Iraqi Journal for Computer Science and Mathematics

Volume 5 | Issue 4 Article 9

2024

A Comprehensive Analysis of Partition Dimensions in Efavirenz Abacavir Lamivudine Doravirine of Anti-HIV Drug Structures

R. Nithya Raj
Department of Mathematics, Hindustan Institute of Technology and Science, Chennai 603 103, India, nithyarajmaths@gmail.com

R. Sundara Rajan
Department of Mathematics, Hindustan Institute of Technology and Science, Chennai 603 103, India

Hijaz Ahmad
Near East University, Operational Research Center in Healthcare, TRNC Mersin 10, Nicosia, 99138, Turkey AND Department of Mathematics, Faculty of Science, Islamic University of Madinah, Madinah, Saudi Arabia

Recommended Citation

Raj, R. Nithya; Rajan, R. Sundara; and Ahmad, Hijaz (2024) "A Comprehensive Analysis of Partition Dimensions in Efavirenz Abacavir Lamivudine Doravirine of Anti-HIV Drug Structures," *Iraqi Journal for Computer Science and Mathematics*: Vol. 5: Iss. 4, Article 9.
DOI: https://doi.org/10.52866/2788-7421.1212
Available at: https://ijcsm.researchcommons.org/ijcsm/vol5/iss4/9

IRAQI JOURNAL FOR COMPUTER SCIENCE AND MATHEMATICS 2024;5:100–107

RESEARCH ARTICLE

A Comprehensive Analysis of Partition Dimensions in Efavirenz Abacavir Lamivudine Doravirine of Anti-HIV Drug Structures

R. Nithya Raj [a,*], **R. Sundara Rajan** [a], **Hijaz Ahmad** [b,c]

[a] Department of Mathematics, Hindustan Institute of Technology and Science, Chennai 603 103, India
[b] Near East University, Operational Research Center in Healthcare, TRNC Mersin 10, Nicosia, 99138, Turkey
[c] Department of Mathematics, Faculty of Science, Islamic University of Madinah, Madinah, Saudi Arabia

ABSTRACT

The partition dimension of a graph in chemical graph theory refers to a graph invariant used to analyze the structural properties of molecules. It represents the minimum number of clusters or resolving partition set required to uniquely identify each vertex in the graph based on the neighborhoods within their respective clusters. In the context of chemical graph theory, the vertices of the graph correspond to atoms, and edges represent bonds between these atoms in a molecular structure. Determining the partition dimension of a chemical graph helps in understanding the relationships between molecular components and their spatial arrangements. It assists in the analysis of molecular conformations, structure-activity relationships, and drug design by identifying the smallest number of distinct clusters or resolving partition sets necessary to uniquely define the local environment of each atom in the molecule. The partition dimension is a valuable metric in computational chemistry, offering insights into molecular complexity, aiding in the prediction of molecular properties, and facilitating the discovery of new drug candidates with specific structural characteristics. In this work, we have calculated the partition dimension of certain ANTI-HIV drug molecular structures.

Keywords: Partition resolving set, Partition dimension, ANTI-HIV drug structures

1. Introduction

Acquired Immunodeficiency Syndrome (AIDS), caused by the Human Immunodeficiency Virus (HIV), stands as one of the most challenging and globally impactful health crises of our time. Since its identification in the early 1980s, the HIV/AIDS pandemic has spurred extensive research, public health initiatives, and medical interventions. This insidious virus, which attacks the immune system, has far-reaching consequences, affecting millions of lives worldwide. Understanding the virology, transmission, and socioeconomic impact of HIV is paramount in the ongoing efforts to prevent new infections, improve treatment modalities, and ultimately work towards a world free of the devastating effects of AIDS. This introduction delves into the multifaceted aspects of the AIDS HIV virus, shedding light on its complexities, the progress made in its management, and the challenges that persist in the pursuit of global health equity. Antiretroviral drugs, vital in the treatment of Human Immunodeficiency Virus (HIV) infection, exhibit diverse molecular structures that contribute to their therapeutic efficacy. These structures are carefully designed to interfere with various stages of the HIV life cycle, preventing the virus from replicating and progressing within the host's immune system. Efavirenz, a non-nucleoside reverse transcriptase inhibitor (NNRTI), disrupts the virus's ability to convert its RNA into DNA by binding to the reverse transcriptase enzyme. Abacavir, a nucleoside reverse transcriptase inhibitor (NRTI), incorporates itself into the

Received 25 July 2024; accepted 10 March 2024.
Available online 25 November 2024

* Corresponding author.
E-mail address: nithyarajmaths@gmail.com (R. N. Raj).

