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Chemical Invariant Analysis of Drug Structures Using Multi-Criteria Decision-Making Approaches: TOPSIS and SAW

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ABSTRACT: Extensive research in recent years has shown the strong relationship between many physicochemical and biological features, including medication toxicity, melting and boiling points, and topological descriptors of chemical structures. For describing molecular graphs and forecasting these crucial characteristics, topological indices (TIs) have become extremely effective mathematical tools. Chain oxides, chain silicate networks, sheet oxide networks, and sheet silicates are among the molecular drug frameworks whose structural properties are examined in this work using a comprehensive topological analysis.. We measure the molecular complexity and connectivity of these structures using a variety of topological indices, such as the Randić Index, Augmented Zagreb Index, and Forgotten Topological Index (FTI). In addition, we rank and evaluate the molecular designs based on their topological signatures using Multi-Criteria Decision-Making (MCDM) methods, specifically the Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS) and the Simple Additive Weighting (SAW) technique. The results provide light on the relative effectiveness of different indices and frameworks for making decisions when evaluating the pharmacological and chemical properties of possible therapeutic options.

Keywords: Topological indices, Randic index, Zagreb Index, TOPSIS and SAW.

Contents

1 Introduction 1

2 Preliminaries 2

3 Network Structures 3

4 Motivation and Application 6

5 Important Results 6

6 Conclusion 16

1. Introduction

One important contribution is the introduction of mathematical ”graph theory” to chemistry [1]. Chemical graph theory is a branch of graph theory that explores the relationship between chemical compounds and processes. Chemical graph theory states that atoms and bonds are represented by nodes and edges, respectively, in molecules, which are represented as chemical graphs. They illustrate their chemical structures in chem informatics. Predicting (quantitative) structure activity and structural properties, an important subject in chem informatics, is based on similar graph traits. Graph theory allows for the reduction of these graphs to indices or descriptors that reflect the molecular properties. [2]. Topological indices are numerical values linked to chemical composition that are used to relate chemical structure to physical properties, chemical reactivity, and biological activity. Building correlations between molecular graph structures and properties is a popular use for these distance-based graphical indices. The physicochemical characteristics and bioactivity of chemical compounds can be predicted using topological indicators. [3] The rapid advancement of chemical and pharmaceutical processes has led to the production of numerous unique nanomaterials, crystals, and drugs, according to Gao et al. [4]. The load on researchers is increased by the large number of chemical experiments required for the evaluation of these diverse substances. The physical behaviors, chemical characteristics, and biological characteristics of topological molecules, including their melting point, boiling temperature, and drug

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toxicity, are closely linked to their structures, according to Katritzky et al. [5]. Chain oxides, chain silicates, sheet oxides, and sheet silicates all have unique structural arrangements that contribute to their value in a variety of sectors.

One-dimensional chains of oxide ions make up chain oxides, which are frequently observed in transition metals such as molybdenum and vanadium. Chain oxides are frequently used in sensor development, catalysis, and battery technology owing to their high electrical conductivity and redox activities. Their utility in some structural applications may be restricted by their an-isotropic characteristics and potential for mechanical fragility. Single or double chains of silicon-oxygen tetrahedra form chain silicates, also known as isosilicates. Chain silicates, which are found in minerals such as pyroxenes and amphibious, are long-lasting, thermally stable, and are utilized extensively in glass, ceramics, and construction. Low electrical conductivity is their main disadvantage, and some materials, such as asbestos, pose health hazards. Materials such as titanium dioxide (TiO_2) are examples of sheet oxides that have a two-dimensional layered structure. These structures are ideal for environmental applications, including water and air purification, as well as solar cell components, because of their enormous surface area and photo-catalytic qualities. Although they are helpful for batteries and catalysis, inadequate inter-layer bonding may restrict their mechanical strength. Layered silicon-oxygen tetrahedra make up sheet silicates (phyllosilicates), which are the building blocks of minerals, such as mica, talc, and different types of clay. These materials are useful for water treatment, insulation, and cosmetics because they are thermally stable, chemically robust, and have excellent ion-exchange capabilities. The use of certain sheet silicates in applications requiring greater structural integrity may be limited because of their softness and potential for water absorption. The behaviors of various drug architectures, including chain oxides, chain silicate networks, sheet oxide networks, and sheet silicates, were examined in this study using Multi criteria decision-making techniques including TOPSIS and SAW. For the first time, this study uses specific MCDM approaches to rate multiple pharmacological architectures. The TOPSIS ranking approach looks at decision-making issues from both a quantitative and qualitative perspective. More accurate and quick answers to real-world problems are provided by it than by any other MCDM technique. Moreover, this method has the benefits of simplicity, rationality, high processing efficiency, and the capacity to mathematically express the relative performance of each option. However, the simple additive weighting method is one of the most fundamental and popular weighted average techniques. The benefit of this method is that it maintains the relative order of the variables while translating the original data in a proportionate linear fashion. Using the SAW approach requires that the decision matrix be standardized to a scale that is comparable to all other ratings that are currently in use.

2. Preliminaries

If there is a connection between any two vertices in a graph, then the graph's vertex and edge sets are connected. Simply put, a network is a connected graph devoid of loops and many edges. Any graph with atoms at its vertices and bonds between them that indicate an underlying chemical structure is called a chemical graph. Any two vertices in a graph that are connected indicate that the vertex and edge sets of the graph are connected. A network is just a connected graph with numerous edges and no loops. An underlying chemical structure can be inferred from any graph that has atoms at its vertices and bonds between them. Cheminformatics is a relatively new topic that blends chemistry, mathematics, and information science. It uses quantitative structure-property relationships (QSPR) and structure-activity relationships (QSAR) to predict the biological activities and properties of chemical substances. Physical-chemical characteristics and topological indices such the Wiener, Szeged, and Randić indices were used in the QSAR/QSPR investigation. The ABC index and Zagreb index are used to forecast a chemical compound's bioactivity. Topological indices of various graph families have been the subject of extensive research to date, and this research is significant because of their chemical significance. Chemical reactivity, biological activity, and other physico-chemical properties are said to be correlated with chemical structure by a topological index, which is actually a numerical number associated with chemical composition.. The process of transforming a molecular graph into a number that characterizes the network's topology is actually the basis of topological indices.

