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Research Article

Computing the Edge Metric Dimension of the Line Graph of the Molecular Graphs of Some Classes of Antiviral Drugs, with Focus on Mpox Treatments

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Abstract: The study of viral infections, particularly those caused by monkeypox (Mpox), is crucial due to its significant public health impact and awareness. Graph theory, which is instrumental in understanding the topology of networks in various disciplines, is applied to studying antiviral drug structures to explore these antiviral drugs' structural and physicochemical properties using invariants such as metric dimension and edge metric dimension. These invariants offer insights into their mechanisms of action and potential for developing more effective therapies. The edge metric dimension is a graph theoretical parameter or invariant that allows for uniquely identifying all edges in a graph or bonds in a molecular graph through a chosen subset of vertices or atoms in a molecular graph, known as the edge resolving set. Line graphs can be applied in chemistry (modeling molecular structures), network theory, and computer science to solve problems like edge coloring and matching. In this paper, we specifically focus on the concept of edge metric dimension in a line graph of antiviral drug structures, which allows for the distinct identification of edges of their corresponding antiviral drug structures through the use of edge-resolving sets. This approach and results obtained not only enhances our knowledge and understanding of molecular interactions but also supports the advancement of effective therapeutic solutions in response to emerging health challenges such as Mpox disease. The following antiviral drug structures, namely Acyclovir, Brincidofovir, Cidofovir, Famciclovir, Tecovirimat, and Valacyclovir, are investigated in this study.

***Keywords*:** edge metric dimension, edge resolving set, antiviral drugs, line graph

MSC: 05C92

1. Introduction

The chemical graph theory, sometimes known as molecular graph, plays a great role in understanding the complex structure of a molecule in investigating the chemical and physical properties of different chemical compounds by means of topological and resolvability parameters. Chemical structures have atoms and bonds, which can be represented as vertices

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and edges, respectively, in the chemical graph. The chemical graph theory originated in the 1870s, when the renowned British mathematician Arthur Cayley published his paper "On the mathematical theory of isomers" [1]. The publication of several books and papers is another indication of the development of the chemical graph theory. The study of the molecular graph and the line graph of glass using the approach of M-polynomial and graph invariants such as topological indices and Banhatti indices was discussed in [2, 3]. Shi et al. investigated (QSPR) analysis in molecular graphs of some anticancer drugs with temperature indices approach [4]. Another interesting application of graph theory different from chemical graph theory is fuzzy graph theory, see [5–7]. Based on the invariants of chemical graph theory, such as metric dimension and edge metric dimension, have a great role in uniquely representing a series of molecular compounds and analyzing their abstract structures [8].

The virus known as monkeypox (MPXV), recently renamed as Mpox virus, which belongs to the orthopoxvirus family, is the cause of the uncommon viral disease known as monkeypoxis (MPX), recently renamed as Mpox. The countries of central and western Africa with rainforests are the most affected areas in the continent. When testing of African animal blood samples was conducted, it was found that many African rodents had indications of Mpox infection, which was originally identified at laboratory in Copenhagen, Denmark in 1958. However, there are still mysteries and doubts about the truth of the real origin of this disease; considering the fact that the originally infected monkeys that were reported in Denmark in 1958 were brought from Singapore not from Africa [9–11]. The 1922 outbreak in Alto Uruguay, Brazil, involving Mycetes seniculus and Cebus capucinus monkeys, is also mentioned in this original report; these monkeys developed typical pustules and passed away in large numbers during a concurrent pox outbreak that is currently thought to be smallpox [9–12]. Many doubts concerning the Mpox Virus's natural origin in humans and animals are brought up by these investigations [13].

Monkeys, certain mammals, and bird species are most likely to be affected by the Mpox virus. In 1970, the virus was discovered in people residing in isolated parts of Africa, leading to the first human report of Mpox ever. From 1981 to 1986, the Democratic Republic of the Congo (formerly Zaire) recorded 37 confirmed instances of Mpox [14]. Mpox outside Africa was first recorded in the United States of America in 2003. As of May 2022, the following non-African nations have been involved in Mpox cases: One instance each from the United States, Australia, France, Israel, Sweden, the Netherlands, and Switzerland; forty cases from Spain; twenty-three cases from Portugal; six cases from Canada; four cases from Belgium; three cases from Italy; and three cases from Germany [15]. The transmission of Mpox from one animal to another or one person to another can be by direct contact with the victim through bodily fluids, by respiratory droplets, by infected animal bites, or by contaminating with things having a virus, such as clothing, bedding, or linens, through blood, or lesions (cutaneous or mucosal) of animals that are affected, such as rats, monkeys, dormice, and rope/tree squirrels [13, 15]. Mpox typically takes 6-13 days to incubate, but it can take up to 21 days in certain circumstances. The invasion phase and skin eruption are the two phases or periods of the Mpox infection shortly after the incubation period [13]. The symptoms of Mpox are somehow related to other viral diseases; initially, the victim will feel headache, fever, backache, muscle aches, a general feeling of discomfort, exhaustion, myalgia, and swollen lymph nodes [14]. Due to our limited knowledge of the Mpox virus and its possible effects (similar to COVID-19), further research is required, which includes creating a database of skin images of affected individuals [16, 17].

Acyclovir is an antiviral drug approved by the U.S. Food and Drug Administration (FDA) to treat and/or prevent the recurrence of certain types of herpes simplex virus (HSV) infections, including genital herpes, varicella-zoster virus (VZV) infections, including chicken pox (primary varicella infection) and shingles. Brincidofovir is an oral antiviral drug used to treat human smallpox infections. It may also be used to treat another type of orthopoxvirus infection called Mpox. Cidofovir is an injectable antiviral drug used to treat cytomegalovirus (CMV) retinitis in patients diagnosed with AIDS. Famciclovir is an antiviral drug approved by the FDA for treating herpes simplex (HSV) and varicella-zoster virus (VZV) infections. Valacyclovir (Valaciclovir) is an antiviral prescription medicine used to treat various herpes infections, particularly genital herpes episodes or outbreaks. Tecovirimat is an antiviral drug that manages and treats all orthopoxviruses, including Mpox, vaccinia, cowpox, rabbitpox, ectromelia, and Variola (smallpox) virus. The FDA approved Tecovirimat in July 2018.

Treatment for human Mpox currently lacks a licensed remedy or appropriate evidence-based recommendation; in order to treat symptoms, control complications, and avoid long-term effects, clinical management is implemented; an

interim clinical management guideline has been released by the World Health Organization (WHO) recently [18, 13]. The antiviral drugs that were originally developed to treat smallpox are now being used to treat Mpox, including Brincidofovir and Tecovirimat [16].

The concept of edge metric dimension, often referred to as edge metric basis, asserts that the entire edge set of a structure can be uniquely identified by selecting an edge metric generator from the vertices set. The study of edge metric dimension was first introduced in [19] and a substantial amount of works have been published since it first appeared, for more research works on edge metric dimension see [11, 20–31]; for the edge metric dimension of chemical graphs [8, 22, 28, 32–34]. The concept of vertices resolvability facilitates the study of the structural properties of the structure and enables the unique identification of antiviral drug structures.

