

# RETRACTED: Vertex metric resolvability of COVID antiviral drug structures

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## 1. Introduction

Cholera, flu, and plague were the most terrifying pandemics in the past few centuries, these disease caused millions of inhabitants of this world to death. In November of 2019 year, there was the first case of COVID-19 (Coronavirus) recorded, and up to 3<sup>rd</sup> of April, 1,116,643 confirmed positive cases, and around 59,158 dying were recorded. These statistics are given by the world health organizations. Not only the human's health infected by this pandemic but also the economy of the world was disrupted because it spread over the world after emerging from the seafood market of Wuhan city in China [18]. The viral structure and genetic sequence of betacoron-

avirus also known as novel corona or 2019-nCoV shares with the MERS-CoV which is middle eastern respiratory syndrome coronavirus. As there is no specific drug is available for this pandemic virus currently. To tackle this pathogen there is an urgent need for antiviral agents. Researchers experimented with some existing antiviral operatives [30, 38, 53, 56, 59] and obtained some productive outcomes to tackle the transmission and infection of COVID-19. Theaflavin, hydroxychloroquine, chloroquine, thalidomide, and arbidol are some antiviral compounds.

Remdesivir (GS5734) were helped to prevent the infection of the Ebola virus, having a broad spectrum activity a nucleotide analog drug [54]. It is reported in [47, 57], chloroquine is considered an antiviral drug that is also broad-spectrum. This antiviral helps to prevent autoimmune disease and malaria. This antiviral tested for the treatment of corona-virus to lower the impact of infections of fever and later

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Table 1  
Basic notions

Terminologies	Notations
Structure	$G_{Structure}$
Vertex set	$V(G_{Structure})$
Edge set	$E(G_{Structure})$
locating set	$ls$
locating number	$ln$
locating set with different cardinality	$ls'$
location of a vertex with respect to locating set $v$	$l(v ls)$
fault-tolerant locating set	$ls_f$
fault-tolerant locating number	$ln_f$
fault-tolerant locating set with different cardinality	$ls'_f$

on this was found helpful. By inhibiting T cell activation, hydroxy-chloroquine supposed by cytokine storm conclusively reduces the acute evolution of COVID-19. Hydroxy-chloroquine and chloroquine approved by FDA as an emergency corona-virus treatment on 30<sup>rd</sup> march of 2020, reported by Forbes. For the inhibitor production of corona-virus by using theaflavin as a lead compound, it is researched and suggested by [30]. For hepatitis C, B, A viruses, and influenza as well, theaflavin shows a vast span of antiviral activity [14, 58]. For the medical benefit of black tea, a polyphenol chemical is found liable.

By a molecular graph in this draft, we consider a transformation from a chemical structure to a molecular graph by assuming atoms and chemical bonds between them are nodes and edges respectively, and this theory is already established, for more detail, one can view some recent literature [9, 16, 21, 23, 40, 42, 49]. Graph theory is also used in different applied sciences and even in the construction of different mathematical theories, for example, fuzzy theory studied in terms of graphs in the literature available by [7, 8, 31–36].

**Definition 1.1.** [26] “Suppose  $\aleph(V(\aleph), E(\aleph))$  is an undirected graph of a chemical structure (network) with  $V(\aleph)$  is called as set of principal nodes (vertex set) and  $E(\aleph)$  is the set of branches (edge set). The distance between two principal nodes  $\zeta_1, \zeta_2 \in V(\aleph)$ , denoted as  $d(\zeta_1, \zeta_2)$  is the minimum count of edges between  $\zeta_1 - \zeta_2$  path.”

**Definition 1.2.** [26] “Suppose  $R \subset V(\aleph)$  is the subset of principal nodes set and defined as  $R = \{\zeta_1, \zeta_2, \dots, \zeta_s\}$ , and let a principal node  $\zeta \in V(\aleph)$ . The identification or locations  $r(\zeta|R)$  of a principal node  $\zeta$  with respect to  $R$  is actually a

$s$ —ordered distances  $(d(\zeta, \zeta_1), d(\zeta, \zeta_2), \dots, d(\zeta, \zeta_s))$ . If each principal node from  $V(\aleph)$  have unique identification according to the ordered subset  $R$ , then this subset renamed as a resolving set of network  $\aleph$ . The minimum numbers of the elements in the subset  $R$  is actually the metric dimension of  $\aleph$  and it is denoted by the term  $dim(\aleph)$ .”

**Definition 1.3.** [26] “A particular chosen ordered subset which were actually resolving set symbolize by  $R$  of a network  $\aleph$  is considered to be a fault-tolerant network denoted by  $(R_f)$ , now if for each member of  $\zeta \in R$ , with the condition  $R \setminus \zeta$  is also remain a resolving set for the network  $\aleph$ . The minimum number of elements in the fault-tolerant resolving set is known as the fault-tolerant metric dimension and described as  $dim_f(\aleph)$ .”

In the above definitions a graph or a chemical structure is shown with symbol  $\aleph$ , notation  $r(\zeta|R)$  shows the position of a vertex  $\zeta$  with respect to the resolving set or locating set  $R$ , and for the fault-tolerant set they used the symbol  $R_f$ ,  $dim(\aleph)$  is used for the metric dimension of a graph  $\aleph$ , fault-tolerant metric is notated by the symbol  $dim_f(\aleph)$ .

Very few and recent literature on the topic of metrics and their generalization are given here. In [10], polycyclic aromatic compounds are discussed on the topic of metric and its generalization. A chemical structure is discussed in [19], they mentioned two-dimensional lattice is discussed with the idea of metric and of that structure. Cellulose network is considered in [20], by the same concept of distance-based theory of graph. Generalized concepts are given by [25, 28, 29, 46]. A computer network is discussed in [39] with the concept of distance graph theory. Generalized families of and structures of the graph are detailed in [1–3, 6, 52].