Randić proposed in 1975 that a graph's topological connectivity index, or RI(G), be defined as the sum of its weights. [6], i.e.,

$$RI\left(G\right)=\sum_{u\,v\in E\left(G\right)}\frac{1}{\sqrt{d_d(u)d_d(v)}}.$$

The "branching index" or "molecular connectivity index" was the initial names given to this measure, which was useful for assessing the extent of branching.. These days, it is frequently called the Randić index [7]. The generic Randić index was created in 1998 by Bollobás and Erdös [8], who extended this index by substituting any real integer for $\frac{-1}{2}$ is

$$RI^{a}\left(G\right)=\sum_{u\,v\in E\left(G\right)}\left[d_d\left(u\right)d_d\left(v\right)\right]^{a} \text{—}(1)$$

Randić showed a relationship between a number of physicochemical parameters and the Randić index [9]. Dvořák et al. [10] recently demonstrated that a new index,
$RI^{'}\left(G\right)$, can be added if$RI\left(G\right)\geq\frac{rad(G)}{2}$, where $rad\left(G\right)$ indicates the radius of G.
Their primary goal was to establish this new index in the following manner:
$RI^{'}\left(G\right)=\sum_{u\,v\in E\left(G\right)}\frac{1}{\max\{d_d(u)d_d(v)\}}$
The improved Zagreb index (AZI), a novel topological metric derived from the ABC index, was proposed recently by Furtula et al. [16] as
$AZI\left(G\right)=\sum_{u\,v\in E\left(G\right)}\left(\frac{d_d(u)d_d(v)}{d_d(u)+d_d(v)-2}\right)^{3}$—(2)
The ABC index is not as predictive as this. He demonstrated how to use the AZI to precisely forecast the heat of formation in octanes and heptanes. [?]. One could conclude that just this index passed the tests of the examination. Therefore, this index should be used when developing quantitative structure–property connections [11]. The forgotten topological index, often known as the F-index, was defined by Gao et al. [12] and is expressed as

$$FI\left(G\right)=\sum_{u\,v\in E\left(G\right)}\left[d_d(u)^{2}+d_d(v)^{2}\right] \text{—}(3)$$

De et al. [13] gave a summary of the fundamental characteristics of the forgotten topological index and showed how it may enhance the physical-chemical application of the Zagreb index.

3. Network Structures

This study examines a number of medication molecular structures in addition to their physiochemical characteristics, such as density, complexity, melting and boiling points, and molecular weight. Its fundamental structure, disaccharide, has a high energy stability [14].
This section's primary goal is to calculate a few topological indices for the chain oxide COX_nmolecular network, as shown in Figure. 1. In [15], Hayat et al. investigated a range of degree-based topological indices for different structures. For additional research on other graph families' topological indices [16,17,18].

It is evident that $G_1=COX_n$contains $3n$ edges and $2n+1$ vertices. A one-dimensional chain of oxide ions, frequently connected by metal cautions, makes up a chain oxide. Although they can be flexible along the chain direction, these structures are often less rigid than networks. The edges of G_1 are divided into three subsets. The number of the three edge kinds is displayed in Table 1. We provide an explicit computation formula for a few of the Chain Oxide indices displayed in Figure:1 based on Table 1.

Table 1: Edge Partitions of Chain oxide

d_u,d_v where $uv\in E\left(G_1\right)$	$(2,2)$	$(2,4)$	$(4,4)$
Number of edges	2	$2n$	$n-2$

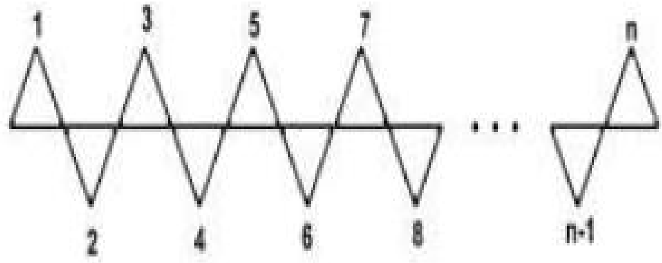

Figure 1: The molecular graph of Chain oxide

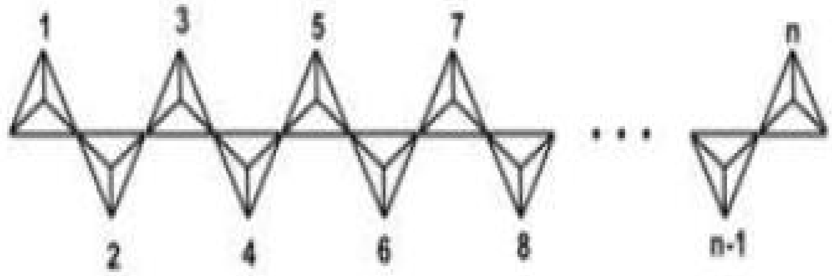

Figure 2: Chain Silicate Network for dimension n

The molecular graph$G_2 = CS_n$, Figure 2: is now under consideration. The facts that $3n+1$ vertices and $6n$ edges are readily apparent.

Silicates with silicon-oxygen tetrahedra forming chains are called isosilicates. There are two main types: Single Chain Silicates: A single chain is formed when two oxygen's are shared by each silicon tetrahedron. Pyroxenes are one example. Double Chain Silicates: Amphiboles and other more complicated structures are created when two single chains are joined by shared oxygen's. Chain silicates are helpful for materials that need strength in one dimension since they are frequently fibrous and strong along the chain axis. We divide G_2 edges into three partitions. The number of the three edge kinds is displayed in Table 2.

Table 2: Edge Partitions of Chain Silicate Network

d_u, d_v where $uv \in E(G_1)$	$(3,3)$	$(3,6)$	$(6,6)$
Number of edges	$n+4$	$2(2n-1)$	$n-2$

The molecular graph$G_3 = OX_n$, Figure:3., is currently under consideration. The fact that $9n^2+3n$ and $18n^2$ is vertices and edges readily apparent.