The line graph of graph G denoted by $L(G)$ is the graph whose vertices are the edges of the graph G, and two vertices are adjacent if the corresponding edges of G share a single common vertex in G. In chemical graph theory, line graphs can be used to identify structural isomers by focusing on the relationships between bonds; chemists can compare how molecules are connected differently; line graphs can be used to visualize which bonds share atoms and how these bonds interact, aiding in the understanding of resonance structures; for complex molecules such as naphthalene (polycyclic hydrocarbons) line graphs can represent the way different ring systems are interconnected by bonds, making it easier to study their bond-related properties; line graphs are useful in edge coloring problems, which can help in analyzing the types of bonds within a molecule. Much research was done in mathematics on the resolvability of line graphs, to mention a few [35–42]; however, most of the studies conducted were on the metric dimension. In 2023, Masmali et al. computed the edge metric dimension of COVID-19 antiviral drug structures such as Arbidol, malaria, carboxylic, thalidomide, and theaflavin [22]. In this study, we compute the edge metric dimension of the line graph of antiviral drug structures, namely Acyclovir, Brincidofovir, Cidofovir, Famciclovir, Tecovirimat, and Valacyclovir.

2. Preliminaries

In this study, we focus mainly on relationships and interactions of atoms and then bonds in their corresponding line graphs. We therefore employ a two-dimensional (2D) model to construct molecular graphs for simplicity and clarity.

Let $G = (V(G),\ E(G))$ be a molecular graph, let $V_A,\ V_B,\ V_C,\ V_F,\ V_T,\ V_V$ and $E_A,\ E_B,\ E_C,\ E_F,\ E_T,\ E_V$ be sets of vertices (nodes/atoms) and edges (bonds) of molecular graphs acyclovir, Brincidofovir, Cidofovir, Famciclovir, Tecovirimat, Valacyclovir respectively; where $V_A = \{v_i :\ i = 1,\ \ldots,\ 20\}$, $V_B = \{v_i :\ i = 1,\ \ldots,\ 42\}$, $V_C = \{v_i :\ i = 1,\ \ldots,\ 23\}$, $V_F = \{v_i :\ i = 1,\ \ldots,\ 25\}$, $V_T = \{v_i :\ i = 1,\ \ldots,\ 35\}$, $V_V = \{v_i :\ i = 1,\ \ldots,\ 28\}$. If v_x and v_y are any two adjacent nodes in $V(G)$ then $v_xv_y \in E(G)$; similarly, $v_x^l,\ v_y^l \in V(L(G))$ then $v_x^lv_y^l \in E(L(G))$. Figures 1-6 illustrates molecular structures, molecular graphs and their corresponding line graphs. We denote the edge metric dimension of line graph of the molecular graph G by $\alpha_e(L(G))$.

3. Main results

In this section, the molecular graph structures of the antiviral drugs used to treat viral infections including Mpox such as Valacyclovir, Cidofovir, Famciclovir, Acyclovir, Brincidofovir, and Tecovirimat are considered in computing the edge metric dimension of their corresponding line graphs.

Theorem 1 Let G_C be the molecular graph of antiviral drug Cidofovir, and $L(G_C)$ be its corresponding line graph, then; $\alpha_e(L(G_C)) = 4$.

Proof. The line graph of Cidofovir with nodes v_x^l and v_y^l are connected by a $v_x^lv_y^l$ edge, Figure 1 shows molecular structure, molecular graph and its corresponding line graph of Cidofovir; then the number of nodes required to uniquely identify all the edges of the line graph of Cidofovir is four. We will show this result by the double inequality approach. For the upper bound $\alpha_e(L(G_C)) \leq 4$, we consider the edge resolving set $W_e^l = \{v_2^l,\ v_6^l,\ v_{21}^l,\ v_{23}^l\}$, shown below are the unique representations of all the edges of $L(G_C)$; then the cardinality of the edge resolving set is 4, which implies that $\alpha_e(L(G_C)) \leq 4$.

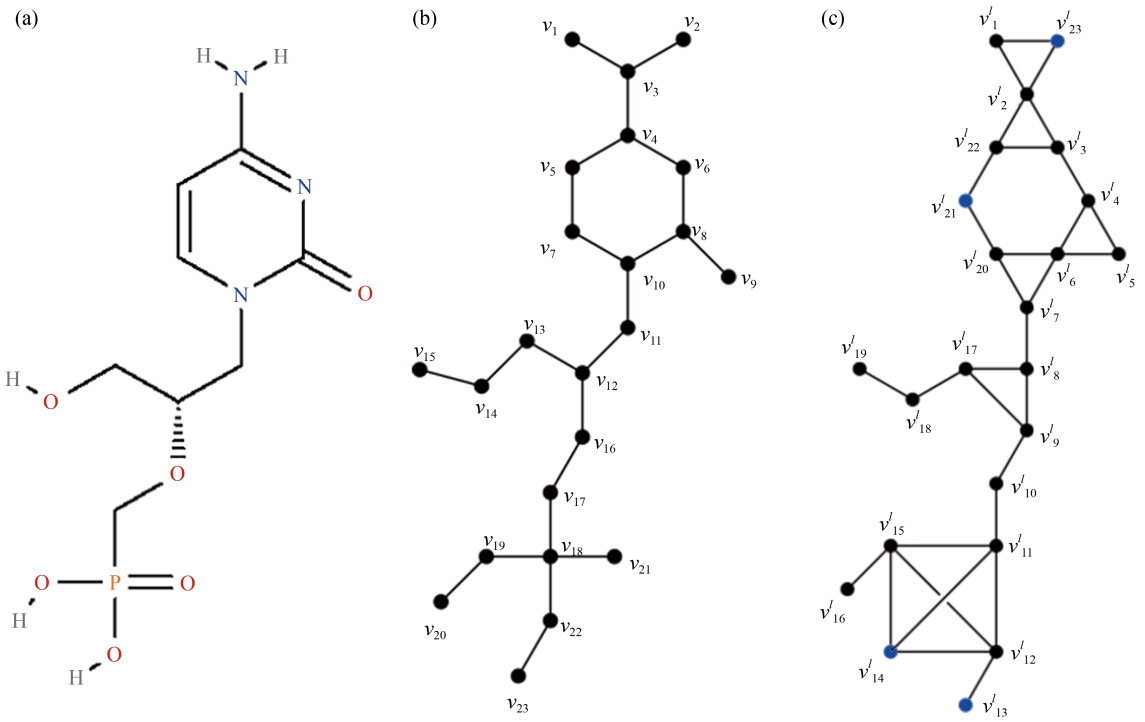


Figure 1. (a) Molecular structure of cidofovir, (b) Molecular graph of cidofovir, and (c) line graph of cidofovir