https://doi.org/10.52866/2788-7421.1212

growing viral DNA chain, inhibiting further synthesis. Lamivudine, another NRTI, competes with natural building blocks for incorporation into the viral DNA, thereby impeding its elongation. Doravirine, a newer generation NNRTI, hinders the reverse transcription process by binding specifically to the viral reverse transcriptase enzyme. These molecular structures exemplify the strategic design of antiretroviral drugs, targeting key viral enzymes or processes essential for replication. Understanding these structures is fundamental to appreciating the nuanced mechanisms by which these drugs combat HIV, ultimately contributing to improved treatment outcomes for individuals living with the virus. Based on information from the World Health Organization (WHO), an estimated 480,000 to 1.0 million individuals lost their lives due to HIV-related causes, and approximately 1.0 to 2.0 million people contracted HIV in the year 2020. The transmission of this virus has surged rapidly, with the alarming observation that no fully recognized drug or vaccine exists for its administration. Nevertheless, certain medications have demonstrated the ability to partially control the virus to some extent. In this context, specific topological descriptors for the chemical structures of tenofovir, employed in the treatment of HIV, have been identified as detailed in [1]. Mamika et al. [30], discussed the Signless laplacian energy of interval-valued fuzzy graph and its applications to build an algorithm that helps in solving some real-life problems. Consequently, Faisal et al. [31], studied decision-making techniques based on similarity measures of possibility interval fuzzy soft environment. Finally, Ahmed et al. [32], used mathematical modeling techniques with applications in biosciences to predict COVID-19 in various.

Some pre-existing drugs have been approved for use and efficacy by researchers to control and manage the deadly virus. These include reverse transcriptase inhibitors that are nucleoside or non-nucleoside. A molecule's topology is fundamentally a non-numerical mathematical unit. The topology of a molecule is essentially a non-numerical mathematical concept. Many measurable characteristics of a molecule are often represented by specific numerical values. To establish a connection between molecular topology and real chemical attributes, the conversion of relevant details embedded in the chemical structure to numeric values becomes crucial, ultimately giving rise to the emergence of topological indices. Thus, the topological index of a molecular graph is considered a non-empirical numerical quantity that determines the framework of the molecule along with its diverging sequence. In other words, these topological indices are functions that map the chemical structure to a real value.

In this paper, we consider a transformation from a chemical structure to a graph representation when discussing a molecular graph. Assumed by this transformation are nodes representing atoms and edges representing the chemical bonds between them. For more detailed information, one can refer to recent literature [2–6].

Following is the division of the remaining sections of the paper. Preliminaries and basic concepts are given in Section 2 and the main findings are listed in Section 3. The final observation of the findings is in Section 4, and the conclusion and further future directions are discussed in Section 5 respectively.

2. Basis concepts

Definition 2.1. *Let $B = (V(B), E(B))$ represent a basic connected undirected graph of a chemical network (structure), with $V(B)$ representing the set of nodes set or vertex set and $E(B)$ representing the set edges set, also known as the branches. The distance between two nodes, often denoted as $d(u, v)$ or $dist(u, v)$ is the length of the shortest path connecting those vertices. The distance is the minimum number of edges that must be traversed to go from vertex u to vertex v in the given graph B.*

Definition 2.2. *Consider $L = \{l_1, l_2, l_3, \ldots, l_s\} \subset V(B)$ is an ordered subset of the set of primary nodes then for a primary node $l \in V(B)$ the identification/position of a primary node l in relation to L is arranged in measurements $(d(l, l_1), d(l, l_2), d(l, l_3), \ldots, d(l, l_s))$. If the ordered subset L assigns a unique identity to each principal node in $V(B)$, then this subset is known as a resolving set of chemical network structures. The metric dimension of is the lowest number of elements in the subset L, which is indicated by the term $dim(B)$.*

Definition 2.3. *Given a vertex t in a molecular graph structure $V(B)$ and a subset P of $V(B)$ the distance between t and P is denoted as $d(t, P)$ and is defined as the minimum distance between t and any vertex x in P expressed as $d(t, P) = min\{d(t, x)|x \in P\}$. Let $\pi = \{P_1, P_2, P_3, \ldots, P_k\}$ be an k ordered resolving partition set of $V(B)$. The representation of a vertex t with respect to π is the k tuple $\{d(t, P_1), d(t, P_2), d(t, P_3), \ldots, d(t, P_k)\}$. A partition π of a graph B is termed a resolving partition if each distinct vertex in B possesses a unique representation with respect to π. The partition dimension, $Pd(B)$, is the smallest number of subsets that can be created with the given set $V(B)$.*

Table 1 lists the different notations and symbols in the context of metrics and their generalizations. A variety of applications for these ideas are explained by the literature included in the text:

Table 1. Fundamental notations.

Terminologies	Notation
Structure	$B_{Structure}$
Node set [NS]	$V(B_{Structure})$
Edge set [ES]	$E(B_{Structure})$
Resolving set [RS]	ls
Resolving number [RN]	l_n
Partition resolving number	prn
Partition resolving set [PRS]	π
Representation of a vertex x with respect to partition resolving set π	$r(x\|\pi)$
Function providing the PLS elements of Figs. 1 to 4	x_i

The very limited and recent literature that is available here is on metrics and their generalization. The topic of metric dimension and its generalization is explored in relation to polycyclic aromatic compounds in [7]. In [8], a two-dimensional lattice is discussed along with the concept of metric dimension and that structure. They also discussed a chemical structure. The same idea of distance-based graph theory is applied to cellulose networks in [9]. In [10], the idea of distance graph theory is used to discuss a computer network. References [11–15] provide specific information on broad classes of connected data patterns (graphs). In general, the literature surveyed encompasses a broad spectrum of applications and extensions of metrics dimension across diverse fields such as chemistry, networking, and graph theory. These investigations are likely to enhance our comprehension of metrics dimension and their relevance in varied contexts.

