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EMPOWERMENTS OF CHEMICAL STRUCTURES USED FOR CURING LUNGS INFECTIONS BY MODERN INVARIANTS

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Abstract

Lungs infection curing medicines can be investigated and improved by Cheminformatics which is a combination of chemistry, computer, and mathematics. Cheminformatics involves graph theory and its tools. Any number that can be uniquely calculated by a graph is known as a graph invariant. In chemical graph theory, chemical compounds are converted into graphs with atoms as vertex and bonds as edges. Many topological indices have been developed for the determination of physical properties of chemical structures of compounds. The study computed newly prepared topological invariants, K-Banhatti Sombor Invariants, Dharwad Invariants, and Quadratic-Contraharmonic Invariants of chemical structures used in lungs infection and corona curing medicine to explore their characteristics such as remdesivir, chloroquine, hydroxychloroquine, and theaflavin. The calculated results are valuable and helpful in understanding the deep physical and chemical behavior of these chemical structures in the human body. These results will also be useful for researchers to understand how these chemical structures can be constructed and improved with different physical and chemical properties.

Keywords: Topological Invariants; K-Banhatti; Sombor Indices; Maple; Network Graph; Molecular Graph; Theaflavin; Chloroquine; Lungs Infection; Hydroxychloroquine; Remdesivir.

1. INTRODUCTION

Corona disease is also a severe form of lungs infection. Coronaviruses are the type of viruses that have crown-like spikes on their surfaces. Two major forms of coronaviruses are found in severe acute respiratory syndrome SARS and Middle East respiratory

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syndrome MERS [1]. In December 2019 a new strain of SARS COV-2 was reported in Wuhan china[2]. The SARS Cov-2 that causes LUNGS INFECTIONenters the human through the mouth, nose and eyes. It moves to the back of nasal passages to the lungs where it multiplies and spreads to other body tissues [3]. COVID-19 symptoms are cough, fever, shortness of breath, headache, loss of taste, sore throat, congestion or runny nose, nausea or vomiting and diarrhea. Symptoms usually appear 1 to 14 days after infection [4]. The most common drugs used in the treatment of LUNGS INFECTIONare chloroquine, hydroxychloroquine, remdesivir and theaflavin. Chloroquine and hydroxychloroquine [5] belong to the same molecular drugs. Both have antiviral potential but Hydroxychloroquine has a better formulation against malaria, and viral infections and is immunity-boosting [6]. Remedisivir is another FDA-approved drug used for the treatment of COVID-19. Theaflavin is a natural product extracted from the plant Black tea. It is a polyphenolic compound and has broad-spectrum antiviral activities against various viruses such as Influenza, hepatitis C, and in vitro against COVI-19. However, it is given intravenously in hospitals [7]. The pharmacological potential of drugs can be assayed through their molecular structures. Recently topological indices or mathematical graph has been used by many researchers in the preparation of synthetic structures and improving statistical features of drugs [8]. As another arising science is developed with the help of computer sciences, mathematics and chemistry called cheminformatics, whose significant segments incorporate Quantitative structure-activity relationship (QSAR) and Quantitative structure-property relationships (QSPR) and the segments can add to the examination of physicochemical characteristics of synthetic mixtures. QSAR is a modeling tool used to solve the topology of networks or structure of compounds and modeled the efficient and best performer networks or structures. QSPR is also a modeling tool which correlates the properties of a network structures with the help of mathematical equation or expression. It also provides the quantitative relationship between properties of networks or chemical structures. Angles of topology in the form of numeric value can be portrayed with the help of graph because of invariant.

In chemical graph theory, chemical compounds are converted into graphs with atoms as vertex and bonds as edges [9]. Many topological indices have been developed for the determination of physical properties of chemical structures of compounds.