The expression for $r(v_\xi^l v_{\xi+1}^l \mid W_e^l)$ is defined as follows. For $\xi = 1, \ldots, 3$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = \left(\left\lfloor \frac{\xi}{3} \right\rfloor + 1,\ 2,\ 10-\xi,\ 11-\xi \right),$$

for $\xi = 4, \ldots, 6$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = \left(\left\lfloor \frac{\xi}{5} \right\rfloor + 3,\ 3 - \left\lfloor \frac{\xi}{5} \right\rfloor,\ 11-\xi,\ 12-\xi \right),$$

for $\xi = 7, \ldots, 12$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = \left(\xi - 2,\ \xi - 5,\ 11 - \xi + \left\lfloor \frac{\xi}{11} \right\rfloor,\ 12-\xi \right),$$

for $\xi = 14,\ 15$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (10,\ 7,\ \xi - 14,\ 2),$$

for $\xi = 17,\ 18$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 10,\ \xi - 13,\ \xi - 13,\ \xi - 12),$$

and for $\xi = 20,\ 21$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (23 - \xi,\ 0,\ \xi - 14,\ \xi - 13).$$

$$r\left(v_x^l v_y^l \mid W_e^l\right) = \begin{cases} v_8^l v_{17}^l \to (6,\ 3,\ 4,\ 5), \\ v_9^l v_{17}^l \to (7,\ 4,\ 3,\ 4), \\ v_2^l v_{22}^l \to (1,\ 1,\ 8,\ 9), \\ v_2^l v_{23}^l \to (0,\ 2,\ 9,\ 10), \\ v_3^l v_{22}^l \to (2,\ 1,\ 8,\ 9), \\ v_6^l v_{20}^l \to (4,\ 1,\ 6,\ 7), \\ v_7^l v_{20}^l \to (4,\ 1,\ 5,\ 6), \\ v_4^l v_6^l \to (3,\ 2,\ 6,\ 7), \\ v_1^l v_{23}^l \to (0,\ 3,\ 10,\ 11), \\ v_{12}^l v_{14}^l \to (10,\ 7,\ 0,\ 1), \\ v_{11}^l v_{14}^l \to (9,\ 6,\ 0,\ 2), \\ v_{12}^l v_{15}^l \to (10,\ 7,\ 1,\ 1), \\ v_{11}^l v_{15}^l \to (9,\ 6,\ 1,\ 2). \end{cases}$$

Now, in order to achieve the equality sign, we need to show the lower bound, that is $\alpha_e(L(G_C)) \geq 4$. Let us assume, if possible, that the cardinality of the edge resolving set is 3. Then we can choose any subset of cardinality 3 from the set $V(L(G_C))$, let $\mathscr{S}_e^l = \{v_a^l,\ v_b^l,\ v_c^l :\ a \neq b \neq c;\ a,\ b,\ c \in \{1,\ 2,\ \ldots,\ 23\}\}$, where $\mathscr{S}_e^l \subset V(L(G_C))$. If $\mathscr{S}_e^l = \{v_a^l,\ v_b^l,\ v_c^l :\ a \neq b \neq c;\ a,\ b,\ c \in \{1,\ 2,\ \ldots,\ 23\}\}$, then there are at least three pairs of edges that can not be uniquely identified by $\mathscr{S}_e^l$, for instance, for $i < j < k$ there exist $i,\ j,\ k \in \{1,\ 2,\ \ldots,\ 21\}$ such that $r(v_i^l v_{i+2}^l | \mathscr{S}_e^l) = r(v_{i+1}^l v_{i+2}^l | \mathscr{S}_e^l)$, $r(v_{i+2}^l v_j^l | \mathscr{S}_e^l) = r(v_j^l v_{j+1}^l | \mathscr{S}_e^l)$, $r(v_k^l v_{k+2}^l | \mathscr{S}_e^l) = r(v_{k+2}^l v_{k+3}^l | \mathscr{S}_e^l)$, a contradiction; so our assumption is wrong, we can not choose any subset of cardinality three to identify all edges of Cidofovir, hence $\alpha_e(L(G_C)) \geq 4$.

Theorem 2 Let G_V be the molecular graph of antiviral drug Valacyclovir, and $L(G_V)$ be its corresponding line graph, then; $\alpha_e(L(G_V)) = 4$.

Proof. The number of nodes required to uniquely identify all the edges of the line graph of Valacyclovir is four, the line graph of Valacyclovir with nodes v_x^l and v_y^l are connected by $v_x^l v_y^l$ edge, Figure 2 shows molecular structure, molecular graph and its corresponding line graph of Valacyclovir; then we will show this result by double inequality approach, for the upper bound $\alpha_e(L(G_V)) \leq 4$, we consider the edge resolving set $W_e^l = \{v_1^l,\ v_9^l,\ v_{25}^l,\ v_{29}^l\}$, shown below are the unique representations of all the edges of $L(G_V)$, then the cardinality of the edge resolving set is 4, and this proves the upper bound, which implies that $\alpha_e(L(G_V)) \leq 4$.

The expression for $r(v_\xi^l v_{\xi+1}^l \mid W_e^l)$ is defined as follows. For $\xi = 1,\ 2$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 1,\ 5 - \xi,\ 14 - \xi,\ 14 - \xi),$$

for $\xi = 3,\ \ldots,\ 5$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 2,\ 5 - \xi,\ 12,\ 12),$$

for $\xi = 6,\ 7$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (4,\ \xi - 6,\ 11,\ 11),$$

for $\xi = 8,\ \ldots,\ 10$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (5,\ \xi - 6,\ 18 - \xi,\ 18 - \xi),$$

for $\xi = 12,\ \ldots,\ 15$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 6,\ \xi - 7,\ 18 - \xi,\ 18 - \xi),$$

for $\xi = 16,\ \ldots,\ 18$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = \left(\xi - 6,\ \xi - 7,\ 19 - \xi,\ 19 - \xi + \left\lfloor \frac{\xi}{18} \right\rfloor\right),$$

for $\xi = 19,\ 20$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 7,\ \xi - 8,\ 0,\ \xi - 17),$$

for $\xi = 22,\ 23$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 10,\ \xi - 11,\ \xi - 20,\ 23 - \xi),$$

for $\xi = 25,\ 26$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 23,\ 3,\ 36 - \xi,\ 36 - \xi),$$

for $\xi = 27,\ 28$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 24,\ 2,\ 37 - \xi,\ 37 - \xi).$$

$$r\left(v_x^l v_y^l \mid W_e^l\right) = \begin{cases} v_1^l v_3^l \to (0,\ 3,\ 12,\ 12), \\ v_3^l v_{25}^l \to (1,\ 3,\ 11,\ 11), \\ v_4^l v_{25}^l \to (2,\ 2,\ 11,\ 11), \\ v_5^l v_7^l \to (3,\ 1,\ 11,\ 11), \\ v_7^l v_{28}^l \to (4,\ 1,\ 10,\ 10), \\ v_8^l v_{28}^l \to (4,\ 2,\ 10,\ 10), \\ v_{10}^l v_{29}^l \to (4,\ 3,\ 9,\ 9), \\ v_{11}^l v_{29}^l \to (4,\ 3,\ 8,\ 8), \\ v_{16}^l v_{18}^l \to (10,\ 9,\ 2,\ 2), \\ v_{18}^l v_{22}^l \to (11,\ 10,\ 2,\ 1), \\ v_{19}^l v_{21}^l \to (12,\ 11,\ 1,\ 2), \\ v_{19}^l v_{22}^l \to (12,\ 11,\ 1,\ 1), \\ v_{22}^l v_{24}^l \to (12,\ 11,\ 2,\ 0), \\ v_{25}^l v_{27}^l \to (2,\ 3,\ 10,\ 10), \\ v_{27}^l v_{29}^l \to (3,\ 3,\ 9,\ 9), \\ v_{28}^l v_{29}^l \to (4,\ 2,\ 9,\ 9). \end{cases}$$