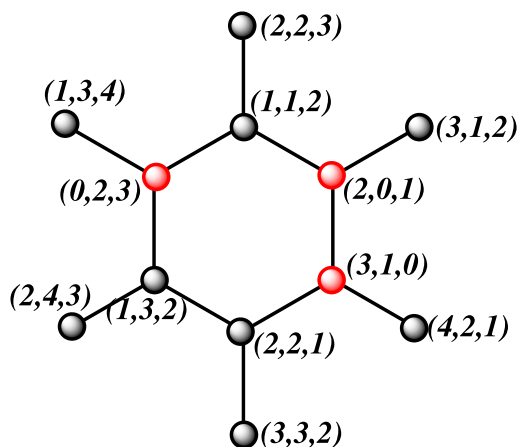


Fig. 1. Example of a locating number.

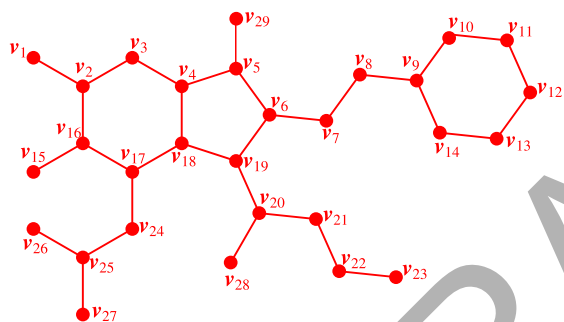


Fig. 2. Arbidol COVID antiviral drug structure.

Fault-tolerant concept of generalized structures are measured in [5, 11, 22, 43, 44]. Some interconnection computer networks are studied by [45] in the form of the fault-tolerant concept of metric of a graph. A chemical oxide-related structure is discussed in

[51] and crystal structures are done by [27], a hollow coronoid chemical structure is detailed in [26].

The very first use of metric dimension in 1975 by [50] and he named this concept as locating set. Later in 1976, two independent researchers from the computer science field named this concept as resolving set found in [15]. This idea is also named as the metric basis in the pure mathematical study of graphs and structures, available in [12, 13]. There are many generalized versions of metric dimension or locating set and fault-tolerant locating set is one of them introduced by [17]. Given below are mathematical terminologies of our main research work and also methodologies are presented as well.

**Example 1.4.** Figure 1 shows an example of locating numbers. The structure shown in the Figure 1 is a polycyclic aromatic hydrocarbon series first structure. It has three locating numbers, locating set or the vertices in the locating set highlighted with red color, and the representation of each node (vertex) is attached in the figure.

Metric dimension has many applied ways in which combinatorial optimization, robot roving, in complex games, in image processing, pharmaceutical chemistry, polymer industry, and in the electric field as well. All these applications are found in [4, 24, 41, 48, 50].

## 2. Main Results

In this section, we will include our main results of metric and fault-tolerant metric locating set of some structures, for example, arbidol, chloroquine, hydroxy-chloroquine, thalidomide, and theaflavin.

Table 2  
Locations of the nodes of  $G_{Arbidol}$ .

$l(v I_S)$	$v_{10}$	$v_{23}$	$v_{27}$	$i$ -range
$v_i$	$10 - i$	$10 - i$	6	$i = 1, 3$
$v_i$	$10 - i$	$10 - i$	5	$i = 2, 4$
$v_i$	$10 - i$	$i + 1$	6	$i = 5$
$v_i$	$10 - i$	$i - 1$	$i$	$i = 6, \dots, 10$
$v_i$	$i - 10$	$i - 1$	$i$	$i = 11, 12$
$v_i$	$10 - i$	$23 - i$	$24 - i$	$i = 13$
$v_i$	$i - 12$	$23 - i$	$24 - i$	$i = 14$
$v_i$	$10 - i$	$i - 1$	$i$	$i = 15, 16, 17$
$v_i$	$24 - i$	$23 - i$	$i - 14$	$i = 18, 19$
$v_i$	$i - 14$	$23 - i$	$i - 14$	$i = 20, 21, 22, 23$
$v_i$	$i - 16$	$i - 17$	2	$i = 24, 26$
$v_i$	$i - 16$	$i - 17$	1	$i = 25$
$v_i$	10	9	0	$i = 27$
$v_i$	$35 - i$	4	7	$i = 28$
$v_i$	$35 - i$	7	7	$i = 29$

Given below are the node and bond set of arbidol COVID antiviral drug structure. The order (total count of nodes) and size (total count of edges) of this arbidol structure is  $|V(G_{\text{Arbidol}})| = 29$ ,  $|E(G_{\text{Arbidol}})| = 31$ , respectively. Moreover, the molecular graph of Arbidol and labeling used in our main results are shown in the Figure 2. Some of the topological properties of this structure are available in the reference [37, 55].  $V(G_{\text{Arbidol}}) = \{v_i : i = 1, 2, \dots, 29\}$   
 $E(G_{\text{Arbidol}}) = \{v_i v_{i+1} : i = 1, 2, \dots, 13,$   
 $i = 15, 16, \dots, 22, i = 24, 25, 26\} \cup \{v_2 v_6, v_4 v_{18},$   
 $v_5 v_{29}, v_6 v_{19}, v_9 v_{14}, v_{20} v_{28}, v_{17} v_{24}, v_{25} v_{27}\}.$

**Theorem 2.1.** Let  $G_{\text{Arbidol}}$  be a graph of arbidol COVID antiviral drug structure. Then the locating number of  $G_{\text{Arbidol}}$  is three.