There are fewer precise partitions available and frequently only bounds are given because the partition dimension [PD] is a more complicated idea than the metric dimension [MD]. For example, bounds are provided in reference [16] for partitioning a generalized set of convex polytopes, and similar bounds are provided in reference [17]. Partitioning is demonstrated using a chemical fullerene graph in [18], and bounds for another chemical structure are given in [19]. [20] presents partition sets for specific nanotubes and sheets, and [21] discusses the two-dimensional lattice structure. The partition dimension is computed for a variety of broad Characteristics defining graph families and classes in references [22–26].

The metric dimension has many applications in various fields, such as image processing, robotic roving, complex games, combinatorial optimization, pharmaceutical chemistry, the polymer industry, and the electric field. The list of these applications is complete in [27–29]. In the field of robotics, the partitioning of a vertex set according to metric properties holds significance for optimizing robot roving strategies [29]. Partition dimensions are used by the Djokovic-Winkler relation in chemistry to confirm and identify networks. In addition, metric dimension is used in hierarchical data structures, image processing, pattern recognition, and mastermind games. The metric dimension, in general, has a broad range of useful applications that are pertinent to numerous fields that require effective and efficient problem-solving techniques.

3. Main result

The main findings of our partition resolving a set of different structures will be shown in this section, such as Efavirenz, Abacavir, Lamivudine, and Doravirine.

Theorem 3.1. *Let $B_{efavirenz}$ be a graph of efavirenz anti- HIV drug structure depicted as a network of nodes and edges. In this structure, the total number of edges, also referred to as the size, is 23, while the total number of nodes, also known as the order, is 21. Additionally, Fig. 1 displays the molecular graph of the labeling and structure of the anti-HIV drug efavirenz, which was utilized to illustrate our main findings. Then, the $B_{efavirenz}$ partition resolving set is less than or equal to 4.*
$V(B_{efavirenz}) = \{a_r : r = 1, 2, 3, \ldots, 21\}$ $E(B_{efavirenz}) = \{a_r a_{r+1} : r = 1, 2, 3, \ldots, 7\} \cup \{a_r a_{r+1} : r = 9, 10\} \cup \{a_r a_{r+1} : r = 12, 13, 14\} \cup \{a_r a_{r+1} : r = 16, 17, 18)\} \cup \{a_6 a_8, a_3 a_9, a_{14} a_{16}, a_3 a_{12}, a_{19} a_{10}, a_{12} a_{18}, a_2 a_{20}, a_2 a_{21}\}$.

Proof. Let $\pi = \{\pi_1, \pi_2, \pi_3, \pi_4\}$ where $\pi_1 = \{a_1\}$ $\pi_2 = \{a_{20}\}$, $\pi_3 = \{a_7, a_{11}\}$ and $\pi_4 = V(B_{efavirenz}) \setminus \{\pi_1 \cup \pi_2 \cup \pi_3\}$ be a partition resolving set of $B_{efavirenz}$.

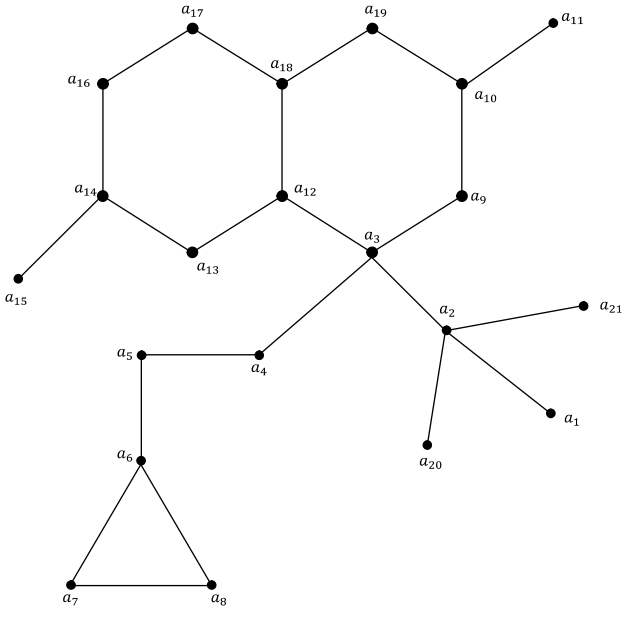

Fig. 1. Molecular graph of efavirenz.

Table 2. Identification of each node of $B_{efavirenz}$.

