2023) 1–8. doi: 10.3389/fncom.2022.1023585.

[11] X. Guo, M. Faheem, Z. Zahid, W. Nazeer, J. Li. Fault-Tolerant Resolvability in Some Classes of Line Graphs, *Mathematical Problems in Engineering*, 2020(2020) 1–8. doi: 10.1155/2020/1436872.

[12] K. Azhar, S. Zafar, A. Kashif, Z. Zahid. Fault-Tolerant Partition Resolvability in Chemical Graphs, *Polycyclic Aromatic Compounds*, (2022) 1–11. doi: 10.1080/10406638.2022.2156559.

[13] H. Raza, S. Hayat, M. Imran, X. Pan. Fault-Tolerant Resolvability and Extremal Structures of Graphs, *Mathematics*, 7(2019) 79.

[14] Ali N. A. Koam, A. Ahmad, M. Ibrahim, M. Azeem. Edge Metric and Fault-Tolerant Edge Metric Dimension of Hollow Coronoid, *Mathematics*, 9(2021) 1405. doi: 10.3390/math9121405.

[15] H. Wang, M. Azeem, M. F. Nadeem, A. Rehman, A. Aslam. On Fault-Tolerant Resolving Sets of Some Families of Ladder Networks, *Complexity*, 2021(2021) 1–6. doi: 10.1155/2021/9939559.

[16] M. A. Johnson. Structure-activity maps for visualizing the graph variables arising in drug design, *Journal of Biopharmaceutical Statistics*, 3(1993) 203–236.

[17] A. Sebő, E. Tannier. On metric generators of graphs, *Mathematics of Operations Research*, 29(2004) 383–393.

[18] A. Ahmad, A. N. A. Koam, M. H. F. Siddiqui, M. Azeem, Resolvability of the smartphone structure and applications in electronics, *Ain Shams Engineering Journal*, 2021. doi: 10.1016/j.asej.2021.09.014.

[19] S. Khuller, B. Raghavachari, A. Rosenfeld, Landmarks in graphs, *Discrete Applied Mathematics*, 70(1996) 217–229.

[20] Y. Tu, S. Ali, M. Azeem, M. Arshad, G. Haidar, H. K. Thabet, "Optimizing emergency response services in urban areas through the fault-tolerant metric dimension of hexagonal nanosheet, *Scientific Reports*, 15(1)(2025) DOI:10.1038/s41598-025-16684-0

[21] G. Chartrand, L. Eroh, M. A. O. Johnson, R. Ortrud. Resolvability in graphs and the metric dimension of a graph, *Discrete Applied Mathematics*, 105(2000) 99–113.

[22] P. Manuel, R. Bharati, I. Rajasingh, M. C. Monica. On minimum metric dimension of honeycomb networks, *Discrete Algorithms*, 6(2008) 20–27.

[23] A. Piperno. Search Space Contraction in Canonical Labeling of Graphs, *arXiv preprint*, (2008) arXiv:0804.4881.

[24] S. Söderberg, H. Shapiro. A combinatory detection problem, *American Mathematical Monthly*, 70(1963) 1066–1070.

[25] V. Chvátal. Mastermind, *Combinatorica*, 3(1983) 125–129.

[26] J. B. Liu, A. Zafari, Z. Hassan. Metric Dimension, Minimal Doubly Resolving Sets, and the Strong Metric Dimension for Jellyfish Graph and Cocktail Party Graph, *Complexity*, (2020) 9407456. doi: 10.1155/2020/9407456.

[27] J. Kratica, M. Čangalović, V. Kovačević-Vujčić. Computing minimal doubly resolving sets of graphs, *Computers and Operations Research*, 37(2009) 2149–2159. doi: 10.1016/j.cor.2008.08.002.

[28] H. M. A. Siddiqui, M. Imran. Computing the metric and partition dimension of H-Naphtalenic and VC5C7 nanotubes, *Journal of Optoelectronics and Advanced Materials*, 17(2015) 790–794.

[29] G. Haidar, M. U. I. Khan, S. Ali, W. Khan. Fault-tolerant topological indices of graph joins with applications in multi-swarm drone networks, *Computer Networks*, (2025) doi: 10.1016/j.comnet.2025.111517.