**Proof.** The locating number or metric dimension of graph of arbidol COVID antiviral drug structure is three. To prove this statement we have chosen a locating set with cardinality three and stated as  $l_s(G_{\text{Arbidol}}) = \{v_{10}, v_{23}, v_{27}\}$ . Now to make this statement valid we have provided the representations of each node of the arbidol COVID antiviral drug structure which are given in the Table 2.

Given locations  $l(v|l_s)$  of each node of graph of arbidol COVID antiviral drug structure is distinct and fulfill the definitions of locating set. This proved that the locating number  $ln(G_{\text{Arbidol}}) \leq 3$  of graph of arbidol COVID antiviral drug structure. To make this assertion exact we need to prove that  $ln(G_{\text{Arbidol}}) \geq 3$  and following by contradiction we will have  $ln(G_{\text{Arbidol}}) = 2$ . Now, to make this assertion false, we have developed some following cases.

Let  $l_s' = \{v_i, v_j : i \neq j, i, j = 1, 2, \dots, 29\}$ , is a chosen subset with cardinality two, candidate for the locating set. Then same position  $l(v_\alpha|l_s') = l(v_\beta|l_s') = (d(v_\alpha, v_i), d(v_\beta, v_i) + 1)$ . This prevails for the each possibility of taking locating set with two cardinality, so there is no single subset eligible for the locating set.

Hence proved that  $ln(G_{\text{Arbidol}}) = 3$ . □

**Theorem 2.2.** Let  $G_{\text{Arbidol}}$  be a graph of arbidol COVID antiviral drug structure. Then the fault-tolerant locating number of  $G_{\text{Arbidol}}$  is five.

**Proof.** The fault-tolerant locating number or fault-tolerant metric dimension of graph of arbidol COVID antiviral drug structure is five. To prove this state-

ment we have chosen a fault-tolerant locating set with cardinality five and stated as  $l_{s_f}(G_{\text{Arbidol}}) = \{v_{10}, v_{11}, v_{21}, v_{24}, v_{27}\}$ . Now to make this statement valid we have provided the representations of each node of the arbidol COVID antiviral drug structure which are given below.

$$l(v_i|l_{s_f}) = \left\{ \begin{array}{l} (10 - i, 11 - i, 8 - i, 4, 6), \\ \text{if } i = 1, 3; \\ (10 - i, 11 - i, 8 - i, 3, 5), \\ \text{if } i = 2, 4; \\ (10 - i, 11 - i, i - 1, 4, 6), \\ \text{if } i = 5; \\ (10 - i, 11 - i, i - 3, i - 2, i), \\ \text{if } i = 6, \dots, 10; \\ (i - 10, |i - 11|, i - 3, i - 2, i), \\ \text{if } i = 11, 12; \\ (10 - i, i - 1, 21 - i, 22 - i, 24 - i), \\ \text{if } i = 13; \\ (i - 12, i - 11, 21 - i, 22 - i, 24 - i), \\ \text{if } i = 14; \\ (10 - i, 25 - i, 21 - i, 18 - i, i), \\ \text{if } i = 15, 16, 17; \\ (24 - i, 25 - i, 21 - i, i - 16, i - 14), \\ \text{if } i = 18, 19; \\ (i - 14, i - 13, |21 - i|, i - 16, i - 14), \\ \text{if } i = 20, 21, 22, 23; \\ (i - 16, i - 15, i - 19, i - 24, 2), \\ \text{if } i = 24, 26; \\ (i - 16, i - 15, i - 19, i - 24, 1), \\ \text{if } i = 25; \\ (10, 12, 7, 2, 0), \\ \text{if } i = 27; \\ (35 - i, 8, 2, 5, 7), \\ \text{if } i = 28; \\ (35 - i, 7, 5, 5, 7), \\ \text{if } i = 29. \end{array} \right.$$

Given locations  $l(v|s_f)$  of each node of graph of arbidol COVID antiviral drug structure is distinct and fulfill the definitions of fault-tolerant locating set. This proved that the fault-tolerant locating number  $ln_f(G_{Arbidol}) \leq 5$  of graph of arbidol COVID antiviral drug structure. To make this assertion exact, we need to prove that  $ln_f(G_{Arbidol}) \geq 5$  and following by contradiction we will have  $ln_f(G_{Arbidol}) = 4$ . Now, to make this assertion false, we have developed some following cases.

Let  $ls'_f = \{v_i, v_j : i \neq j, i, j = 1, 2, \dots, 29\}$ , is a chosen subset with cardinality four, candidate for the fault-tolerant locating set. Then same position  $l(v_\alpha|ls'_f) = l(v_\beta|ls'_f) = (d(v_\alpha, v_i), d(v_\beta, v_i) + 1, d(v_\beta, v_i) + 2)$ . This prevails for the each possibility of taking fault-tolerant locating set with four cardinality, so there is no single subset eligible for the fault-tolerant locating set.

Hence proved that  $ln_f(G_{Arbidol}) = 5$ .  $\square$

Given below are the node and bond set of chloroquine COVID antiviral drug structure. The order (total count of nodes) and size (total count of edges) of this chloroquine structure is  $|V(G_{Chloroquine})| = 22$ ,  $|E(G_{Chloroquine})| = 23$ , respectively. Moreover, the molecular graph of Chloroquine and labeling used in our main results are shown in the Figure 3. Some of the topological properties of this structure are available in the reference [37, 55].

$$V(G_{Chloroquine}) = \{v_i : i = 1, 2, \dots, 22\}$$

$$E(G_{Chloroquine}) = \{v_i v_{i+1} : i = 1, 2, \dots, 13, \\ i = 15, i = 17, \dots, 20\} \cup \{v_2 v_{21}, \\ v_5 v_{20}, v_6 v_{17}, v_8 v_{22}, v_{12} v_{15}, v_{15} v_{16}\}.$$

**Theorem 2.3.** Let  $G_{Chloroquine}$  be a graph of chloroquine COVID antiviral drug structure. Then the locating number of  $G_{Chloroquine}$  is two.