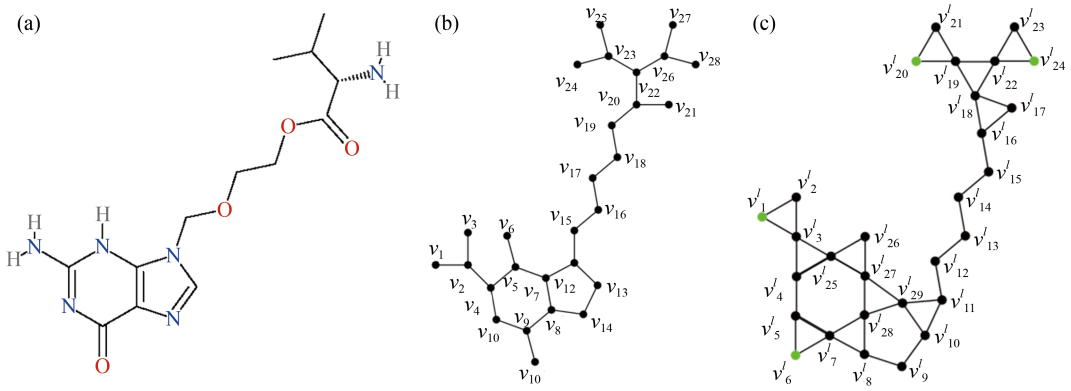


Figure 2. (a) Molecular structure of Valacyclovir, (b) Molecular graph of Valacyclovir, and (c) line graph of Valacyclovir

Again, in order to achieve the equality sign, we need to show the lower bound, that is $\alpha_e(L(G_V)) \geq 4$. Let us assume, if possible, that the cardinality of the edge resolving set is 3. Then we can choose any subset of cardinality 3 from the set $V(L(G_V))$, let $\mathscr{S}_e^l = \{v_a^l,\ v_b^l,\ v_c^l :\ a \neq b \neq c;\ a,\ b,\ c \in \{1,\ 2,\ \ldots,\ 29\}\}$, where $\mathscr{S}_e^l \subset V(L(G_V))$. If $\mathscr{S}_e^l = \{v_a^l,\ v_b^l,\ v_c^l : a \neq b \neq c;\ a,\ b,\ c \in \{1,\ 2,\ \ldots,\ 29\}\}$, then there are at least five pairs of edges that can not be uniquely identified by $\mathscr{S}_e^l$, for instance, there exist $i,\ j \in \{4,\ \ldots,\ 21\}$ and $\delta,\ \beta \in \{1,\ \ldots,\ 8\}$ such that $r(v_i^l v_{i+\delta}^l | \mathscr{S}_e^l) = r(v_j^l v_{j+\beta}^l | \mathscr{S}_e^l)$, a contradiction; so our asssumption is wrong, we can not choose any subset of cardianlity three to identify all edges of Valacyclovir, hence $\alpha_e(L(G_V)) \geq 4$.

Theorem 3 Let G_F be the molecular graph of antiviral drug Famciclovir, and $L(G_F)$ be its corresponding line graph, then; $\alpha_e(L(G_F)) = 4$.

Proof. Four nodes are needed to uniquely identify every edge in the line graph of Famciclovir, which has nodes v_x^l and v_y^l connected by a $v_x^l v_y^l$ edge, Figure 3 shows molecular structure, molecular graph and its corresponding line graph

of Famciclovir; using the double inequality method, we shall demonstrate this result. We examine the edge resolving set $W_e^l = \{v_2^l,\ v_{12}^l,\ v_{20}^l,\ v_{26}^l\}$ in order to get the upper bound $\alpha_e(L(G_F)) \leq 4$. Since each edge in $L(G_F)$ has a unique representation as shown below, the edge resolving set's cardinality is 4; this suggests that $\alpha_e(L(G_F)) \leq 4$.

The expression for $r(v_\xi^l v_{\xi+1}^l \mid W_e^l)$ is defined as follows. For $\xi = 1,\ 2$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (1,\ 6-\xi,\ 11-\xi,\ 11-\xi),$$

for $\xi = 3,\ \ldots,\ 6$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi-1,\ 6-\xi,\ 8,\ 8),$$

for $\xi = 7,\ \ldots,\ 9$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (5,\ \xi-7,\ 14-\xi,\ 14-\xi),$$

for $\xi = 10,\ \ldots,\ 12$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi-4,\ \xi-7,\ 14-\xi,\ 4),$$

for $\xi = 13,\ \ldots,\ 15$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = \left(\xi-4,\ \xi-7,\ 1-\left\lfloor \frac{\xi}{15} \right\rfloor,\ \xi-8\right),$$

for $\xi = 18,\ \ldots,\ 19$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi-16,\ 21-\xi,\ 28-\xi,\ 28-\xi),$$

for $\xi = 22,\ 23$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi-14,\ \xi-17,\ \xi-18,\ 24-\xi),$$

for $\xi = 24,\ 25$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi-14,\ \xi-17,\ \xi-18,\ 25-\xi).$$

$$r\left(v_x^l v_y^l \mid W_e^l\right) = \begin{cases} v_1^l v_{17}^l \to (0,\ 6,\ 11,\ 11), \\ v_2^l v_{17}^l \to (0,\ 5,\ 10,\ 10), \\ v_2^l v_{18}^l \to (1,\ 4,\ 10,\ 10), \\ v_3^l v_{18}^l \to (2,\ 4,\ 9,\ 9), \\ v_4^l v_{21}^l \to (3,\ 2,\ 7,\ 7), \\ v_5^l v_{20}^l \to (4,\ 2,\ 8,\ 8), \\ v_5^l v_{21}^l \to (4,\ 2,\ 7,\ 7), \\ v_6^l v_{20}^l \to (4,\ 1,\ 9,\ 9), \\ v_8^l v_{21}^l \to (4,\ 1,\ 7,\ 7), \\ v_9^l v_{21}^l \to (4,\ 2,\ 6,\ 6), \\ v_{11}^l v_{22}^l \to (7,\ 4,\ 4,\ 3), \\ v_{12}^l v_{22}^l \to (8,\ 5,\ 3,\ 3), \\ v_{14}^l v_{16}^l \to (10,\ 7,\ 0,\ 6), \\ v_{24}^l v_{26}^l \to (10,\ 7,\ 6,\ 0). \end{cases}$$