$r(a_r\|\pi)$	π_1	π_2	π_3	π_4	Range
a_r	r-1	r+1	r+4	δ_r	r=1
a_r	r-1	r-1	6-r	0	$r = 2, 3$
a_r	r-1	r-1	7-r	δ_r	$4 \le r \le 7$
a_r	r-2	r-6	1	0	$r = 8$
a_r	r-6	r-6	11-r	δ_r	$9 \le r \le 11$
a_r	r-9	r-9	r-8	0	$12 \le r \le 15$
a_r	22-r	22-r	21-r	0	$16 \le r \le 18$
a_r	5	5	2	0	$r = 19$
a_r	2	0	5	δ_r	$r = 20$
a_r	2	2	5	0	$r = 21$

To prove π is a partition resolving number, it is enough to show that all the vertices $\{a_r; 1 \le r \le 21\}$ of $B_{efavirenz}$ have unique representations with regard to π. For $1 \le r \le 21$ the representation a_r of $B_{efavirenz}$ with regard to π are shown in Table 2.

$$\delta_r = \begin{cases} 1 & \text{if } r \in 1, 7, 11, 20 \\ 0 & \text{if } otherwise \end{cases}$$

Given identification $r(a_r|\pi)$ each node of efavirenz of anti-*HIV* drug structure is unique and fulfills the definition of partition resolving set. This proved that the partition resolving number $prn(B_{efavirenz}) \le 4$ of the graph of efavirenz of anti-*HIV* drug structure. □

Theorem 3.2. *Let $B_{abacavir}$ be a graph of abacavir anti- HIV drug structure depicted as a network of nodes and edges. The total number of nodes in this structure, referred to as the order, is 21, while the total number of edges, known as the size, is 24 respectively. Moreover, Fig. 2 shows the molecular graph of the abacavir anti-HIV molecular structure and labeling used to demonstrate our major results. Then the partition resolving number of $B_{abacavir}$ is equal to 3. $V(B_{abacavir}) = \{b_r : r = 1, 2, 3, \ldots, 21\}$, $E(B_{abacavir}) = \{b_r b_{r+1} : r = 1, 2, 3, \ldots, 11\} \cup \{b_r b_{r+1}) : r = 18, 19\} \cup \{b_{10}b_{13}, b_{13}b_{14}, b_8b_{14}, b_7b_{15}, b_{15}b_{16}, b_5b_{16}, b_{16}b_{17}, b_{17}b_{19}, b_4b_{18}, b_2b_{21}, b_1b_{21}\}$.*

Table 3. Identification of each node of $B_{abacavir}$.

$r(b_r\|\pi)$	π_1	π_2	π_3	Range
b_r	$r-1$	$12-r$	δ_r	$1 \le r \le 12$
b_r	$22-r$	$r-10$	0	$r = 13, 14$
b_r	$21-r$	$r-9$	0	$r = 15, 16$
b_r	6	8	0	$r = 17$
b_r	$r-14$	$r-9$	0	$r = 18$
b_r	$r-14$	$r-10$	0	$r = 19, 20$
b_r	1	$\frac{r+1}{2}$	0	$r = 21$

Proof. Let $\pi = \{\pi_1, \pi_2, \pi_3\}$ where $\pi_1 = \{b_1\}$ $\pi_2 = \{b_{12}\}$, and $\pi_3 = V(B_{abacavir}) \setminus \{\pi_1 \cup \pi_2\}$ be a partition resolving set of $B_{abacavir}$ To prove π is a partition resolving set, it is enough to show that all the vertices $\{b_i : 1 \le i \le 21\}$ of $B_{abacavir}$ have distinct representation with respect to π. For $1 \le i \le 21$ the representation b_i of $B_{abacavir}$ with respect to π are shown in Table 3.

$$\delta_r = \begin{cases} 1 & \text{if } r \in 1, 12 \\ 0 & \text{if } otherwise \end{cases}$$

Given identification $r(b_i|\pi)$ each node of abacavir of anti-HIV drug structure is unique and fulfills the definition of partition resolving set. This

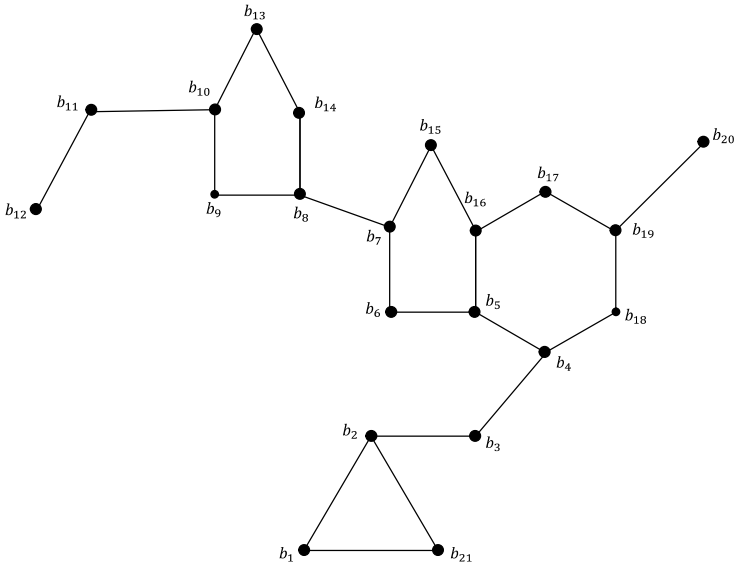

Fig. 2. Molecular graph of abacavir.