**Proof.** The locating number or metric dimension of graph of chloroquine COVID antiviral drug structure is two. To prove this statement we have chosen a locating set with cardinality two and stated as  $ls(G_{Chloroquine}) = \{v_3, v_{14}\}$ . Now to make this statement valid we have provided the representations of each node of the chloroquine COVID antiviral drug structure which are given in the Table 3.

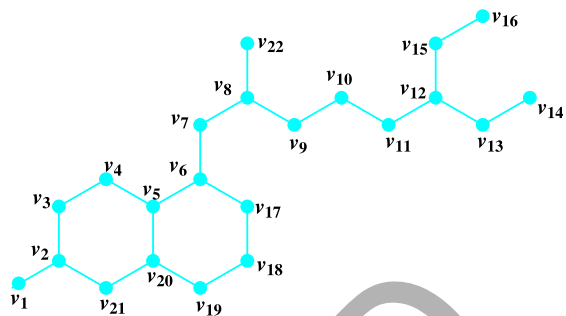


Fig. 3. Chloroquine COVID antiviral drug structure

Table 3  
Locations of the nodes of  $G_{Chloroquine}$ .

$l(v s)$	$v_3$	$v_{14}$	$i$ -range
$v_i$	$ i - 3 $	$14 - i$	$i = 1, 2, \dots, 14$
$v_i$	$i - 5$	$i - 12$	$i = 15, 16$
$v_i$	$i - 13$	$i - 8$	$i = 17$
$v_i$	$23 - i$	$i - 8$	$i = 18, 19$
$v_i$	$23 - i$	$i - 10$	$i = 20, 21$
$v_i$	$i - 18$	$i - 15$	$i = 22$

Given locations  $l(v|s)$  of each node of graph of chloroquine COVID antiviral drug structure is distinct and fulfill the definitions of locating set. This proved that the locating number  $ln(G_{Chloroquine}) \leq 2$  of graph of chloroquine COVID antiviral drug structure. To make this assertion exact we need to prove that  $ln(G_{Chloroquine}) \geq 2$  and following by contradiction we will have  $ln(G_{Chloroquine}) = 1$ . Now, this is not true because this statement is reserved for path graph.

Hence proved that  $ln(G_{Chloroquine}) = 2$ .  $\square$

**Theorem 2.4.** Let  $G_{Chloroquine}$  be a graph of chloroquine COVID antiviral drug structure. Then the fault-tolerant locating number of  $G_{Chloroquine}$  is five.

**Proof.** The fault-tolerant locating number or fault-tolerant metric dimension of graph of chloroquine COVID antiviral drug structure is five. To prove this statement we have chosen a fault-tolerant locating set with cardinality five and stated as  $ls_f(G_{Chloroquine}) = \{v_{13}, v_{14}, v_{18}, v_{19}, v_{20}\}$ . Now to make this statement valid we have provided the representations of each node of the chloroquine COVID antiviral drug structure which are given below.

$$l(v_i|ls_f) = \begin{cases} (13-i, 14-i, 6-i, 5-i, 4-i), & \text{if } i = 1, 2; \\ (13-i, 14-i, 8-i, 7-i, 6-i), & \text{if } i = 3, 4; \\ (13-i, 14-i, 8-i, i-3, i-4), & \text{if } i = 5, 6; \\ (|13-i|, 14-i, i-4, i-3, i-4), & \text{if } i = 7, 8, \dots, 14; \\ (i-13, i-12, i-6, i-5, i-6), & \text{if } i = 15, 16; \\ (i-9, i-8, 18-i, 19-i, 20-i), & \text{if } i = 17, 18; \\ (i-9, i-8, i-18, 19-i, 20-i), & \text{if } i = 19; \\ (i-11, i-10, i-18, i-19, 20-i), & \text{if } i = 20; \\ (i-11, i-10, i-18, i-19, i-20), & \text{if } i = 21; \\ (i-16, i-15, i-18, i-16, i-17), & \text{if } i = 22. \end{cases}$$

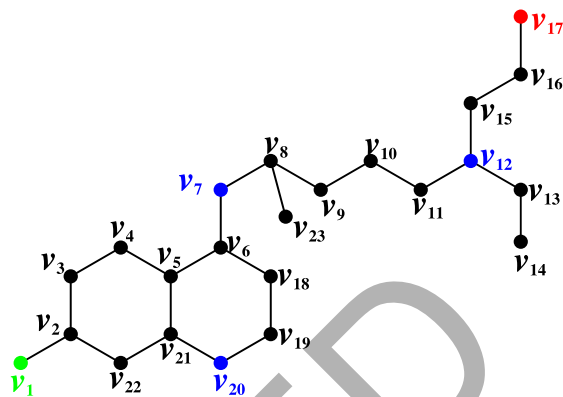


Fig. 4. Hydroxy-Chloroquine COVID antiviral drug structure

Table 4  
Locations of the nodes of  $G_{Hydroxy}$ .

$l(v ls)$	$v_3$	$v_{14}$	$i$ -range
$v_i$	$ i-3 $	$14-i$	$i = 1, 2, \dots, 14$
$v_i$	$i-5$	$i-12$	$i = 15, 16, 17$
$v_i$	$i-14$	$i-9$	$i = 18$
$v_i$	$24-i$	$i-9$	$i = 19, 20$
$v_i$	$24-i$	$i-11$	$i = 21, 22$
$v_i$	$i-17$	$i-16$	$i = 23$

Given locations  $l(v|ls_f)$  of each node of graph of chloroquine COVID antiviral drug structure is distinct and fulfill the definitions of fault-tolerant locating set. This proved that the fault-tolerant locating number  $ln_f(G_{Chloroquine}) \leq 5$  of graph of chloroquine COVID antiviral drug structure. To make this assertion exact, we need to prove that  $ln_f(G_{Chloroquine}) \geq 5$  and following by contradiction we will have  $ln_f(G_{Chloroquine}) = 4$ . Now, to make this assertion false, we have developed some following cases.