Metals or other elements act as bridges between the two-dimensional layers of oxide ions that make up sheet oxide networks. By sliding over one another, these layers can produce special qualities. Frequently have good thermal and electrical properties and a layered, sheet-like shape. The edges of G_3 are divided into two partitions. The quantity of the two types of edges is displayed in Table 3.

The molecular graph$G_4 = SL_n$, Figure:4, is currently under consideration. The fact that vertices $15n^2+3n$ and edges $36n^2$ are readily apparent.

Two-dimensional sheets of silicon-oxygen tetrahedra, each sharing three oxygen's with its neighbors,

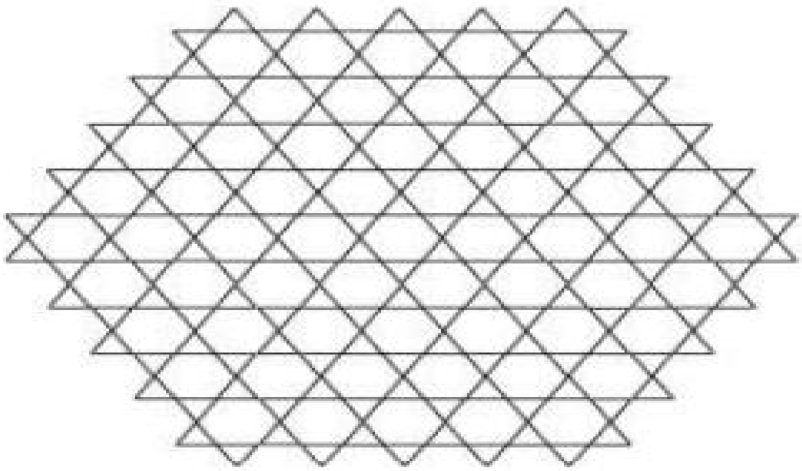

Figure 3: Sheet Oxide Network

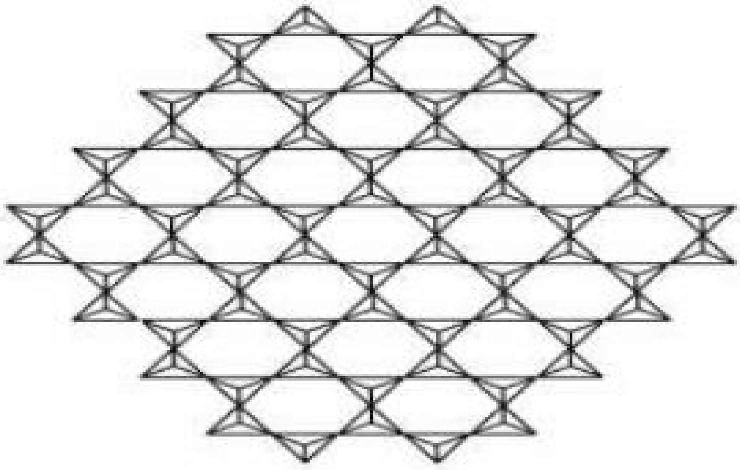

Figure 4: Sheet Silicate

Table 3: Edge Partitions of Sheet Oxide Network

d_u, d_v where $uv \in E(G_1)$	$(2,4)$	$(4,4)$
Number of edges	$12n$	$(18n^2 - 12n)$

are found in phyllosilicates. These configurations provide materials that split readily along the sheet planes because they have weak bonding between sheets but strong bonding in two dimensions. The edges of G_4 are divided into three edge partitions. Table 4 shows the number of two types of edges.

Table 4: Edge Partitions of Sheet Silicate

d_u, d_v where $uv \in E(G_1)$	$(3,3)$	$(3,6)$	$(6,6)$
Number of edges	$6n$	$(18n^2 + 6n)$	$(18n^2 - 12n)$

4. Motivation and Application

They have unique structural properties that make chain oxides, chain silicate networks, sheet oxide networks, and sheet silicates useful in a wide range of fields. The primary uses for each type are as follows:

Oxides in chains: Chain oxides are perfect for fast-charging lithium-ion batteries because they allow for rapid ion transport. Chain oxides can be used as catalysts and catalytic supports because of their stability and surface characteristics. Chain oxides are used more often in ceramics and sensors because they increase electrical conductivity.

Chain Silicate Networks: The thermal stability of chain silicates, such as pyroxenes, makes them suitable for use in heat-resistant ceramics. Rock formation and soil composition depend heavily on pyroclastic and amphibole minerals. Abrasives for cutting, polishing, and grinding are hard inosilicates.

Sheet Oxide Networks: Transistors, resistors, and capacitors all use transition metal sheet oxides. Sheet oxides are perfect for chemical and environmental catalysis because of their layered structure and active sites. Sheet oxides are useful for detecting pollutants because of their high surface area and sensitivity. Sheet Silicates: In cosmetics, talc and mica offer a smooth texture and adhesion. Sheet silicates based on clay are utilized in insulation, cement, tiles, and bricks. Phyllosilicates increase the mineral richness and water retention of soil. Talc is perfect for industrial lubrication because of its layered structure. used to increase durability and heat resistance in rubber, paints, and polymers.

5. Important Results

Theorem 5.1 *Graph, G. Examine chain oxide COX_n's graph G_1 Next, the general randic index represents* $RI^a(G_1) = (32n - 24)^a$

Proof: The General Randic index is $RI^a(G) = \sum\limits_{u\,v \in E(G)} [d_d(u)\, d_d(v)]^a$

$= (|E_1|(2*2) + |E_2|(2*4) + |E_3|(4*4))^a$

$= (2(4) + 2n(8) + (n-2)(16))^a$ $RI^a(G_1) = (32n - 24)^a$

□

Theorem 5.2 *Examine chain oxide COX_n's graph G_1 Next, the Augmented Zagreb index represents* $AZI(G_1) = \frac{944}{27}n - \frac{592}{27}$

Proof: The Augmented Zagreb index is

$AZI(G) = \sum\limits_{u\,v \in E(G)} \left(\frac{d_d(u)d_d(v)}{d_d(u)+d_d(v)-2}\right)^3 = |E_1|\left[\frac{2*2}{2+2-2}\right]^3 + |E_2|\left[\frac{2*4}{2+4-2}\right]^3 + |E_3|\left[\frac{4*4}{4+4-2}\right]^3 = (2)[2]^3 + (2n)[2]^3 + (n-2)\left[\frac{8}{3}\right]^3$ $AZI(G_1) = \frac{944}{27}n - \frac{592}{27}$