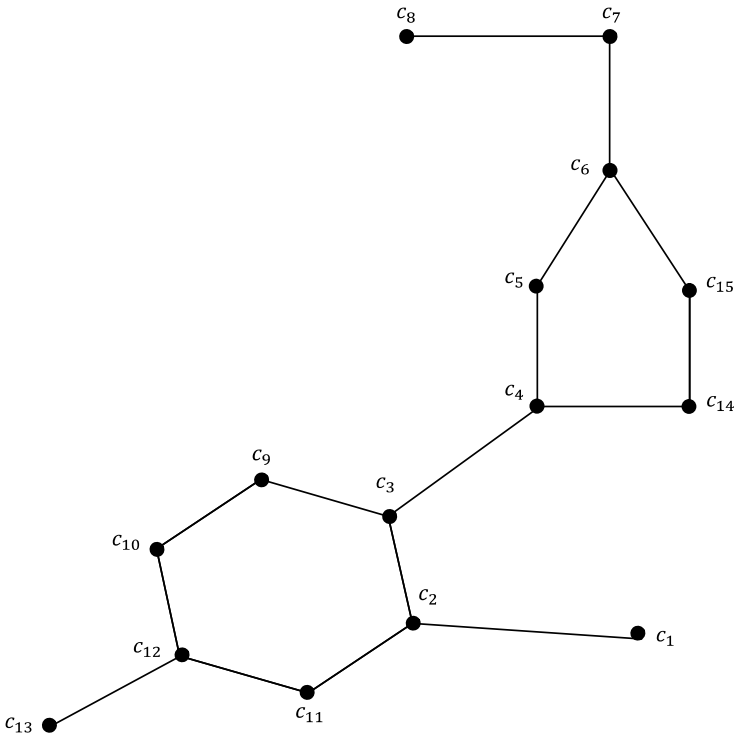

Fig. 3. Molecular graph of lamivudine.

demonstrated that the partition resolving number $prn(B_{abacavir}) = 3$ of a graph of abacavir of anti-HIV drug structure. □

Theorem 3.3. *Let $B_{lamivudine}$ be a graph of efavirenz anti- HIV drug structure is depicted as a network of nodes and edges. In this structure. This structure's total number of edges, or size, is 16, while its total number of nodes, or order, is 15 respectively. Moreover, Fig. 3 shows the molecular graph of the lamivudine anti-HIV molecular structure and labeling used to demonstrate our major results. Then the partition resolving number of $B_{lamivudiner}$ is equal to 3.* $V(B_{lamivudine}) = \{c_r : r = 1, 2, 3, \ldots, 15\}$, $E(B_{lamivudine}) = \{c_r c_{r+1} : r = 1, 2, 3, \ldots, 7\} \cup \{c_r c_{r+1} : r = 11, 12\} \cup \{c_3c_9, c_9c_{10}, c_{10}c_{12}, c_2c_{11}, c_6c_{15}, c_4c_{14}, c_{14}c_{15}\}$.

Proof. Let $\pi = \{\pi_1, \pi_2, \pi_3\}$ where $\pi_1 = \{c_1\}$ $\pi_2 = \{c_8\}$, and $\pi_3 = V(B_{lamivudine}) \setminus \{\pi_1 \cup \pi_2\}$ be a partition resolving a set of $B_{lamivudine}$ To prove π is a partition resolving set, it is enough to show that all the vertices $\{c_r : 1 \le r \le 15\}$ of $B_{lamivudine}$ have distinct representation with respect to π. For $1 \le r \le 15$ the representation c_r of $B_{lamivudine}$ with respect to π are shown in Table 4.

$$\delta_r = \begin{cases} 1 & \text{if } r \in 1, 8 \\ 0 & \text{if } otherwise \end{cases}$$

Table 4. Identification of each node of $B_{lamivudine}$.

$r(c_r\|\pi)$	π_1	π_2	π_3	Range
c_r	$r-1$	$8-r$	δ_r	$1 \le r \le 8$
c_r	$r-6$	$r-3$	0	$r = 9, 10$
c_r	$r-9$	$r-4$	0	$11 \le r \le 13$
c_r	$r-10$	$n-r+3$	0	$r = 14, 15$

Given identification $r(c_r|\pi)$ each node of lamivudine of anti-*HIV* drug structure is unique and fulfills the definition of partition resolving set. This shows that the partition resolving number $pln(B_{lamivudine}) = 3$ of the graph of lamivudine of anti-*HIV* drug structure. □