Let  $ls'_f = \{v_i, v_j : i \neq j, i, j = 1, 2, \dots, 22\}$ , is a chosen subset with cardinality four, candidate for the fault-tolerant locating set. Then same position  $l(v_\alpha|ls'_f) = l(v_\beta|ls'_f) = (d(v_\alpha, v_i), d(v_\beta, v_i) + 1, d(v_\beta, v_i) + 2)$ . This prevails for the each possibility of taking fault-tolerant locating set with four cardinality, so there is no single subset eligible for the locating set.

Hence proved that  $ln_f(G_{Chloroquine}) = 5$ .  $\square$

Given below are the node and bond set of hydroxy-chloroquine COVID antiviral drug structure. The order (total count of nodes) and size (total count of edges) of this hydroxy-chloroquine structure is  $|V(G_{Hydroxy})| = 23$ ,  $|E(G_{Hydroxy})| = 24$ , respectively. Moreover, the molecular graph of hydroxy-chloroquine and labeling used in our main results are shown in the Figure 4. Some of the topological properties of this structure are available in the reference [37, 55].

$$V(G_{Hydroxy}) = \{v_i : i = 1, 2, \dots, 23\}$$

$$E(G_{Hydroxy}) = \{v_i v_{i+1} : i = 1, 2, \dots, 13, i = 15, 16, i = 18, \dots, 21\} \cup \{v_2 v_{22}, v_5 v_{21}, v_6 v_{18}, v_8 v_{23}, v_{12} v_{15}\}.$$

**Theorem 2.5.** Let  $G_{Hydroxy}$  be a graph of hydroxy-chloroquine COVID antiviral drug structure. Then the locating number of  $G_{Hydroxy}$  is two.

**Proof.** The locating number or metric dimension of graph of hydroxy-chloroquine COVID antiviral drug structure is two. To prove this statement we have chosen a locating set with cardinality two and stated as  $ls(G_{Hydroxy}) = \{v_3, v_{14}\}$ . Now to make this statement valid we have provided the representations of each node of the hydroxy-chloroquine COVID antiviral drug structure which are given in the Table 4.

Given locations  $l(v|ls)$  of each node of graph of hydroxy-chloroquine COVID antiviral drug structure is distinct and fulfill the definitions of locating set. This proved that the locating number  $ln(G_{Hydroxy}) \leq 2$  of graph of hydroxy-chloroquine COVID antiviral drug structure. To make this assertion exact we need to prove that  $ln(G_{Hydroxy}) \geq 2$  and following by contradiction we will have  $ln(G_{Hydroxy}) = 1$ . Now, this is not true because this statement is reserved for path graph.

Hence proved that  $ln(G_{Hydroxy}) = 2$ .  $\square$

**Theorem 2.6.** Let  $G_{Hydroxy}$  be a graph of hydroxy-chloroquine COVID antiviral drug structure. Then the fault-tolerant locating number of  $G_{Hydroxy}$  is five.

**Proof.** The fault-tolerant locating number or fault-tolerant metric dimension of graph of hydroxy-chloroquine COVID antiviral drug structure is five. To prove this statement we have chosen a fault-tolerant locating set with cardinality five and stated as  $ls_f(G_{Hydroxy}) = \{v_{13}, v_{14}, v_{19}, v_{20}, v_{21}\}$ . Now to make this statement valid we have provided the representations of each node of the hydroxy-chloroquine COVID antiviral drug structure which are given below.

$$l(v_i|ls_f) =$$

- (13 - i, 14 - i, 6 - i, 5 - i, 4 - i), if i = 1, 2;
- (13 - i, 14 - i, 8 - i, 7 - i, 6 - i), if i = 3, 4, 5;
- (13 - i, 14 - i, 8 - i, i - 3, i - 4), if i = 6;
- (|13 - i|, 14 - i, i - 4, i - 3, i - 4), if i = 7, 8, ..., 14;
- (i - 13, i - 12, i - 6, i - 3, i - 6), if i = 15, 16, 17;
- (i - 9, i - 9, 19 - i, 20 - i, 21 - i), if i = 18, 19;
- (i - 9, i - 9, i - 19, 20 - i, 21 - i), if i = 20;
- (i - 11, i - 11, i - 19, i - 20, 21 - i), if i = 21;
- (i - 11, i - 11, i - 19, i - 20, i - 21), if i = 22;
- (i - 16, i - 16, i - 18, i - 17, i - 17), if i = 23.

Given locations  $l(v_i|ls_f)$  of each node of graph of hydroxy-chloroquine COVID antiviral drug structure is distinct and fulfill the definitions of fault-tolerant locating set. This proved that the fault-tolerant locating number  $ln_f(G_{Hydroxy}) \leq 5$  of graph of hydroxy-chloroquine COVID antiviral drug structure. To make this assertion exact, we need to prove that  $ln_f(G_{Hydroxy}) \geq 5$  and following by contradiction we will have  $ln_f(G_{Hydroxy}) = 4$ . Now, to make this assertion false, we have developed some following cases.