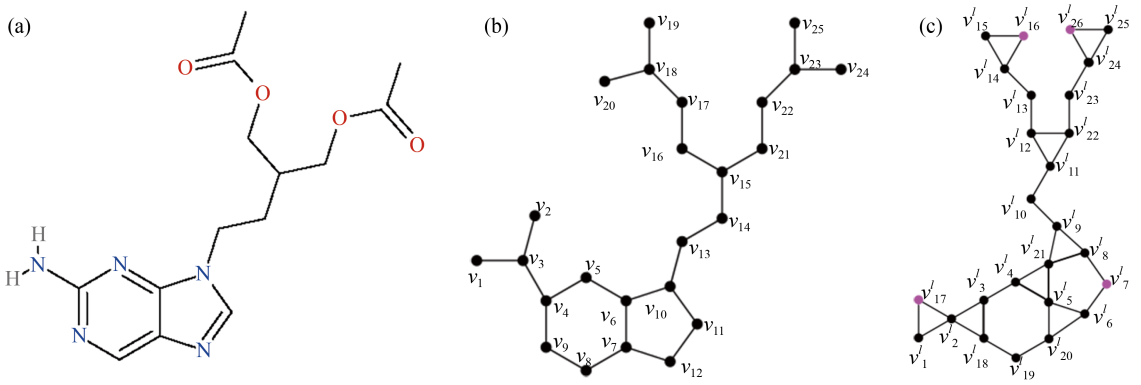


Figure 3. (a) Molecular structure of Famciclovir, (b) Molecular graph of Famciclovir, and (c) line graph of Famciclovir

Showing the lower bound, $\alpha_e(L(G_F)) \geq 4$, is necessary to obtain the equality sign. For the sake of argument, let us assume that the edge resolving set has cardinality three. After that, we can select any subset of cardinality 3 from the set $V(L(G_F))$. Let $\mathscr{S}_e^l = \{v_a^l,\ v_b^l,\ v_c^l :\ a \neq b \neq c;\ a,\ b,\ c \in \{1,\ 2,\ \ldots,\ 26\}\}$, where $\mathscr{S}_e^l \subset V(L(G_F))$. There is at least one pair of edges that cannot be uniquely identified by $\mathscr{S}_e^l$ if $\mathscr{S}_e^l = \{v_a^l,\ v_b^l,\ v_c^l :\ a \neq b \neq c;\ a,\ b,\ c \in \{1,\ 2,\ \ldots,\ 26\}\}$. For example, there exist $i,\ j \in \{4,\ \ldots,\ 20\}$ and $\delta,\ \beta \in \{1,\ \ldots,\ 6\}$ such that $r(v_i^l v_{i+\delta}^l | \mathscr{S}_e^l) = r(v_j^l v_{j+\beta}^l | \mathscr{S}_e^l)$, which contradicts our assumption; we cannot select any subset of cardinality three to uniquely identify every edge of Famciclovir; hence, $\alpha_e(L(G_F)) \geq 4$.

Theorem 4 Let G_A be the molecular graph of antiviral drug acyclovir, and $L(G_A)$ be its corresponding line graph, then; $\alpha_e(L(G_A)) = 3$.

Proof. The line graph of acyclovir, where nodes v_x^l and v_y^l are connected by a $v_x^l v_y^l$edge, Figure 4 shows molecular structure, molecular graph and its corresponding line graph of acyclovir; requires three nodes to uniquely identify all the edges in the line graph. We will demonstrate this result using a double inequality approach. For the upper bound $\alpha_e(L(G_A)) \leq 3$, we consider the edge resolving set $W_e^l = \{v_1^l,\ v_7^l,\ v_{20}^l\}$. Shown below are the unique representations

of all the edges of $L(G_A)$, leading to the conclusion that the cardinality of the edge resolving set is 3, which implies $\alpha_e(L(G_A)) \leq 3$.

The expression for $r(v_\xi^l v_{\xi+1}^l \mid W_e^l)$ is defined as follows. For $\xi = 1, \ldots, 4$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 1,\ 4 - \xi,\ 8),$$

for $\xi = 5,\ 6$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (4,\ \xi - 5,\ 7),$$

for $\xi = 7, \ldots, 9$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (5,\ \xi - 5,\ 13 - \xi),$$

for $\xi = 10, \ldots, 13$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 5,\ \xi - 6,\ 13 - \xi),$$

for $\xi = 18,\ 19$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 15,\ 2,\ 24 - \xi).$$

$$r\left(v_x^l v_y^l \mid W_e^l\right) = \begin{cases} v_1^l v_{16}^l \to (0,\ 4,\ 9), \\ v_2^l v_{16}^l \to (1,\ 3,\ 8), \\ v_2^l v_{17}^l \to (1,\ 3,\ 7), \\ v_3^l v_{17}^l \to (2,\ 2,\ 7), \\ v_3^l v_{21}^l \to (2,\ 2,\ 8), \\ v_4^l v_6^l \to (3,\ 1,\ 7), \\ v_5^l v_{21}^l \to (3,\ 1,\ 8), \\ v_6^l v_{19}^l \to (4,\ 1,\ 6), \\ v_7^l v_{19}^l \to (4,\ 2,\ 6), \\ v_9^l v_{20}^l \to (4,\ 3,\ 5), \\ v_{10}^l v_{20}^l \to (4,\ 3,\ 4), \\ v_{14}^l v_{15}^l \to (9,\ 8,\ 0), \\ v_{17}^l v_{18}^l \to (2,\ 3,\ 6). \end{cases}$$

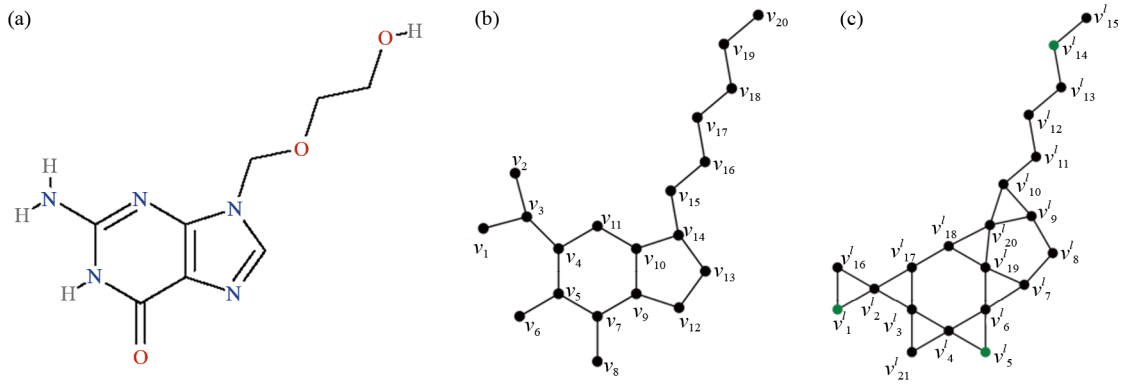


Figure 4. (a) Molecular structure of Acyclovir, (b) Molecular graph of Acyclovir, and (c) line graph of acyclovir

On the other hand, we need to show the lower bound, that is $\alpha_e(L(G_A)) \geq 3$. Let us assume, if possible, that the cardinality of the edge resolving set is 2. Then we can choose any subset of cardinality 2 from the set $V(L(G_A))$, let $\mathscr{S}_e^l = \{v_a^l,\ v_b^l :\ a \neq b;\ a,\ b \in \{1,\ 2,\ \ldots,\ 21\}\}$, where $\mathscr{S}_e^l \subset V(L(G_A))$. If $\mathscr{S}_e^l = \{v_a^l,\ v_b^l :\ a \neq b;\ a,\ b \in \{1,\ 2,\ \ldots,\ 21\}\}$, then there are at least six pairs of edges that can not be uniquely identified by $\mathscr{S}_e^l$, for instance, for some $i,\ j \in \{3,\ 4,\ \ldots,\ 16\}$ there exist $\delta,\ \beta \in \{1,\ \ldots,\ 5\}$ such that $r(v_i^l v_{i+\delta}^l | \mathscr{S}_e^l) = r(v_j^l v_{j+\beta}^l | \mathscr{S}_e^l)$, a contradiction; so our assumption is wrong, we can not choose any subset of cardinality two to identify all edges of acyclovir, hence $\alpha_e(L(G_A)) \geq 3$.