Theorem 3.4. *The graph $B_{doravirine}$ anti-HIV drug structure is represented by a network of nodes and edges. The entire number of nodes in this structure, also known as the order is 29, whereas the total number of edges, also known as the size, is 31 respectively. Moreover, Fig. 4 shows the molecular graph of the doravirine anti-HIV molecular structure and labeling used to demonstrate our major results. Then the partition resolving number of $B_{doravirine}$ is less than or equal to 4.* $V(B_{doravirine}) = \{d_r : r = 1, 2, 3, \ldots, 29\}$, $E(B_{doravirine}) = \{d_r d_{r+1} : r = 1, 2, 3, \ldots, 10\} \cup \{d_r d_{r+1} : r = 12, 13, 14, 15, 16\} \cup \{d_r d_{r+1} : r = 18, 19, 20\} \cup \{d_{19}d_{24}, d_{12}d_{22}, d_{22}d_{23}, d_6d_{22}, d_{14}d_{18}, d_3d_{12}, d_8d_{25}, d_{25}d_{26}, d_{10}d_{26}, d_9d_{27}, d_2d_{28}, d_2d_{29}, d_{24}d_{16}\}$

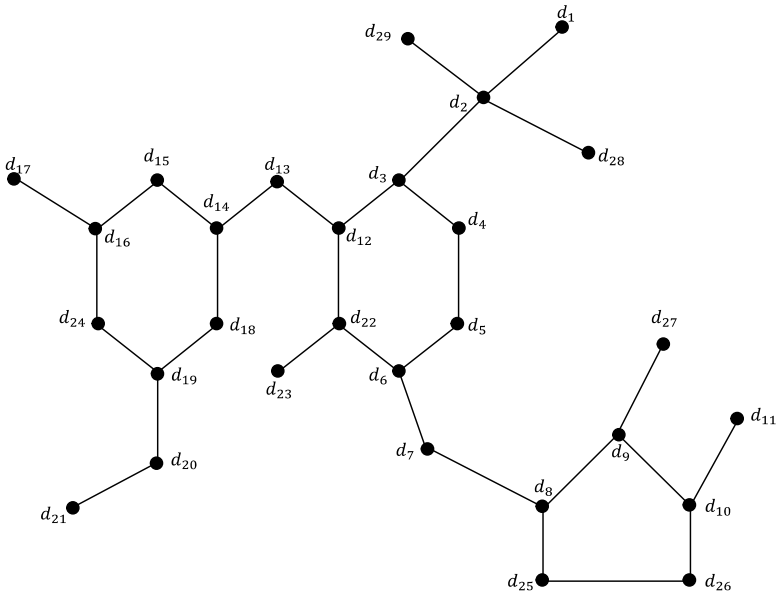

Fig. 4. Molecular graph of doravirine.

Proof. Let $\pi = \{\pi_1, \pi_2, \pi_3, \pi_4\}$ where $\pi_1 = \{d_1\}$ $\pi_2 = \{d_4, d_{29}\}$, $\pi_3 = \{d_{17}, d_{27}\}$ and $\pi_4 = V(B_{doravirine}) \setminus \{\pi_1 \cup \pi_2 \cup \pi_3\}$ be a partition resolving set of $B_{doravirine}$. To prove π is a partition resolving set, it is enough to show that all the vertices $\{d_i : 1 \leq r \leq 29\}$ of $B_{doravirine}$ have unique representation with respect to π. For $1 \leq r \leq 29$ the representation d_i of $B_{doravirine}$ with respect to π are shown in Table 5.

$$\delta_r = \begin{cases} 1 & \text{if } r \in 1, 4, 17, 27, 29 \\ 0 & \text{if } otherwise \end{cases}$$

Given identification $r(d_i|\pi)$ each node of doravirine of anti-HIV molecular structure is unique and fulfills the definition of partition resolving set. This shows that the partition resolving number $prn(B_{doravirine}) \leq 4$ of the graph of doravirine of anti-HIV molecular structure. □

Table 5. Identification of each node of $B_{doravirine}$.

$r(d_r\|\pi)$	π_1	π_2	π_3	π_4	Range
d_r	$r-1$	$3-r$	$9-r$	δ_r	r = 1
d_r	$r-1$	$3-r$	$9-r$	0	r = 2
d_r	$r-1$	$4-r$	6	0	$r=3$
d_r	$r-1$	$4-r$	6	δ_r	$r=4$
d_r	$r-1$	$r-4$	$10-r$	0	$5 \leq r \leq 9$
d_r	$r-1$	$r-4$	$12-r$	0	$r=10,11$
d_r	$r-9$	$r-10$	$17-r$	0	$12 \leq r \leq 16$
d_r	$r-9$	$r-10$	$17-r$	δ_r	$r=17$
d_r	$r-12$	$r-13$	4	0	$r=18$
d_r	$r-12$	$r-13$	$r-16$	0	$19 \leq r \leq 21$
d_r	$r-18$	$r-19$	$r-17$	0	$r=22,23$
d_r	$r-16$	$r-17$	2	0	$r=24$
d_r	$r-17$	$r-20$	3	0	$r=25,26$
d_r	$r-18$	6	0	δ_r	$r=27$
d_r	2	0	8	0	$r=28$
d_r	2	0	8	δ_r	$r=29$

4. Final observation

The findings of this study indicate that efavirenz and doravirine can split into four subgroups within their partition-resolving sets, whereas abacavir and lamivudine show a partition dimension of three. In order to represent the structures of these antibiotic HIV molecular graphs, the article investigates the use of vertex matrices in molecular graph theory. Table 6 provides a further summary.