Let  $ls'_f = \{v_i, v_j : i \neq j, i, j = 1, 2, \dots, 23\}$ , is a chosen subset with cardinality four, candidate for the fault-tolerant locating set. Then same

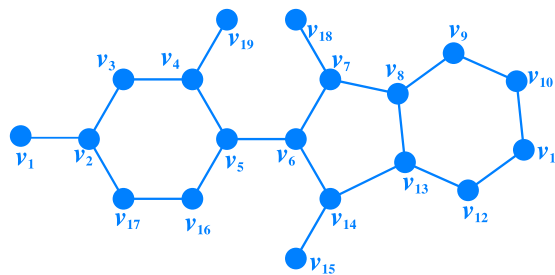


Fig. 5. Thalidomide COVID antiviral drug structure

position  $l(v_\alpha|ls'_f) = l(v_\beta|ls'_f) = (d(v_\alpha, v_i), d(v_\beta, v_i) + 1, d(v_\beta, v_i) + 2)$ . This prevails for the each possibility of taking fault-tolerant locating set with four cardinality, so there is no single subset eligible for the fault-tolerant locating set.

Hence proved that  $ln_f(G_{Hydroxy}) = 5$ .  $\square$

Given below are the node and bond set of thalidomide COVID antiviral drug structure. The order (total count of nodes) and size (total count of edges) of this thalidomide structure is  $|V(G_{Thalidomide})| = 19$ ,  $|E(G_{Thalidomide})| = 21$ , respectively. Moreover, the molecular graph of Thalidomide and labeling used in our main results are shown in the Figure 5. Some of the topological properties of this structure are available in the reference [37, 55].

$$V(G_{Thalidomide}) = \{v_i : i = 1, 2, \dots, 19\}$$

$$E(G_{Thalidomide}) = \{v_i v_{i+1} : i = 1, 2, \dots, 14, i = 16\} \cup \{v_2 v_{17}, v_4 v_{19}, v_7 v_{18}, v_5 v_{16}, v_6 v_{14}, v_8 v_{13}\}.$$

**Theorem 2.7.** Let  $G_{Thalidomide}$  be a graph of Thalidomide COVID antiviral drug structure. Then the locating number of  $G_{Thalidomide}$  is two.

**Proof.** The locating number or metric dimension of graph of Thalidomide COVID antiviral drug structure is two. To prove this statement we have chosen a locating set with cardinality two and stated as  $ls(G_{Thalidomide}) = \{v_6, v_{18}\}$ . Now to make this statement valid we have provided the representations of each node of the Thalidomide COVID antiviral drug structure which are given in the Table 5.

Given locations  $l(v_i|ls)$  of each node of graph of Thalidomide COVID antiviral drug structure is distinct and fulfill the definitions of locating set. This proved that the locating number  $ln(G_{Thalidomide}) \leq 2$  of graph of Thalidomide COVID antiviral drug structure. To make this assertion exact we need to prove that  $ln(G_{Thalidomide}) \geq 2$  and following by contradiction we will have  $ln(G_{Thalidomide}) = 1$ . Now, this is not true because this statement is reserved for path graph.

Table 5  
Locations of the nodes of  $G_{\text{Thalidomide}}$ .

$l(v ls)$	$v_6$	$v_{18}$	$i$ -range
$v_i$	$ i - 6 $	$ 7 - i  + 1$	$i = 1, 2, \dots, 10$
$v_i$	$15 - i$	$16 - i$	$i = 11, 12, 13$
$v_i$	$15 - i$	$i - 13$	$i = 14$
$v_i$	$2$	$i - 13$	$i = 15$
$v_i$	$i - 14$	$i - 12$	$i = 16, 17$
$v_i$	$i - 16$	$i - 18$	$i = 18$
$v_i$	$i - 16$	$i - 14$	$i = 19$

Hence proved that  $ln(G_{\text{Thalidomide}}) = 2$ . □

**Theorem 2.8.** Let  $G_{\text{Thalidomide}}$  be a graph of Thalidomide COVID antiviral drug structure. Then the fault-tolerant locating number of  $G_{\text{Thalidomide}}$  is four.

**Proof.** The fault-tolerant locating number or fault-tolerant metric dimension of graph of Thalidomide COVID antiviral drug structure is five. To prove this statement we have chosen a fault-tolerant locating set with cardinality five and stated as  $ls_f(G_{\text{Thalidomide}}) = \{v_3, v_{14}, v_{15}, v_{19}\}$ . Now to make this statement valid we have provided the representations of each node of the Thalidomide COVID antiviral drug structure which are given below.

$$l(v_i|ls_f) = \left\{ \begin{array}{l} (|i - 3|, 7 - i, 8 - i, |i - 4| + 1), \\ \text{if } i = 1, 2, \dots, 6; \\ (|i - 3|, i - 5, i - 4, |i - 4| + 1), \\ \text{if } i = 7; \\ (|i - 3|, i - 6, i - 5, |i - 4| + 1), \\ \text{if } i = 8, 9, 10; \\ (|i - 3|, |i - 14|, 15 - i, |i - 4| + 1), \\ \text{if } i = 11; \\ (18 - i, |i - 14|, 15 - i, 18 - i), \\ \text{if } i = 12, 13, 14; \\ (i - 10, |i - 14|, 15 - i, i - 10), \\ \text{if } i = 15; \\ (19 - i, i - 13, i - 12, i - 13), \\ \text{if } i = 16, 17; \\ (i - 13, i - 15, i - 14, i - 13), \\ \text{if } i = 18 \\ (i - 17, i - 15, i - 14, i - 19), \\ \text{if } i = 19. \end{array} \right.$$

Given locations  $l(v|ls_f)$  of each node of graph of Thalidomide COVID antiviral drug structure is distinct and fulfill the definitions of fault-tolerant locating set. This proved that the fault-tolerant locating number  $ln_f(G_{\text{Thalidomide}}) \leq 4$  of graph of Thalidomide COVID antiviral drug structure. To make this assertion exact, we need to prove that  $ln_f(G_{\text{Thalidomide}}) \geq 4$  and following by contradiction we will have  $ln_f(G_{\text{Thalidomide}}) = 3$ . Now, to make this assertion false, we have developed some following cases.