□

Theorem 5.3 *Examine chain oxide COX_n's graph G_1 Next, the F-index represents* $FI\left(G_1\right) = 72n - 48$

Proof: The F-index is
$FI\left(G\right) = \sum\limits_{u\,v \in E(G)} \left[d_d(u)^2 + d_d(v)^2\right] = |E_1|\left[2^2 + 2^2\right] + |E_2|\left[2^2 + 4^2\right] + |E_3|\left[4^2 + 4^2\right]$
$= (2)\left[8\right] + (2n)\left[20\right] + (n-2)\left[32\right]$ $FI\left(G_1\right) = 72n - 48$

□

Theorem 5.4 *Examine the chain Silicate Network C_n's graph G_2 .Next the general randic index represents* $RI^a\left(G_2\right) = \left(117n - 72\right)^a$

Proof: The General Randic index is
$RI^a\left(G\right) =$
$\sum\limits_{u\,v \in E(G)} \left[d_d\left(u\right) d_d\left(v\right)\right]^a$

$= \left(|E_1|\left(3*3\right) + |E_2|\left(3*6\right) + |E_3|\left(6*6\right)\right)^a$

$= \left(\left(n+4\right)\left(9\right) + \left(4n-2\right)\left(18\right) + \left(n-2\right)\left(36\right)\right)^a$

$RI^a\left(G_2\right) = \left(117n - 72\right)^a$

□

Theorem 5.5 *Examine the chain Silicate NetworkC_n's graph G_2 .Next the Augmented Zagreb index represents* $AIG\left(G_2\right) = 172.7142\,n - 81.7553$

Proof: The Augmented Zagreb index is
$AZI\left(G\right) = \sum\limits_{u\,v \in E(G)} \left(\frac{d_d(u)d_d(v)}{d_d(u)+d_d(v)-2}\right)^3$

$= |E_1|\left[\frac{3*3}{3+3-2}\right]^3 + |E_2|\left[\frac{3*6}{3+6-2}\right]^3 + |E_3|\left[\frac{6*6}{6+6-2}\right]^3$

$= \left(n+4\right)\left[\frac{9}{4}\right]^3 + \left(4n-2\right)\left[\frac{18}{7}\right]^3 + \left(n-2\right)\left[\frac{18}{5}\right]^3$

$AIG\left(G_2\right) = 172.7142\,n - 81.7553$

□

Theorem 5.6 *Examine the chain Silicate NetworkC_n's graph G_2 .Next the F-index represents* $FI\left(G_2\right) = 270\,n - 162$

Proof: The F-index is
$FI\left(G\right) = \sum\limits_{u\,v \in E(G)} \left[d_d(u)^2 + d_d(v)^2\right]$

$= |E_1|\left[3^2 + 3^2\right] + |E_2|\left[3^2 + 6^2\right] + |E_3|\left[6^2 + 6^2\right]$

$= \left(n+4\right)\left[18\right] + \left(4n-2\right)\left[45\right] + \left(n-2\right)\left[72\right]$

$FI\left(G_2\right) = 270\,n - 162$

□

Theorem 5.7 *Examine the Sheet Oxide NetworkOX_n's graph G_3. Next the general randic index represents* $RI^a\left(G_3\right) = \left(288\, n^2 - 96n\right)^a$

Proof: The General Randic index is
$RI^a\left(G\right) = \sum\limits_{u\, v \in E(G)} \left[d_d\left(u\right) d_d\left(v\right)\right]^a$

$= \left(\left|E_1\right|\left(2*4\right) + \left|E_2\right|\left(4*4\right)\right)^a$

$= \left(\left(12n\right)\left(8\right) + \left(18n^2 - 12n\right)\left(16\right)\right)^a \ RI^a\left(G_3\right) = \left(288\, n^2 - 96n\right)^a$

□

Theorem 5.8 *Examine the Sheet Oxide NetworkOX_n's graph G_3. Next the Augmented Zagreb index represents* $AIG\left(G_3\right) = \frac{1024}{3}\, n^2 - \frac{1184}{9}\, n$

Proof: The Augmented Zagreb index is $AZI\left(G\right) = \sum\limits_{u\, v \in E(G)} \left(\frac{d_d(u) d_d(v)}{d_d(u)+d_d(v)-2}\right)^3 = \left|E_1\right|\left[\frac{2*4}{2+4-2}\right]^3 + \left|E_2\right|\left[\frac{4*4}{4+4-2}\right]^3$
$= \left(12n\right)\left[2\right]^3 + \left(18n^2 - 12n\right)\left[\frac{8}{3}\right]^3 \ AIG\left(G_3\right) = \frac{1024}{3}\, n^2 - \frac{1184}{9}\, n$

□

Theorem 5.9 *Examine the Sheet Oxide NetworkOX_n's graph G_3. Next the F-index represents* $FI\left(G_3\right) = 576\, n^2 - 144\, n$

Proof: The F-index is $FI\left(G\right) = \sum\limits_{u\, v \in E(G)} \left[d_d(u)^2 + d_d(v)^2\right] = \left|E_1\right|\left[2^2 + 4^2\right] + \left|E_2\right|\left[4^2 + 4^2\right]$
$= \left(12\, n\right)\left[20\right] + \left(18n^2 - 12n\right)\left[32\right] \ FI\left(G_3\right) = 576\, n^2 - 144\, n$

□

Theorem 5.10 *Examine the Sheet Oxide NetworkSL_n's graph G_4 .Next the general randic index represents* $RI^a\left(G_3\right) = \left(972n^2 - 270n\right)^a$

Proof: The General Randic index is $RI^a\left(G\right) = \sum\limits_{u\, v \in E(G)} \left[d_d\left(u\right) d_d\left(v\right)\right]^a$
$= \left(\left|E_1\right|\left(3*3\right) + \left|E_2\right|\left(3*6\right) + \left|E_3\right|\left(6*6\right)\right)^a$
$= \left(\left(6n\right)\left(9\right) + \left(18n^2 + 6n\right)\left(18\right) + \left(18n^2 - 12n\right)\left(36\right)\right)^a \ RI^a\left(G_3\right) = \left(972n^2 - 270n\right)^a$