The partition dimension of antibiotic HIV-drug structures, including Efavirenz, Abacavir, Lamivudine, and Doravirine, plays a crucial role in their pharmacokinetics and pharmacodynamics. Understanding the partition dimension is essential for predicting drug behavior within biological systems, optimizing drug delivery, and enhancing therapeutic efficacy. These drugs exhibit unique structural features that influence their partitioning behavior, affecting factors such as absorption, distribution, metabolism, and excretion. Investigating the partition dimension of these antibiotic HIV drugs provides

Table 6. Overview of the results.

Graphs	Partition resolving number [PRN]
$B_{efavirenz}$	≤ 4
$B_{abacavir}$	3
$B_{lamivudine}$	3
$B_{doravirine}$	≤ 4

valuable insights into their biological activity and aids in the development of more effective treatment strategies for HIV/AIDS.

5. Conclusion and future studies

In this paper, our investigation into the partition dimensions of Efavirenz, Abacavir, Lamivudine, and Doravirine, anti-HIV drug structures, has provided valuable insights into the molecular characteristics of these compounds. The partition dimension, as explored in this study, plays a crucial role in understanding the distribution and behavior of these drugs within biological systems. The unique structural features identified for each drug contribute to our understanding of their pharmacokinetics and potential implications for therapeutic efficacy.

The exploration of partition dimensions in Efavirenz, Abacavir, Lamivudine, and Doravirine opens doors to a deeper understanding of their molecular behavior. Future research endeavors should continue to build upon these findings, aiming to bridge the gap between structural insights and clinical outcomes, ultimately contributing to the advancement of anti-HIV drug development and therapeutic strategies.

Funding

No funding received for this work

Acknowledgement

The authors express their gratitude to the reviewers for their insightful comments, which helped this paper to be presented in a better way.

Conflicts of interest

There is no conflict of interest disclosed by the authors.

References

1. B. D. Shree, R. Jagadeesh, and Siddabasappa, "Application of topological indices of tenofovir chemical structures for the cure of HIV/AIDS patients," *Turkish Journal of Computer and Mathematics Education (TURCOMAT)*, vol. 12, pp. 1693–1706, 2021.
2. H. Ann, K. H. Kim, H. Y. Choi, H. H. Chang, S. H. Han, K. H. Kim, J. S. Lee, Y. S. Kim, K. H. Park, and Y. K. Kim, "Safety and efficacy of ziagen (abacavir sulfate) in HIV-infected Korean patients," *Infection chemotherapy*, vol. 49, pp. 205–212, 2017.
3. T. H. Pham, M. A. Xiao, M. A. Principe, A. Wong, and T. Mesplede, "Pharmaceutical, clinical, and resistance information on doravirine, a novel nonnucleoside reverse transcriptase inhibitor for the treatment of HIV-1 infection," *Drugs in context*, vol. 9, 2020.
4. R. Quercia, C. F. Perno, J. Koteff, K. Moore, C. McCoig, M. S. Clair, and D. Kuritzkes, "Twenty-five years of lamivudine current and future use for the treatment of HIV-1 infection," *Journal of Acquired Immune Deficiency Syndromes*, vol. 78, no. 2, pp. 125–135, 2018.
5. N. Y. Rakhmanina and J. N. Van den Anker, "Efavirenz in the therapy of HIV infection," *Expert Opin Drug Metab Toxicol*, vol. 6, pp. 95–103, 2010.
6. A. E. Rock, J. Lerner, and M. E. Badowski, "Doravirine and its potential in the treatment of HIV," *An Evidence-Based Review of the Emerging Data, HIV/AIDS (Auckland, NZ)*, vol. 12, pp. 201–210, 2020.
7. M. Azeem and M. F. Nadeem, "Metric-based resolvability of polycyclic aromatic hydrocarbons," *The European Physical Journal Plus*, vol. 136, no. 395, 2021.
8. Z. Hussain, M. Munir, M. Choudhary, and S. M. Kang, "Computing metric dimension and metric basis of 2d lattice of alpha-boron nanotubes," *Symmetry*, vol. 10, no. 8, 2018.
9. S. Imran, M. K. Siddiqui, and M. Hussain, "Computing the upper bounds for the metric dimension of cellulose network," *Applied Mathematics E-Notes*, vol. 19, pp. 585–605, 2019.
10. M. F. Nadeem, M. Azeem, and A. Khalil, "The locating number of hexagonal Mobius ladder network," *Journal of Applied Mathematics and Computing*, vol. 66, pp. 149–165, 2021.
11. M. Ahsan, Z. Zahid, S. Zafar, A. Rafiq, M. S. Sindhu, and M. Umar, "Computing the edge metric dimension of convex polytopes related graphs," *Journal of Mathematics and Computer Science*, vol. 22, pp. 174–188, 2021.
12. A. Ahmad, M. Baca, and S. Sultan, "Minimal doubly resolving sets of the necklace graph," *Math. Reports*, vol. 20, no. 70, pp. 123–129, 2018.
13. T. Vetrık and A. Ahmad, "Computing the metric dimension of the categorial product of some graphs," *International Journal of Computer Mathematics*, vol. 94, no. 2, pp. 363–371, 2017.
14. A. Ahmad and S. Sultan, "On minimal doubly resolving sets of circulant graphs," *Acta Mechanica Slovaca*, vol. 21, no. 1, pp. 6–11, 2017.
15. M. Imran, A. Ahmad, O. Al-Mushayt, and S. A. U. H. Bokhary, "On the metric dimension of barycentric subdivision of Cayley graphs cay($z_n \oplus z_m$)," *Miskolc Mathematical Notes*, vol. 16, no. 2, pp. 637–646, 2015.
16. J. B. Liu, M. F. Nadeem, and M. Azeem, "Bounds on the partition dimension of convex polytopes," *Combinatorial Chemistry High Throughput Screening*, vol. 25, no. 3, pp. 547–553, 2022.
17. M. Azeem, M. Imran, and M. F. Nadeem, "Sharp bounds on partition dimension of hexagonal Mobius ladder," *Journal of King Saud University-Science*, vol. 34, no. 2, 101779, 2022.
18. N. Mehreen, R. Farooq, and S. Akhter, "On partition dimension of fullerene graphs," *AIMS Mathematics*, vol. 3, no. 3, pp. 343–352, 2018.
19. A. Shabbir and M. Azeem, "On the partition dimension of trihexagonal α-boron nanotube," *IEEE Access*, vol. 9, pp. 55644–55653, 2021.
20. H. M. A. Siddiqui and M. Imran, "Computing the metric and partition dimension of h-naphtalenic and VC_5C_7 nanotubes," *Journal of Opto electronics and Advanced Materials*, vol. 17, pp. 790–794, 2015.
21. H. M. A. Siddiqui and M. Imran, "Computing metric and partition dimension of 2-dimensional lattices of certain nanotubes," *Journal of Computational and Theoretical Nanoscience*, vol. 11, no. 12, pp. 2419–2423, 2014.