Let  $ls'_f = \{v_i, v_j : i \neq j, i, j = 1, 2, \dots, 19\}$ , is a chosen subset with cardinality three, candidate for the fault-tolerant locating set. Then same position  $l(v_\alpha|ls'_f) = l(v_\beta|ls'_f) = (d(v_\alpha, v_i), d(v_\beta, v_i) + 1)$ . This prevails for the each possibility of taking fault-tolerant locating set with three cardinality, so there is no single subset eligible for the fault-tolerant locating set.

Hence proved that  $ln_f(G_{\text{Thalidomide}}) = 4$ . □

Given below are the node and bond set of theaflavin COVID antiviral drug structure. The order (total count of nodes) and size (total count of edges) of this theaflavin structure is  $|V(G_{\text{Theaflavin}})| = 41$ ,  $|E(G_{\text{Theaflavin}})| = 46$ , respectively. Moreover, the molecular graph of Theaflavin and labeling used in our main results are shown in the Figure 6. Some of the topological properties of this structure are available in the reference [37, 55].

$$V(G_{\text{Theaflavin}}) = \{v_i : i = 1, 2, \dots, 41\}$$

$$E(G_{\text{Theaflavin}}) = \{v_i v_{i+1} : i = 1, 2, \dots, 23, i = 25, 26, \dots, 30\} \cup \{v_1 v_{39}, v_1 v_{40}, v_3 v_8, v_4 v_{40}, v_6 v_{41}, v_1 v_{31}, v_{30} v_{38}, v_{29} v_{37}, v_{27} v_{36}, v_{26} v_{35}, v_{13} v_{28}, v_{16} v_{34}, v_{15} v_{24}, v_{18} v_{23}, v_{22} v_{33}, v_{20} v_{32}\}.$$

**Theorem 2.9.** Let  $G_{\text{Theaflavin}}$  be a graph of Theaflavin COVID antiviral drug structure. Then the locating number of  $G_{\text{Theaflavin}}$  is two.

**Proof.** The locating number or metric dimension of graph of Theaflavin COVID antiviral drug structure is two. To prove this statement we have chosen a locating set with cardinality two and stated as  $ls(G_{\text{Theaflavin}}) = \{v_{31}, v_{41}\}$ . Now to make this statement valid we have provided the representations of each node of the Theaflavin COVID antiviral drug structure which are given in the Table 6.

Given locations  $l(v|ls)$  of each node of graph of Theaflavin COVID antiviral drug structure is distinct and fulfill the definitions of locating set. This proved that the locating number  $ln(G_{\text{Theaflavin}}) \leq 2$



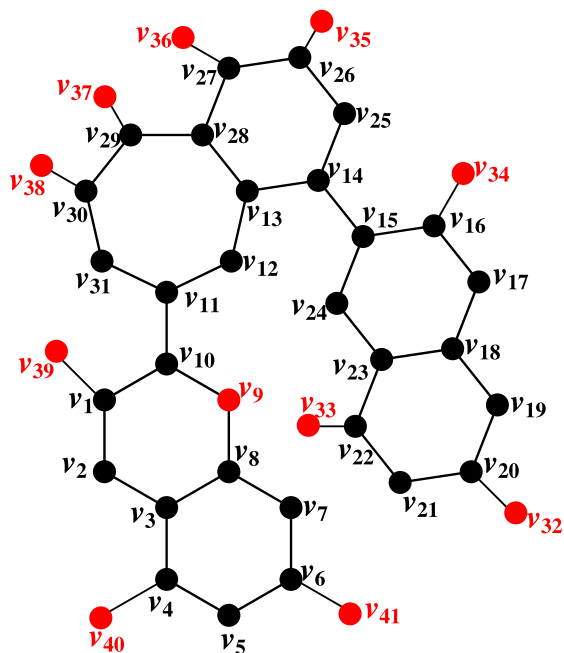


Fig. 6. Theaflavin COVID antiviral drug structure

Table 6  
Locations of the nodes of  $G_{\text{Theaflavin}}$

$l(v ls)$	$v_{33}$	$v_{41}$	$i$ -range
$v_i$	$i + 9$	$7 - i$	$i = 1, 2, \dots, 5$
$v_i$	$19 - i$	$i - 5$	$i = 6, 7, \dots, 15$
$v_i$	$21 - i$	$i - 5$	$i = 16, 17, 18$
$v_i$	$23 - i$	$35 - i$	$i = 19, 20$
$v_i$	$23 - i$	$35 - i$	$i = 21, 22$
$v_i$	$i - 21$	$35 - i$	$i = 23, 24$
$v_i$	$i - 19$	$37 - i$	$i = 25$
$v_i$	$i - 19$	$37 - i$	$i = 26, 27$
$v_i$	$i - 21$	$37 - i$	$i = 28$
$v_i$	$i - 21$	$38 - i$	$i = 29, 30$
$v_i$	$i - 22$	$38 - i$	$i = 31$
$v_i$	$i - 28$	$i - 16$	$i = 32$
$v_i$	$i - 33$	$i - 19$	$i = 33$
$v_i$	$i - 28$	$i - 22$	$i = 34$
$v_i$	$i - 27$	$47 - i$	$i = 35, 36$
$v_i$	$i - 28$	$47 - i$	$i = 37, 38$
$v_i$	$i - 28$	$i - 32$	$i = 39$
$v_i$	$i - 26$	$i - 36$	$i = 40$
$v_i$	$i - 27$	$i - 41$	$i = 41$

of graph of Theaflavin COVID antiviral drug structure. To make this assertion exact we need to prove that  $ln(G_{\text{Theaflavin}}) \geq 2$  and following by contradiction we will have  $ln(G_{\text{Theaflavin}}) = 1$ . Now, this is not true because this statement is reserved for path graph.