This paper first introduces the problem statement with Remdesivir, Chloroquine, Hydroxychloroquine, and Theaflavin Structures. These chemical structures are solved by topological invariants like k-banhatti sombor indices introduced by Gutman in 2021 [10], Quadratic-Contraharmonic indices introduced by V.R Kulli in 2022 [11], and Dharwad indices introduced by V.R Kulli in 2021 [12]. Secondly, review the literature, thirdly discuss the research methodology section, in the fourth section analyze data and in the last section write results and conclude the research. The study has implications in the fields of chemistry, and pharmacy for modeling the purpose of chemical structures, to improve the effectiveness of medications used against corona patients. K-Banhatti Sombor topological invariants and Quadratic- Contraharmonic invariants allow us to accumulate information about algebraic structures and mathematically predict hidden

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properties of various chemical structures such as Remdesivir, Cloroquine, Hydroxychloroquine, and Theaflavin used against corona patients.

2. BACKGROUND

Seven youngsters matured 3 months to 11 years with histologically confirmed interstitial lung illness (ILD) [6 with desquamative interstitial pneumonitis (DIP) and 1 with chronic interstitial pneumonitis] were treated with chloroquine, 10 mg/kg/day. One patient, analyzed late throughout the illness, passed on following three weeks of treatment, in spite of the addition of systemic corticosteroids. Another patient responded to joined therapy with chloroquine and prednisone and had an ordinary lung biopsy following 6 months of treatment. He went through careful fix of mitral valve stenosis and kicked the bucket after broad cerebrum infarction. The other 5 patients responded well to chloroquine therapy with significant improvement in oxygenation inside half a month and in lung function throughout the following couple of months. They stayed well clinically and physiologically, including an ordinary response to gradual activity, during a mean subsequent time of 9.8 years (range 3.5 to 15.7 years). None of the patients has created retinopathy or some other visual complication. Bronchoalveolar lavage was a valuable tool for evaluation of the action of the sickness (prevalence of neutrophils) in 3 out of 4 patients. We propose that chloroquine ought to be considered as a viable treatment in ILD in youngsters. Gradual activity test might be useful for routine development and evaluation of the viability of a particular treatment.

3. LITERATURE REVIEW

Gao et al developed several topological indices for the graphene and chemical compounds used for the treatment of cancer [13]. Kimrani reported topological indices for eight antiviral drugs including lopinavir, ritonavir, arbidol, and thalidomide via M-polynomial and NM-polynomials and performed QSPR and QSAR topological indices to predict the strength of these medicines used for the treatment of LUNGS INFECTION[14].

An outbreak of SARS- CoV-2 originated in Wuhan china in December 2019. The virus spread globally and causes millions of death due to COVID-19 across the world and the World health organization declared this disease a pandemic in March 2020 [15]. This pandemic created a socio-economic burden on societies.WHO has recommended preventive measures to control the spread of the pandemic such as quarantining suspects, the physical distancing of at least 3 ft, frequent hand washing and the use of face masks [16].

Remdesivir is a phosphoramidite product of pyrrole [triazine 4-amino] adenine having an antiviral potential against a wide range of viral infections [17]. The FDA approved this drug for COVID-19 treatment on May 1, 2020. Remdesivir was also approved by the European Commission on July 3, 2020. Remdesivir is a nucleoside that can terminate chain RdRp from SARS COVID-19 and it is reported by Gordon in a study that RdRp is

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the target of remedsivir against MERS- COV and SARS COV-1 strains[18]. Remdesivir can inhibit SARS-CoV-1 and MERS-CoV replication in several *in vitro* studies as reported in primary human airway epithelial cell cultures [19].

Chloroquine is a quinoline that is substituted by a 5-diethylamino pentane-2-2yl amino group at 4 positions and by chlorine at 7 positions.[20] Hydroxychloroquine (HCQ) is derivative of chloroquine (CQ) in which one of the ethyl groups is hydroxylated at position 2. Both drugs have strong antimalarial potential. These are weak bases and increase endosomal pH in host intracellular organelles thereby inhibiting the autophagosome-lysosome fusion and inactivating the enzymes required for viruses' replication. More than 80 clinical trials have been registered worldwide for covid-19 treatment [21].