□

Theorem 5.11 *Examine the Sheet Oxide NetworkSL_n's graph G_4 .Next the Augmented Zagreb index represents* $AIG\left(G_4\right) = 1145.8604\, n^2 - 389.5107\, n$

Proof: The Augmented Zagreb index is $AZI\left(G\right) = \sum\limits_{u\, v \in E(G)} \left(\frac{d_d(u) d_d(v)}{d_d(u)+d_d(v)-2}\right)^3$
$= \left|E_1\right|\left[\frac{3*3}{3+3-2}\right]^3 + \left|E_2\right|\left[\frac{3*6}{3+6-2}\right]^3 + \left|E_3\right|\left[\frac{6*6}{6+6-2}\right]^3$
$= \left(6n\right)\left[\frac{9}{8}\right]^3 + \left(18n^2 + 6n\right)\left[\frac{18}{7}\right]^3 + \left(18n^2 - 12n\right)\left[\frac{36}{10}\right]^3$
$AIG\left(G_4\right) = 1145.8604\, n^2 - 389.5107\, n$

□

Theorem 5.12 *Examine the Sheet Oxide Network SL_n's graph G_4 .Next the the F-index represents* $FI\left(G_3\right) = 576\, n^2 - 144\, n$

Proof: The F-index is $FI\,(G) = \sum\limits_{u\,v \in E(G)} \left[d_d(u)^2 + d_d(v)^2 \right]$

$= |E_1| \left[3^2 + 3^2\right] + |E_2| \left[3^2 + 6^2\right] + |E_3| \left[6^2 + 6^2\right]$
$= (6\,n)\,[18] + \left(18n^2 + 6n\right)[45] + \left(18n^2 - 12n\right)[72]$
$FI\,(G_4) = 2106\,n^2 - 486\,n$

□

A behavioral examination of the chemical structures of anticancer medicinal compounds was the goal of the study, which used several topological indices, such as the Randić index and the augmented Zagreb index. Additionally, the omitted invariants are intended to give analysts and scientists a more economical and effective way to use the eleventh topological indices to determine the physical and chemical characteristics of anticancer drugs, respectively. To give researchers and analysts a more effective and economical way to ascertain the physical and chemical characteristics of anticancer drugs, we also included a weighted evaluation of several topological indices in this study. Two distinct decision-making methods were applied to the weighted assessment chemical in order to achieve this. The first method is called Order Preference by Similarity to Ideal Solution (TOPSIS). The best response and the most likely best solution are the main emphasis of this weighted evaluation. Additionally, it evaluates the precision of molecular compound requirements using mathematics. The 1980s saw the introduction of the multicriteria decision-making technique (MCDM).

The weight distribution indicates the percentage of a medication structure that needs to be considered. Medication structures with various physical and chemical characteristics are advantageous. In this case, we assign them more weight than the others, and the others follow suit (see Figure 10). The following formula was used to apportion weight:
$\sum\limits_{I=1}^{J} W_J^{'} = 1$
1. Whether a medication has a positive or negative effect is referred to as its impact. For instance, what are the best and worst physicochemical features of our medication. It is recommended that data values be handled as standard units for a particular factor.
2. Ideal worst and ideal best: To identify the ideal best and ideal worst, we must first describe the characteristics of the medication compounds in question and then compare each drug's physical characteristics with the previously mentioned characteristics. The five typical features of drug structures include density, melting point, boiling temperature, complexity, and molecular weight. A crucial characteristic of pharmaceutical compounds, whether powders or tablets, is their solid density. This makes it easier for us to determine which materials will sink in a liquid. Substances flow when their densities are lower than those of the liquids they are submerged in. [19]. Consequently, our pharmacological structures are best suited for a low density. In the domains of chemical, biological, and medical sciences, the melting point is one essential physical characteristic that characterizes the transition.. Generally, melting points that are lower have a greater chance of being absorbed than those that are higher. The pharmaceutical industry also uses molecular weight as a crucial feature. When the molecular weight of the polymer decreases, the degree of crystallinity increases [20]. Since the molecular weights of the drug structures were less than 1000 g/mol, we selected medications with low molecular weights. A medicine's boiling point is one of its most important characteristics [21].
TOPSIS: Every property is presumed to be evaluated independently. The metric of likeness to the ideal alternative could be used to grade compromises [22]. The n features (augmented Zagreb index, forgotten topological index, and Randić indices) and m options (drug structures) are listed in Table 1.. We gave the attributes the appropriate weights in order to choose the best option and attain balance between them [23].

Step 1: From Table 6's m choices (drug structures) and n features (Randić indices, increased Zagreb index, and forgotten topological index), create a decision matrix by choosing the most crucial characteristics.

Table 5: Calculated values of the indices

$Alternatives$	$RI(a=1)$	AZI	$RI(a=-1)$	FTI	$RI\ a=\frac{-1}{2}$
$Chainoxide$	8	13.037	0.125	24	2.8284
$ChainSlicateNetwork$	45	90.9589	0.0222	108	6.7082
$SheetoxideNetwork$	192	209.777	0.0052	432	13.8564
$SheetSilicate$	702	756.3496	0.00142	1620	26.4952

Table 6: Calculated values of the indices

$Alternatives$	$RI_1(G)$	$AZI(G)$	$RI_{-1}(G)$	$FI(G)$	$RI_{1/2}(G)$
COX_n	8	13.037	0.125	24	2.8284
C_n	45	90.9589	0.0222	108	6.7082
OX_n	192	209.777	0.0052	432	13.8564
SL_n	702	756.3496	0.00142	1620	26.4952

$$D_{ij}=\begin{cases} d_{11}\ \ d_{12}\ ....\ d_{1n} \\ d_{21}\ \ d_{22}\ ....\ d_{2n} \\ . \\ d_{n1}\, d_{n2}\ ....\ d_{mn} \end{cases}$$