Hence proved that  $ln(G_{\text{Theaflavin}}) = 2$ .  $\square$

**Theorem 2.10.** Let  $G_{\text{Theaflavin}}$  be a graph of Theaflavin COVID antiviral drug structure. Then the fault-tolerant locating number of  $G_{\text{Theaflavin}}$  is four.

**Proof.** The fault-tolerant locating number or fault-tolerant metric dimension of graph of Theaflavin COVID antiviral drug structure is five. To prove this statement we have chosen a fault-tolerant locating set with cardinality five and stated as  $ls_f(G_{\text{Theaflavin}}) = \{v_6, v_{33}, v_{34}, v_{41}\}$ . Now to make this statement valid we have provided the representations of each node of the Theaflavin COVID antiviral drug structure which are given below,

$$l(v_i|ls_f) = \left\{ \begin{array}{l} (|6 - i|, 9 + i, 7 + i, 7 - i), \quad \text{if } i = 1, 2, \dots, 5; \\ (|6 - i|, 19 - i, 17 - i, i - 5), \quad \text{if } i = 6, 7, \dots, 15; \\ (|6 - i|, 21 - i, 17 - i, i - 5), \quad \text{if } i = 16; \\ (|6 - i|, 21 - i, i - 15, i - 5), \quad \text{if } i = 17, 18; \\ (|6 - i|, 23 - i, i - 15, i - 5), \quad \text{if } i = 19, 20; \\ (34 - i, 23 - i, i - 15, 35 - i), \quad \text{if } i = 21; \\ (34 - i, 23 - i, 27 - i, 35 - i), \quad \text{if } i = 22; \\ (34 - i, i - 21, 27 - i, 35 - i), \quad \text{if } i = 23, 24 \\ (34 - i, i - 19, i - 21, 37 - i), \quad \text{if } i = 25 \\ (36 - i, i - 19, i - 21, 37 - i), \quad \text{if } i = 26, 27 \\ (36 - i, i - 21, i - 23, 37 - i), \quad \text{if } i = 28 \\ (37 - i, i - 21, i - 23, 38 - i), \quad \text{if } i = 29, 30 \\ (37 - i, i - 22, 38 - i, 38 - i), \quad \text{if } i = 31 \\ (i - 17, i - 28, 38 - i, i - 16), \quad \text{if } i = 32 \\ (i - 20, i - 33, i - 27, i - 19), \quad \text{if } i = 33 \\ (i - 23, i - 28, i - 34, i - 22), \quad \text{if } i = 34 \\ (46 - i, i - 27, i - 29, 47 - i), \quad \text{if } i = 35, 36 \\ (46 - i, i - 28, i - 30, 47 - i), \quad \text{if } i = 37, 38 \\ (i - 33, i - 28, i - 30, i - 32), \quad \text{if } i = 39 \\ (i - 37, i - 26, i - 28, i - 36), \quad \text{if } i = 40 \\ (i - 40, i - 27, i - 29, i - 41), \quad \text{if } i = 41. \end{array} \right.$$

Given locations  $l(v_i|ls_f)$  of each node of graph of Theaflavin COVID antiviral drug structure is distinct and fulfill the definitions of fault-tolerant locating set. This proved that the fault-tolerant locating number  $ln_f(G_{\text{Theaflavin}}) \leq 4$  of graph of Theaflavin COVID antiviral drug structure. To make this asser-

Table 7  
Summary of the results

$G$	$ln$	$ln_f$
$G_{Arbidol}$	3	5
$G_{Chloroquine}$	2	5
$G_{Hydroxy}$	2	5
$G_{Thalidomide}$	2	4
$G_{Theaflavin}$	2	4

tion exact, we need to prove that  $ln_f(G_{Theaflavin}) \geq 4$  and following by contradiction we will have  $ln_f(G_{Theaflavin}) = 3$ . Now, to make this assertion false, we have developed some following cases.

Let  $ls'_f = \{v_i, v_j : i \neq j, i, j = 1, 2, \dots, 41\}$ , is a chosen subset with cardinality three, candidate for the fault-tolerant locating set. Then same position  $l(v_\alpha | ls'_f) = l(v_\beta | ls'_f) = (d(v_\alpha, v_i), d(v_\beta, v_i) + 1)$ . This prevails for the each possibility of taking fault-tolerant locating set with three cardinality, so there is no single subset eligible for the fault-tolerant locating set.

Hence proved that  $ln_f(G_{Theaflavin}) = 4$ .  $\square$

### 3. Conclusion

As we can see from our main results section, the metric of arbidol is three, while chloroquine, hydroxy-chloroquine, thalidomide, theaflavin has two members in their locating sets. In the fault-tolerant subset of arbidol, chloroquine, hydroxychloroquine, and theaflavin five members and only thalidomide structure contain four members. In short, this article detailed a few COVID-19 antiviral structures in the form of molecular graph theory with the metric of vertices. By this concept of vertex-metric resolvability of COVID antiviral drug structures are uniquely identified and help to study the structural properties of the structure. Moreover, the summary of main results are given in the Table 7. **Advantage and limitation of the proposed work:** As far as the detail about the advantages of this work, we have already mentioned this work is not done on these structures and it is also the novelty of this work. This can help to understand the chemical structure of these medicines or formulas more deeply. The only limitation we found is that all of these structures are finite, there is no generalized structure of these medicinal structures.

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