[30] F. B. Farooq, F. Ahmad, M. K. Jamil, A. Javed, N. A. Alqahtani, Uniquely identifying vertices and edges of a heptagonal snake graph using distance formulas, *AIMS Mathematics*, 10(6)(2025), 15069–15087. doi: 10.3934/math.2025676.

[31] M. Azeem, Cycle-super magic labeling of polyomino linear and zig-zag chains. *Journal of Operations Intelligence* 1.1(2023): 67-81. https://doi.org/10.31181/jopi1120235.

[32] S. Ali, F. Ahmad, M. K. Jamil, The novel resolvability parameter, local edge partition dimension of graphs, Open Journal of Discrete Applied Mathematics (ODAM), 3(2024), pp. 69-71, DOI. 10.30538/psrp-odam2024.0105

[33] S. N. A. Zamri, S. Ali, M. Azeem, H. A. Neamah, B. Almohsen The Mixed Partition Dimension: A New Resolvability Parameter in Graph Theory. IEEE Access (2025). DOI: 10.1109/ACCESS.2025.3534819

[34] S. Ali, M. K. Jamil, The novel resolvability parameter, Face metric dimension of Planar graphs, Open Journal of Discrete Applied Mathematics (ODAM), 1(2025),10.30538/psrp-odam2025.0108

[35] F. Simonraj, A. George. On the metric dimension of silicate stars, *ARPN Journal of Engineering and Applied Sciences*, 5(2015) 2187–2192.

[36] S. Imran, M. K. Siddique, M. Hussain. Computing the upper bounds for metric dimension of cellulose network, *Applied Mathematics*, 19(2019) 585–605.

[37] M. Ahsan, Z. Zahid, S. Zafar, A. Rafiq, M. S. Sindhu, M. Umar. Computing the metric dimension of convex polytopes related graphs, *Mathematics and Computer Science*, 22(2020) 174–188.

[38] Z. Hussain, M. Munir, M. Choudhary, S. M. Kang. Computing metric dimension and metric basis of the 2D lattice of alpha-boron nanotubes, *Symmetry*, 10(2018).

[39] S. Krishnan, B. Rajan. Fault-tolerant resolvability of specific crystal structures, *Applied Mathematics*, 7(2016) 599–604.

[40] A. Ahmad, M. Bača, S. Sultan. Computing the metric dimension of kayak paddle graph and cycles with chord, *Proyecciones Journal of Mathematics*, 39(2)(2020) 287–300.

[41] M. K. Siddiqui, M. Naeem, N. A. Rahman, M. Imran. Computing topological indices of certain networks, *Journal of Optoelectronics and Advanced Materials*, 18(2016) 884–892.

[42] A. R. Ashrafi, T. Došlić, M. Saheli. The eccentric connectivity index of TUC_4C_8 nanotubes, *MATCH Communications in Mathematical and Computer Chemistry*, 65(2011) 221–230.

[43] H. M. A. Siddiqui, M. A. Arshad, M. F. Nadeem, M. Azeem, A. Haider, M. A. Malik. Topological properties of a supramolecular chain of different complexes of N-salicylidene-L-Valine, *Polycyclic Aromatic Compounds*, (2021). doi: 10.1080/10406638.2021.1980060.

[44] M. Maryam, M. Acholi, O. A. AbuGhneim, H. Al-Ezeh. Metric dimension of some path-related graphs, *Global Journal of Pure and Applied Mathematics*, 13(2017) 149–157.

[45] F. Harary, R. A. Melter. On the metric dimension of graphs, *Ars Combinatoria*, 2(1976) 191–195.

[46] A. Estrado-Moreno, J. A. Rodríguez-Velázquez, I. G. Yero. The metric dimension of a graph, *Applied Mathematics and Information Sciences*, 9(6)(2015) 2829–2840.

[47] I. Tomescu, M. Imran. R-sets and the metric dimension of necklace graphs, *Applied Mathematics and Information Sciences*, (in press).

[48] R. Naeem, M. Imran. Metric Dimension and Exchange Property for Resolving Sets in Rotationally-Symmetric Graphs, *Applied Mathematics and Information Sciences*, 8(2014) 1665–1674. doi: 10.12785/amis/080422.

[49] S. Ali, M. K. Jamil, M. Azeem, M. A. Zahid, T. A. Ismail, Double resolving sets and the exchange property with applications in network optimization and cybersecurity, *Materials Chemistry and Physics*, (2025) DOI: 10.1016/j.matchemphys.2025.131289