Theorem 5 Let G_B be the molecular graph of antiviral drug Brincidofovir, and $L(G_B)$ be its corresponding line graph, then; $\alpha_e(L(G_B)) = 4$.

Proof. The edge resolving number for the line graph of the antiviral drug Brincidofovir is four; Figure 5 shows molecular structure, molecular graph and its corresponding line graph of Brincidofovir. We will use the double inequality approach to prove our claim. First we need to show the existence of the upper bound, which is $\alpha_e(L(G_B)) \leq 4$, to this end, let $W_e^l = \{v_1^l,\ v_9^l,\ v_{19}^l,\ v_{21}^l\}$. Clearly, shown below are the unique representations of all edges of the line graph of Brincidofovir, which implies that the cardinality of the edge resolving set is four; hence, $\alpha_e(L(G_B)) \leq 4$.

The expression for $r(v_\xi^l v_{\xi+1}^l \mid W_e^l)$ is defined as follows. For $\xi = 1,\ \ldots,\ 4$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 1,\ 4 - \xi,\ 10 - \xi,\ 11 - \xi),$$

for $\xi = 5,\ \ldots,\ 9$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 1,\ \xi - 5,\ 10 - \xi,\ 11 - \xi),$$

for $\xi = 10,\ 11$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 1,\ \xi - 5,\ 0,\ 2),$$

for $\xi = 12,\ \ldots,\ 31$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 2,\ \xi - 6,\ \xi - 11,\ \xi - 10),$$

for $\xi = 33,\ 34$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 26,\ \xi - 30,\ \xi - 29,\ \xi - 28),$$

for $\xi = 37,\ 38$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 35,\ 2,\ 7,\ 8).$$

$$r\left(v_x^l v_y^l \mid W_e^l\right) = \begin{cases} v_1^l v_{36}^l \to (0,\ 4,\ 10,\ 11), \\ v_2^l v_{36}^l \to (1,\ 3,\ 9,\ 10), \\ v_2^l v_{37}^l \to (1,\ 3,\ 8,\ 9), \\ v_3^l v_{37}^l \to (2,\ 2,\ 8,\ 9), \\ v_6^l v_{40}^l \to (4,\ 1,\ 5,\ 6), \\ v_7^l v_{33}^l \to (6,\ 2,\ 4,\ 5), \\ v_7^l v_8^l \to (7,\ 3,\ 3,\ 4), \\ v_{10}^l v_{12}^l \to (9,\ 5,\ 1,\ 2), \\ v_{12}^l v_{41}^l \to (10,\ 6,\ 1,\ 1), \\ v_{38}^l v_{40}^l \to (3,\ 1,\ 6,\ 7), \\ v_{39}^l v_{40}^l \to (4,\ 1,\ 6,\ 7), \\ v_{41}^l v_{42}^l \to (10,\ 6,\ 1,\ 0). \end{cases}$$

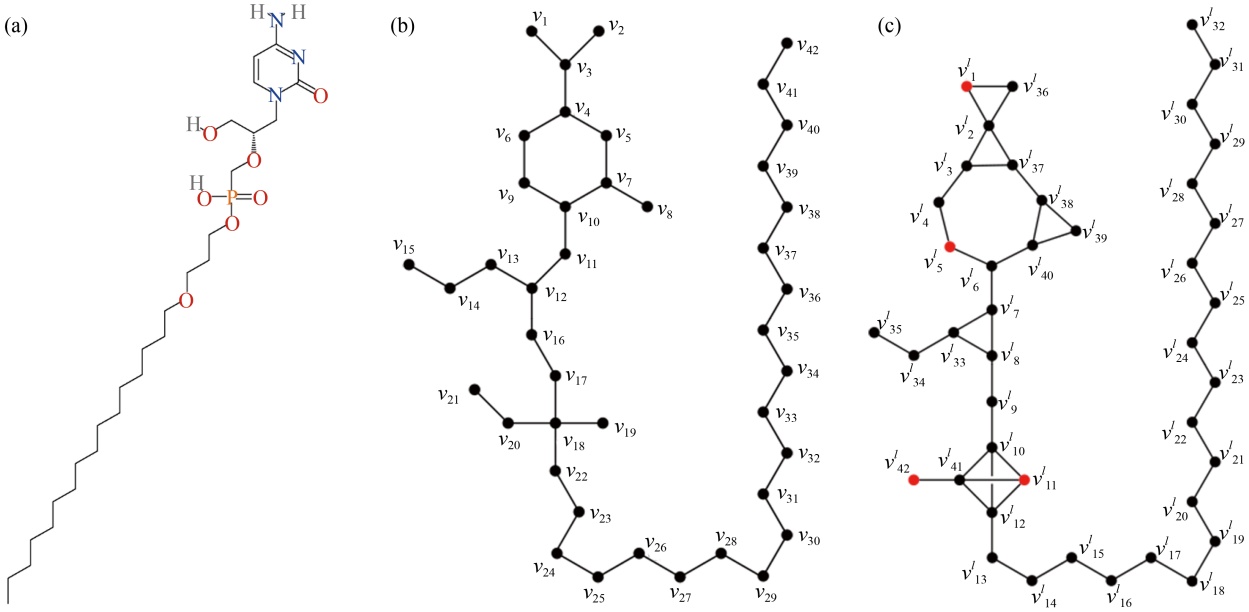
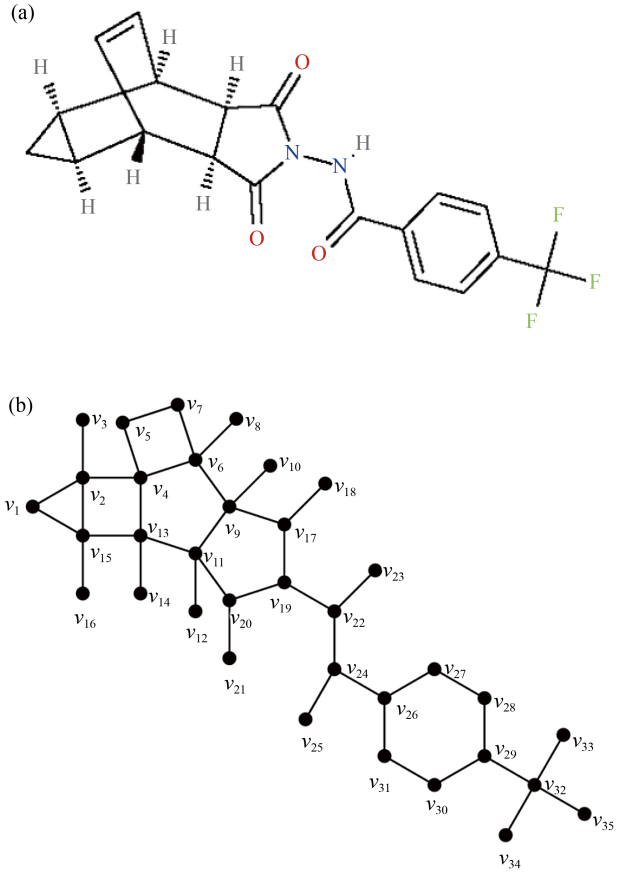