Our choice matrix is now being constructed. D_{ij}, that is

Step 2: Refer to Table 7 to determine the normalized choice matrix in relation to the jth attribute (topological indices) and the normalized value of the ith alternative (drug structure). $H_{ij}=\begin{cases} h_{11}\ \ h_{12}\ ....\ h_{1n} \\ h_{21}\ \ h_{22}\ ....\ h_{2n} \\ . \\ h_{n1}\, h_{n2}\ ....\ h_{mn} \end{cases}$

where $H_{ij} = d_{ij}/\sqrt{\sum_{i=1}^{m} d_{ij}^2}\forall j = 1, 2, ...n\ i = 1, 2, ...m$

Step 3: As indicated in Table 8, compute the weighted normalized decision matrix X_{ij} The normalized weighted value appears to be $X_{ij} = W_j^{'} h_{ij}\ \forall j = 1, 2, ...n$ where $\sum_{I=1}^{J} W_J^{'} = 1$

In this case, we give the topological descriptor with the highest ranking the most weight.
$RI_1(G)$ provides tiny numbers for each drug's structure so that we can assign it the lowest weight (0.20). Since $AZI(G)$ values deviate significantly from $RI_1(G)$,
we give it a bit more weight (0.25). We then allocate weight (0.30) if we observe that $RI_{-1}(G)$ values are greater than$FI(G)$. Finally, we assign$RI_{1/2}(G)$, which has the richest values, a maximum weight of (0.30). $W_j^{'} = 0.20,\ 0.25,\ 0.10,\ 0.30,\ 0.15$

To calculate the normalized decision matrix, using the following formula.

Table 7: Normalized Decision Matrix H_{ij}

$Alternatives$	$RI_1(G)$	$AZI(G)$	$RI_{-1}(G)$	$FI(G)$	$RI_{1/2}(G)$
COX_n	0.01097068	0.01649705	0.98370637	0.01428353	0.09191088
C_n	0.06171005	0.11509962	0.17470625	0.06427588	0.21798776
OX_n	0.26329622	0.26545235	0.04092218	0.25710351	0.45027363
SL_n	0.96267680	0.95708671	0.01117490	0.96413815	0.86098048

Table 8: Weighted Normalized Decision Matrix X_{ij}

$Alternatives$	$RI_1\,(G)$	$AZI\,(G)$	$RI_{-1}\,(G)$	$FI\,(G)$	$RI_{1/2}\,(G)$
$Weight$	0.2	0.25	0.1	0.3	0.15
COX_n	0.00219414	0.00412426	0.09837064	0.00428506	0.01378663
C_n	0.01234201	0.02877491	0.01747063	0.01928276	0.03269816
OX_n	0.05265924	0.06636309	0.00409222	0.07713105	0.06754104
SL_n	0.19253536	0.23927168	0.00111749	0.28924145	0.12914707

Table 9: Positive and negative ideal solutions L^+ and L^- are calculated.

$Alternatives$	$RI_1\,(G)$	$AZI\,(G)$	$RI_{-1}\,(G)$	$FI\,(G)$	$RI_{1/2}\,(G)$
$Weight$	0.2	0.25	0.1	0.3	0.15
COX_n	0.00043883	0.00103107	0.00983706	0.00128552	0.00206799
C_n	0.00246840	0.00719373	0.00174706	0.00578483	0.00490472
OX_n	0.01053185	0.01659077	0.00040922	0.02313932	0.01013116
SL_n	0.03850707	0.05981792	0.00011175	0.08677243	0.01937206
$L^+(bestideal)$	0.03850707	0.05981792	0.00983706	0.08677243	0.01937206
$L^-(worstideal)$	0.00043883	0.00103107	0.00011175	0.00128552	0.00206799

$$X_{ij}=\begin{cases} W_1'h_{11} \;\; W_2'h_{12} \;....\; W_n'h_{1n} \\ W_1'h_{21} \;\; W_2'h_{22} \;....\; W_n'h_{2n} \\ . \\ W_1'h_{n1} \;\; W_2'h_{n2} \;....\; W_n'h_{mn} \end{cases}$$

$$X_{ij}=\begin{cases} W_1'h_{11} \;\; W_2'h_{12} \;....\; W_n'h_{1n} \\ W_1'h_{21} \;\; W_2'h_{22} \;....\; W_n'h_{2n} \\ . \\ W_1'h_{n1} \;\; W_2'h_{n2} \;....\; W_n'h_{mn} \end{cases}$$

Step 4: Find the ideal solutions $L^+$and L^- for the positive and negative cases, respectively (Table 9). To calculate the gap between option i and the optimal option, this is described as

$L^+ = \{x_1^+, ...x_n^+\} = (\max\,(or\ \min)\ X_{ij}/j \in J)$ and the difference between option i and the as-defined minimum alternative $L^- = \{x_1^-, ...x_n^-\} = (\min\,(or\ \max)\ X_{ij}/j \in J)$

Step 5: The n-dimensional Euclidean distance given in Table 10 can be used to calculate the separation measurement. Each choice's separation from the optimal choice is provided by $P_i^+ = \sqrt{\sum_{j=1}^{n} \left(X_{ij} - L_j^+\right)^2}$ and $P_i^- = \sqrt{\sum_{j=1}^{n} \left(X_{ij} - L_j^-\right)^2}$

Step 6: Check your position in relation to the ideal solution (Table 11). What is meant by a closeness toA_i a relative proximity to A is

$O_i^* = \frac{P_i^-}{P_i^+ + P_i^-}$ where $0 < O_i^* < 1\,,\ i = 1, 2, ..., n$ It clear that $O_i^* = 1\ if\ L_i = L^+$ and $O_i^* = 0\ if\ L_i = L^-$

Table 10: Calculation the separation measures P_i^+ and P_i^-.

$Alternatives$	$RI_1\,(G)$	$AZI\,(G)$	$RI_{-1}\,(G)$	$FI\,(G)$	$RI_{1/2}\,(G)$	P_i^+	P_i^-
COX_n	0.000438	0.001031	0.009837	0.001285	0.002067	0.1118594	0.0097253
C_n	0.002468	0.007193	0.001747	0.005784	0.004904	0.1044118	0.0085476
OX_n	0.010531	0.016590	0.000409	0.023139	0.010131	0.0829135	0.0297769
SL_n	0.038507	0.059817	0.000111	0.086772	0.019372	0.0097253	0.1118594

Table 11: Relative proximity to the optimal solution computation O_i^*.