Theaflavin is a polyphenolic bioflavonoid compound that is 3,4,5-trihydroxybenzocyclohepten-6-one which is substituted at positions 1 and 8 by (2R,3R)-3,5,7-trihydroxy-3,4-dihydro-2H-chromen-2-yl groups. It is a natural product that has strong antioxidant and antimicrobial activities [22]. Jang et al reported theaflavin which is the most active constituent of black tea has inhibitory action against the SARS-Cov-2 virus. Theaflavin can inhibit 3 CL proteases required for coronavirus replication. The IC_{50} calculated was 8.55μg/ml [23].

A topological index is a quantity derived from a graph that reflects relevant structural properties of the underlying molecule. It is, in reality, a numerical number associated with the chemical constitution used to correlate chemical structures with specific physical qualities, chemical reactivity, or biological activity. Various topological indices such as atom-bond connectivity indices, Randi indexes, and geometric arithmetic indices can be used to determine a wide range of variables such as physicochemical properties, thermodynamic properties, chemical activity, and biological activity. We investigate the topological properties of two graphs associated with an algebraic structure in this paper by calculating their Randi index, geometric arithmetic indices, atomic bond connectivity indices, harmonic index, Wiener index, reciprocal complementary Wiener index, Schultz molecular topological index, and Harary index [24].

A topological index is created by converting a chemical structure into a numerical value. It links certain physicochemical features of chemical substances with a molecular structure, such as boiling point, stability, and strain energy (graph). It is a numeric number associated with a chemical structure (graph) that characterizes the structure's topology and is invariant under a structure-preserving mapping.

Metal-organic networks (MONs) are a class of chemical compounds made up of metal ions clusters and organic ligands. These are investigated as one, two, or three-dimensional porous material structures and coordination polymer subclasses. MONs are commonly employed in catalysis to separate and purify gases, as well as conducting solids or super-capacitors. In certain cases, these networks are discovered to be stable throughout the removal or solvent of the guest molecules and may be

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rebuilt using alternative chemical substances. Because of the aforementioned qualities, the physical stability and mechanical aspects of these networks have become a hot issue. Topological indices (TIs) are numerical values that predict the inherent correlations between the physicochemical properties of chemical compounds in their basic network. TIs have an important part in theoretical and environmental chemistry, as well as pharmacology, during MON research. In this research, we compute a variety of recently established degree-based TIs for two separate metal-organic networks with increasing layers of metal and organic ligand vertices. There is also a comparison of the several versions of the TIs that have been generated using numerical values and graphs[25].

A topological descriptor/index (also known as a molecular structure descriptor) is a numerical number connected with a chemical composition that is used to correlate chemical structure/network with physical properties, chemical reactivity, or biological activity. Chemical networks require expressions for their topological properties to have quantitative structure-activity and structure-property relationships. These formulations of topological features are provided by topological indices. Topological descriptors based on valency are the oldest and most effective class of descriptors to date. A chemical graph/network is a depiction of a chemical compound's structural formula, with vertices corresponding to the compound's atoms and edges corresponding to chemical bonds. We investigate valency-based topological indices of chemical networks in this research. We conducted some comparison tests on the performance of practically all well-known valency-based indexes using some real-world data [26].

For any number of reaction steps or a total number of reactions, methods to construct a priori all the finite number of conceivable mechanisms of chemical reactions and/or synthetic routes or thermodynamic cycles, which we describe by generic networks, are presented. kind of animal (reactants, products, catalysts, and intermediates). There are no general networks. Limit the sorts of species that may be used, for example, intermediates can be short-lived, limiting the number of species that can be used. Longer-lived, participating in at least two elementary reaction steps, or shorter-lived, participating in at least two elementary reaction steps in a variety of ways The coefficients of step stoichiometry can be more than unity. Reactants alternatively, or products may operate as catalysts or inhibitors. Topologically, species vertices and the broad networks in which they appear are classed. The networks' topological invariants concerning the number of reaction steps are discovered. Mechanisms having desired properties, such as a specified number of generalized catalysts, chains, auto catalysts, and so on, are created by applying the invariants to gradually greater numbers of reaction steps, starting with the simplest prototypes. Because of their importance in chemical oscillations, dynamical instabilities, and self-replicating reactions, autocatalytic networks are given special attention. The malic acid cycle, glycolysis oscillatory cycles, Lotka-Volterra-Prigogine-Glansdorff models, and others are provided as examples. Common topological property is seen in oscillating and/or self-replicating cycles that