Figure 5. (a) Molecular structure of Brincidofovir, (b) Molecular graph of Brincidofovir, and (c) line graph of Brincidofovir

In order to prove the accuracy of our assertion, we need to show that $\alpha_e(L(G_B)) \geq 4$. To this end, let us check if we can choose the edge resolving set of cardinality less than four. Now suppose we choose the edge resolving set of cardinality three; if we let $\mathscr{S}_e^l = \{v_a^l, v_b^l, v_c^l : a \neq b \neq c; a, b, c \in \{1, 2, \ldots, 42\}\}$, where $\mathscr{S}_e^l \subset V(L(G_B))$. For some $i, j \in \{3, \ldots, 18\}$ and $\delta, \beta \in \{1, \ldots, 4\}$, there are at least five pairs of edges that cannot be uniquely identified by $\mathscr{S}_e^l$ such that $r(v_i^l v_{i+\delta}^l | \mathscr{S}_e^l) = r(v_j^l v_{j+\beta}^l | \mathscr{S}_e^l)$. It goes against what we had assumed; we are unable to pick a subset of cardinality three in order to uniquely identify each edge of Brincidofovir; as a result, $\alpha_e(L(G_B)) \geq 4$.

Theorem 6 Let G_T be the molecular graph of antiviral drug Tecovirimat, and $L(G_T)$ be its corresponding line graph, then; $\alpha_e(L(G_T)) = 12$.

Proof. We assert that twelve nodes are required to uniquely identify all the edges of the line graph of antiviral drug Tecovirimat; Figure 6 shows molecular structure, molecular graph and its corresponding line graph of Tecovirimat. To prove our assertion we will employ the double inequality approach, to show the existance of the upper bound, which is $\alpha_e(L(G_T)) \leq 12$, we let $W_e^l = \{v_1^l, v_5^l, v_8^l, v_{10}^l, v_{16}^l, v_{17}^l, v_{18}^l, v_{22}^l, v_{30}^l, v_{36}^l, v_{39}^l, v_{40}^l\}$. Clearly, shown below are the unique representations of all edges of the line graph of the antiviral drug Tecovirimat, which implies that the cardinality of the edge resolving set is twelve; hence, $\alpha_e(L(G_T)) \leq 12$.



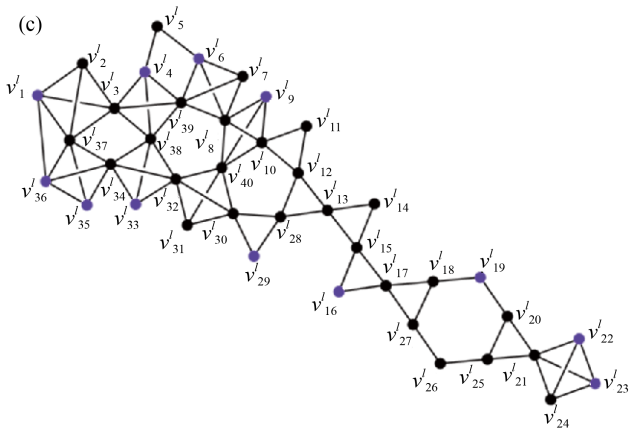


Figure 6. (a) Molecular structure of Tecovirimat, (b) Molecular graph of Tecovirimat, (c) line graph of Tecovirimat

The expression for $r(v_\xi^l v_{\xi+1}^l \mid W_e^l)$ is defined as follows. For $\xi = 1,\ 2$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 1,\ 3-\xi,\ 4-\xi,\ 5-\xi,\ \xi,\ 2,\ 4-\xi,\ 6-\xi,\ 9-\xi,\ 11-\xi,\ 14-\xi,\ 14-\xi),$$

for $\xi = 3,\ 4$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi - 2,\ 0,\ 5-\xi,\ 3,\ \xi - 1,\ \xi - 1,\ 2,\ 4,\ 7,\ 9,\ 12,\ 12),$$

for $\xi = 5,\ 6$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (3,\ \xi - 4,\ 0,\ 2,\ 4,\ 4,\ 3,\ 4,\ 6,\ 8,\ 11,\ 11),$$

for $\xi = 7,\ 8$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (3,\ 2,\ 1,\ 8-\xi,\ 4,\ 4,\ 3,\ 3,\ 5,\ 7,\ 10,\ 10),$$

for $\xi = 9,\ 10$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (4,\ 3,\ 2,\ \xi - 9,\ 4,\ 4,\ 3,\ 3,\ 4,\ 6,\ 9,\ 9),$$

for $\xi = 11$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (5,\ 4,\ 3,\ 2,\ 5,\ 5,\ 4,\ 2,\ 3,\ 5,\ 8,\ 8),$$

for $\xi = 12,\ 13$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi-7,\ \xi-8,\ \xi-9,\ \xi-10,\ 5,\ 5,\ 4,\ 2,\ 2,\ 4,\ 7,\ 7),$$

for $\xi = 14,\ 15$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (7,\ 6,\ 5,\ 4,\ 6,\ 6,\ 5,\ 3,\ 15-\xi,\ 3,\ 6,\ 6),$$

for $\xi = 16,\ 17$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (8,\ 7,\ 6,\ 5,\ 7,\ 7,\ 6,\ 4,\ \xi-16,\ 18-\xi,\ 21-\xi,\ 21-\xi),$$

for $\xi = 18,\ 19$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi-9,\ \xi-10,\ \xi-11,\ \xi-12,\ \xi-10,\ \xi-10,\ \xi-11,\ \xi-13,\ \xi-16,\ 0,\ 21-\xi,\ 21-\xi),$$

for $\xi = 20,\ 21$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (\xi-9,\ \xi-10,\ \xi-11,\ \xi-12,\ \xi-10,\ \xi-10,\ \xi-11,\ \xi-13,\ \xi-17,\ \xi-19,\ 1,\ 21-\xi),$$

for $\xi = 22,\ 23$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (13,\ 12,\ 11,\ 10,\ 12,\ 12,\ 11,\ 9,\ 6,\ 3,\ 0,\ \xi-22),$$

for $\xi = 25,\ 26$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (35-\xi,\ 34-\xi,\ 33-\xi,\ 32-\xi,\ 34-\xi,\ 34-\xi,\ 33-\xi,\ 31-\xi,\ 28-\xi,\ 2,\ \xi-23,\ \xi-23),$$

for $\xi = 28$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (5,\ 4,\ 4,\ 3,\ 4,\ 4,\ 3,\ 0,\ 3,\ 5,\ 8,\ 8),$$