P_i^+	P_i^-	O_i^*
0.111859416	0.009725315	0.079987961
0.104411855	0.008547669	0.075670195
0.082913519	0.029776922	0.264236451
0.009725315	0.111859416	0.920012039

Table 12: Rank the alternatives

Alternatives	O_i^*	*Rank*
COX_n	0.079987961	2
C_n	0.075670195	3
OX_n	0.264236451	4
SL_n	0.920012039	1

As a result, the choice with a value nearer 1 is preferred.

Step 7: Based on Table 12's decreasing order of O_i^*, rank the reference order.

SAW: One multi-criteria decision-making (MCDM) or multi-criteria decision analysis tool is the simple additive weighting approach (SAW), also known as the weighted linear combination or scoring 21method [24]. This method is based on the weighted average. The SAW approach was used to calculate the weighted sum of the performance ratings for each alternative across all criteria [25]. Randić, augmented Zagreb, and forgotten topological indices are among the n attributes, whereas drug structures are among the m choices. The compromise ranking algorithm of the SAW method is made up of the following steps.

Step 1: Create the decision matrix in Table 13 using the m alternatives and n attributes.

$$G_{ij}=\begin{cases} g_{11} \; g_{12} \cdots\cdots g_{1n} \\ g_{21} \; g_{22} \cdots\cdots g_{2n} \\ . \\ g_{n1} \; g_{n2} \cdots\cdots g_{mn} \end{cases}$$

and find each attribute's best values g_j^+ and worst g_j^- values of all the attributes $j = 1, 2, ..., n$

Step 2: We determine the weights using the aforementioned weighted criteria. Additionally, use the formula below to create a normalized choice matrixH_{ij}, here m represents alternatives ,n represents qualities in Table 14. $h_{ij} = \frac{g_{ij}}{\max(g_{ij})}$ and $h_{ij} = \frac{\min(g_{ij})}{g_{ij}}$ $i = 1, 2, ..., m$, $j = 1, 2, ..., n$

Step 3: Use the following formula (Table 16) to get each alternative M_i: $M_i = \sum_{j=1}^{n} W_j \, h_{ij}$ where h_{ij} is the score of the ith alternative with respect to the jth attribute, and $W_j$is the weighted criterion of the attributes

Table 13: The decision matrix G_{ij}

Alternatives	$RI_1\,(G)$	$AZI\,(G)$	$RI_{-1}\,(G)$	$FI\,(G)$	$RI_{1/2}\,(G)$
COX_n	8	13.037	0.125	24	2.8284
C_n	45	90.9589	0.0222	108	6.7082
OX_n	192	209.777	0.0052	432	13.8564
SL_n	702	756.3496	0.00142	1620	26.4952
Best (g_j^+)	8	13	0.00142	24	2.8284
Worst (g_j^-)	702	756.3496	0.125	1620	26.4952

Table 14: Normalized decision matrix H_{ij}

Alternatives	$RI_1\,(G)$	$AZI\,(G)$	$RI_{-1}\,(G)$	$FI\,(G)$	$RI_{1/2}\,(G)$
COX_n	0.01097068	0.01649705	0.98370637	0.01428353	0.09191088
C_n	0.06171005	0.11509962	0.17470625	0.06427588	0.21798776
OX_n	0.26329622	0.26545235	0.04092218	0.25710351	0.45027363
SL_n	0.96267680	0.95708671	0.01117490	0.96413815	0.86098048

Table 15: Normalized decision matrix with weights W_j

Alternatives	$RI_1\,(G)$	$AZI\,(G)$	$RI_{-1}\,(G)$	$FI\,(G)$	$RI_{1/2}\,(G)$
Weight	0.2	0.25	0.1	0.3	0.15
COX_n	0.01139601	0.01723674	1.00000000	0.01481481	0.10675141
C_n	0.06410256	0.12026039	0.17760000	0.06666667	0.21798776
OX_n	0.27350427	0.27735455	0.04160000	0.26666667	0.52297775
SL_n	1.00000000	1.00000000	0.01136000	1.00000000	1.00000000

Table 16: Rank the alternatives

Alternatives	M_i	*Rank*
COX_n	0.127045543	4
hline C_n	0.208418972	3
OX_n	0.208463403	2
SL_n	1.340975809	1