22. E. C. Maritz and T. Vetrık, “The partition dimension of circulant graphs,” *Quaestiones Mathematicae*, vol. 41, no. 1, pp. 49–63, 2018.
23. Z. Hussain, S. M. Kang, M. Rafique, M. Munir, U. Ali, A. Zahid, and M. S. Saleem, “Bounds for partition dimension of *M*-wheels,” *Open Physics*, vol. 17, no. 1, pp. 340–344, 2019.
24. Amrullah, E. T. Baskoro, R. Simanjuntak, and S. Uttunggadewa, “The partition dimension of a subdivision of a complete graph,” *International Conference on Graph Theory and Information Security*, vol. 74, pp. 53–59, 2015.
25. C. Wei, M. F. Nadeem, H. M. A.Siddiqui, M. Azeem, J. B. Liu, and A. Khalil, “On partition dimension of some cycle-related graphs,” *Mathematical Problems in Engineering*, vol. 2021, pp. 1–8, 2021.
26. J. Santoso and Darmaji, “The partition dimension of cycle books graph,” *Journal of Physics Conference Series*, vol. 974, no. 012070, 2018.
27. A. Ahmad, A. N. Koam, M. Siddiqui, and M. Azeem, “Resolvability of the starphene structure and applications in electronics,” *Ain Shams Engineering Journal*, vol. 13, no. 2, 101587, 2022.
28. P. J. Slater, “Leaves of Trees,” *Congressus Numerantium*, vol. 14, pp. 549–559 1975.
29. S. Khuller, B. Raghavachari, and A. Rosenfeld, “Landmarks in graphs,” *Discrete applied mathematics*, vol. 70, no. 3, pp. 217–229, 1996.
30. M. U. Romdhini, F. Al-Sharqi, A. Nawawi, A. Al-Quran, and H. Rashmanlou, “Signless Laplacian energy of interval-valued fuzzy graph and its applications,” *Sains Malaysiana*, vol 52, no. 7, pp. 2127–2137, 2023.
31. F. Al-Sharqi1, A. Al-Quran, and M. U. Romdhini, “Decision-making techniques based on similarity measures of possibility interval fuzzy soft environment,” *Iraqi Journal for Computer Science and Mathematics*, vol 4, no. 4, pp. 18–29, 2023.
32. A. H. Alridha1, A. S. Al-Jilawi, and F. H. A. Alsharify, “Review of mathematical modelling techniques with applications in biosciences,” *Iraqi Journal for Computer Science and Mathematics*, vol. 3, no. 1, pp. 135–144, 2022.