for $\xi = 29,\ 30$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (4,\ 3,\ 3,\ 2,\ 3,\ 3,\ 2,\ \xi-29,\ 4,\ 6,\ 9,\ 9),$$

for $\xi = 31,\ 32$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (3,\ 2,\ 3,\ 2,\ 2,\ 2,\ 32-\xi,\ 2,\ 5,\ 7,\ 10,\ 10),$$

for $\xi = 33,\ 34$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (2,\ 2,\ 3,\ 3,\ 1,\ 34-\xi,\ \xi-33,\ 3,\ 6,\ 8,\ 11,\ 11),$$

for $\xi = 35,\ 36$,

$$r(v_\xi^l v_{\xi+1}^l \mid W_e^l) = (1,\ 39-\xi,\ 40-\xi,\ 4,\ 0,\ \xi-36,\ 2,\ 4,\ 7,\ 9,\ 12,\ 12).$$

$$r\left(v_x^l v_y^l \mid W_e^l\right) = \begin{cases} v_1^l v_3^l \to (0,\ 1,\ 2,\ 3,\ 1,\ 2,\ 2,\ 4,\ 7,\ 9,\ 12,\ 12), \\ v_1^l v_{36}^l \to (0,\ 2,\ 3,\ 4,\ 0,\ 1,\ 2,\ 4,\ 7,\ 9,\ 12,\ 12), \\ v_1^l v_{37}^l \to (0,\ 2,\ 3,\ 4,\ 1,\ 1,\ 2,\ 4,\ 7,\ 9,\ 12,\ 12), \\ v_2^l v_{37}^l \to (1,\ 2,\ 3,\ 4,\ 1,\ 1,\ 2,\ 4,\ 7,\ 9,\ 12,\ 12), \\ v_3^l v_{37}^l \to (1,\ 1,\ 2,\ 3,\ 1,\ 1,\ 2,\ 4,\ 7,\ 9,\ 12,\ 12), \\ v_3^l v_{38}^l \to (1,\ 1,\ 2,\ 3,\ 2,\ 2,\ 1,\ 3,\ 6,\ 8,\ 11,\ 11), \\ v_4^l v_{38}^l \to (2,\ 0,\ 2,\ 3,\ 2,\ 2,\ 1,\ 3,\ 6,\ 8,\ 11,\ 11), \\ v_4^l v_{39}^l \to (2,\ 0,\ 1,\ 2,\ 3,\ 3,\ 2,\ 4,\ 6,\ 8,\ 11,\ 11), \\ v_6^l v_{39}^l \to (2,\ 1,\ 0,\ 2,\ 3,\ 3,\ 2,\ 4,\ 6,\ 8,\ 11,\ 11), \\ v_8^l v_{40}^l \to (3,\ 2,\ 1,\ 1,\ 3,\ 3,\ 2,\ 2,\ 5,\ 7,\ 10,\ 10), \\ v_9^l v_{40}^l \to (4,\ 3,\ 2,\ 0,\ 3,\ 3,\ 2,\ 2,\ 5,\ 7,\ 10,\ 10), \\ v_{12}^l v_{28}^l \to (5,\ 4,\ 3,\ 2,\ 4,\ 4,\ 3,\ 1,\ 3,\ 5,\ 8,\ 8), \\ v_{32}^l v_{40}^l \to (3,\ 2,\ 2,\ 1,\ 2,\ 2,\ 1,\ 2,\ 5,\ 7,\ 10,\ 10), \\ v_{33}^l v_{38}^l \to (2,\ 1,\ 2,\ 3,\ 2,\ 2,\ 0,\ 3,\ 6,\ 8,\ 11,\ 11), \\ v_{38}^l v_{39}^l \to (2,\ 1,\ 1,\ 2,\ 2,\ 2,\ 1,\ 3,\ 6,\ 8,\ 11,\ 11). \end{cases}$$

To make our assertion accurate and precise, we need to show that there is no subset of $V(L(G_T)$ of cardinality less than twelve that can uniquely identify all the edges of the line graph of Tecovirimat. To this end, suppose if possible there is a subset of cardinality eleven, then let $\mathscr{S}_e^l = \{v_a^l,\ v_b^l,\ v_c^l,\ v_d^l,\ v_e^l,\ v_f^l,\ v_g^l,\ v_h^l,\ v_m^l,\ v_n^l,\ v_p^l :\ a \neq b \neq c \neq d \neq e \neq f \neq g \neq h \neq m \neq n \neq p;\ a,\ b,\ c,\ d,\ e,\ f,\ g,\ h,\ m,\ n,\ p \in \{1,\ 2,\ \ldots,\ 40\}\}$, where $\mathscr{S}_e^l \subset V(L(G_T))$. For some $i,\ j \in \{2,\ \ldots,\ 39\}$ and $\delta,\ \beta \in \{1,\ \ldots,\ 15\}$, there are at least two pairs of edges that cannot be uniquely identified by $\mathscr{S}_e^l$ such that $r(v_i^l v_{i+\delta}^l | \mathscr{S}_e^l) = r(v_j^l v_{j+\beta}^l | \mathscr{S}_e^l)$, a contradiction; so our assumption is wrong, we cannot choose any subset of cardinality eleven to identify all edges of Tecovirimat, hence, $\alpha_e(L(G_T)) \geq 12$.

4. Conclusions

In this paper, we computed the edge metric dimension of the line graph of the antiviral drug structures, namely Valacyclovir, Cidofovir, Famciclovir, Acyclovir, Brincidofovir, and Tecovirimat. As we can see from the results presented, only three nodes for Acyclovir and four nodes for Valacyclovir, Cidofovir, Famciclovir, and Brincidofovir are required to

uniquely identify all the edges of their corresponding line graphs, whereas Tecovirimat requires twelve nodes for the same purpose. Knowing the edge metric dimension of the line graph of molecular graphs along with other molecular descriptors can effectively be used to develop predictive models such as Quantitative Structure-Property Relationship (QSPR) model for the behavior of chemical compounds that give insights to scientists or chemists to predict the physiochemical properties of the molecular compounds that will enable them to explore more on the antiviral drugs of viral infections or medicine that will completely cure the disease.

5. Limitations

Computing the edge metric dimension of the line graph of the antiviral drugs may yield interesting mathematical insights; ensuring that the findings have practical chemical relevance or implications for the study of antiviral drugs is crucial. However, the interpretation of the results in linking the gap between theoretical graph analysis and its application in chemistry or pharmacology can be challenging, as it needs to work along with other molecular descriptors for better interpretation and understanding.

Mpox disease and treatment might have a limited number of studies that have been conducted and data compared to more extensively studied diseases, leading to challenges in obtaining comprehensive sets of molecular graphs, particularly molecular graphs of antiviral drugs and their line graphs.

6. Future study

Investigate the vertex metric dimension of the line graph of antiviral drugs for a broader range of antiviral drugs beyond those currently studied.

Investigate Fault-Tolerant Edge Metric Dimensions in the context of the line graph of molecular graphs including antiviral drugs.

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Conflict of interest

Authors declare that there is no conflict of interest.

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