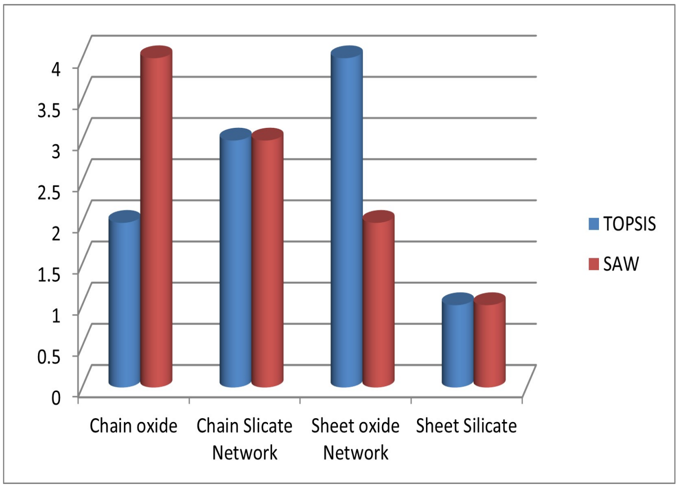

Figure 5: Ranking of TOPSIS and SAW

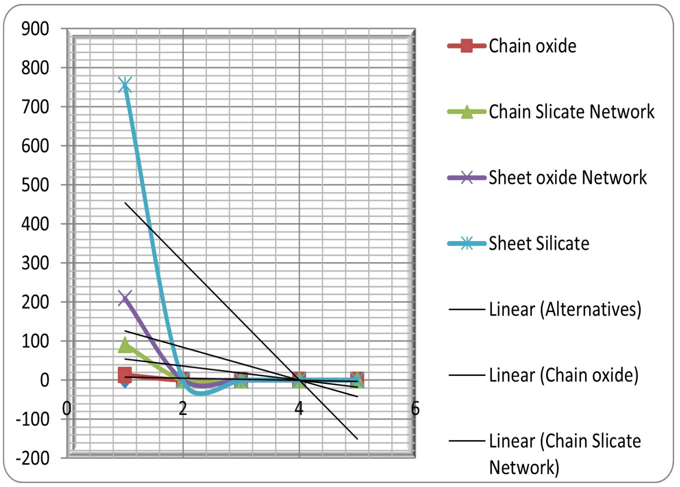

Figure 6: Comparison of alternative using $AZI\,(G)$

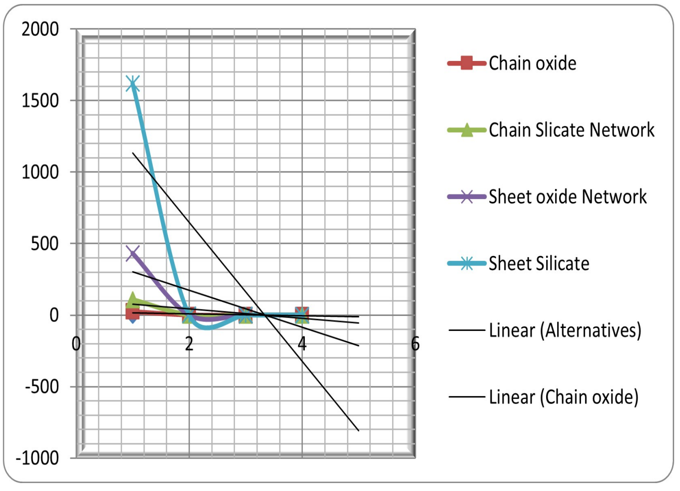

Figure 7: Comparison of alternative using $FI\,(G)$

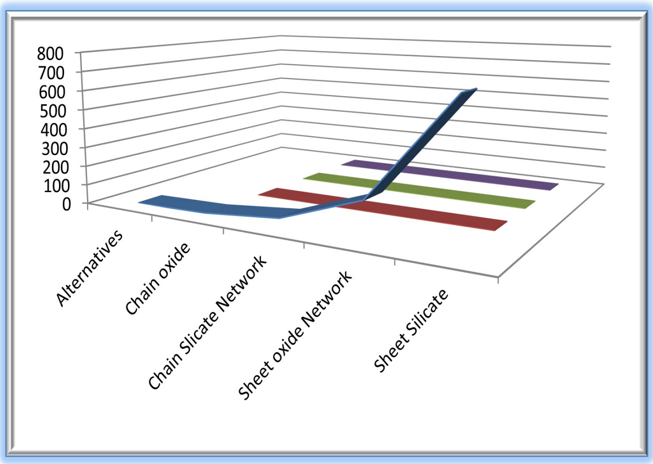

Figure 8: Comparison of alternative using $RI_1(G)$

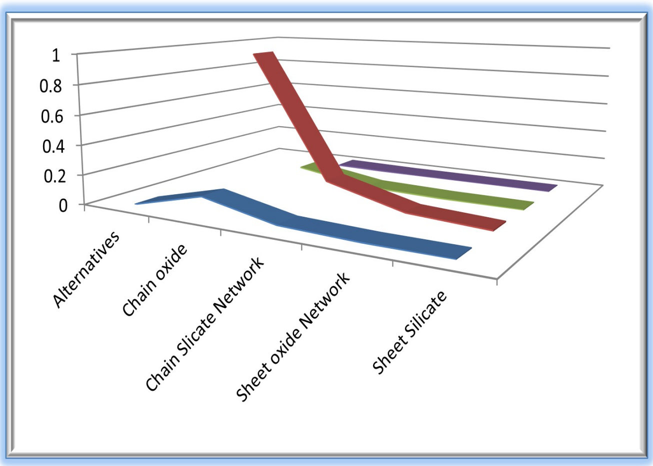

Figure 9: Comparison of alternative using $RI_{-1}(G)$

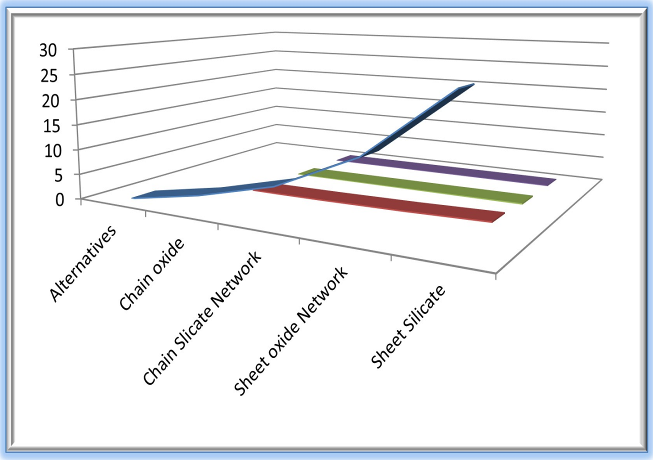

Figure 10: Comparison of alternative using $RI_{1/2}(G)$

6. Conclusion

The molecular structures of medications and their pharmacological and biological properties are closely related, according to a number of drug studies. In this study, utilizing according to the TOPSIS approach, SL_n is the best medication structure since it is closest to the optimal solution. As a result, the drug structures are arranged as follows: OX_n.¿ C_n ¿ COX_n. However, as OX_n and COX_n are ranked opposite in their activities, we have noticed a little altered drug behavior using SAW. The drug structure with the highest ranking in the SAW technique is SL_n. The order of the other structures is COX_n ¿ C_n ¿ OX_n. Additionally, Figures 6–10 show the data plotted using MAPLE and MS Excel, respectively. These theoretical findings could help us understand the topology of the chemical drug structures stated above. As seen in Figure 5, the ranking histogram is produced using Microsoft Excel. These theoretical findings may be useful for rating the drug structures using chemical invariants for future drug evaluations in the domains of medicine, chemistry, drug development, and mathematical chemistry.
Data Availability
The text contains references to the sources utilized in this study.

Conflicts of interest
According to the authors, there are no conflicts of interest.

Author's Contributions
Each author made an equal contribution to this research.

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