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have been cited in diverse settings. The approaches can also be used in a variety of autocatalytic processes that are important in chemical engineering [27-32].

4. Research Methodology

This systematic study will take existing Remdesivir, Chloroquine, Hydroxychloroquine, and Theaflavin Structures associate them with a graph and solve the topology of the graph with the help of k-banhatti Sombor indices, Quadratic- Contraharmonic index, Dharwad index and its reduced forms. The concerning results in the form of formulas will compare with existing results. These deduced results will be used for the modeling and improvement of the effectiveness of corona medicine. This model is very concerning as it solved the topology of Remdesivir, Chloroquine, Hydroxychloroquine, and Theaflavin Structures in numeric and graphical form and gives accurate results. After analysis, a simulation tool maple is used for the verification and validation of results [33-39].

5. Experimental Results

Remdesivir, Chloroquine, Hydroxychloroquine, and Theaflavin Structures are associated with the graph. These are solved through K-Banhatti sombor index, Contraharmonics-Quadratic index, Dharwad index and their other forms.

$$KBSO(G) = \sum_{ue} \sqrt{d_u{}^2 + d_\varrho{}^2} \quad (1)$$

$$KBSO_{r\varrho\underline{d}}(G) = \sum_{ue} \sqrt{(d_u - 1)^2 + (d_\varrho - 1)^2} \quad (2)$$

Eq. (1) and Eq. (2) show the k-banhatti sombor index and its reduced form which will be used for the solution of Remdesivir, chloroquine, Hydroxychloroquine, and Theaflavin Structures.

$$CQI(G) = \sum_{uv \in E(G)} \frac{\sqrt{2(d_G(u)^2 + d_G(v)^2)}}{d_G(u) + d_G(v)} \quad (3)$$

$$QCI(G) = \sum_{uv \in E(G)} \frac{(d_G(u) + d_G(v))}{\sqrt{2(d_G(u)^2 + d_G(v)^2)}} \quad (4)$$

Eq. (3) and Eq. (4) show the Contraharmonic-Quadratic index and Quadratic-Contraharmonic index which will be used for the solution of corona medicines.

$$D(G) = \sum_{ue} \sqrt{du^3 + dv^3} \quad (5)$$

$$RD(G) = \sum_{ue} \sqrt{(du - 1)^3 + (dv - 1)^3} \quad (6)$$

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Eq. (5) and Eq. (6) show the Dharwad index and its reduced form will also be used for the solution of Remdesivir, Chloroquine, Hydroxychloroquine, and Theaflavin Structures.

Table 1: Edge partition of Remdesivir Network

E	ε (du , dv)	De	ε(du , de)	Recurrence
ε_1	ε(1, 2)	1	ε(1, 1)	2
ε_2	ε(1, 3)	2	ε(1, 2)	5
ε_3	ε(1, 4)	3	ε(1, 3)	2
ε_4	ε(2, 2)	2	ε(2, 2)	9
	ε(2, 3)	3	ε(2, 3)	14
	ε(2, 4)	4	ε(2, 4)	4
	ε(3, 3)	4	ε(3, 4)	6
	ε(3, 4)	5	ε(3, 5)	2

$de = du + dv - 2$

Tab. 1 describes the edge partitions of graph Remdesivir given in Fig. 1.

5.1 Main Results of Remdesivir Network

Figure 1: 3D Molecular Structure of Remdesivir

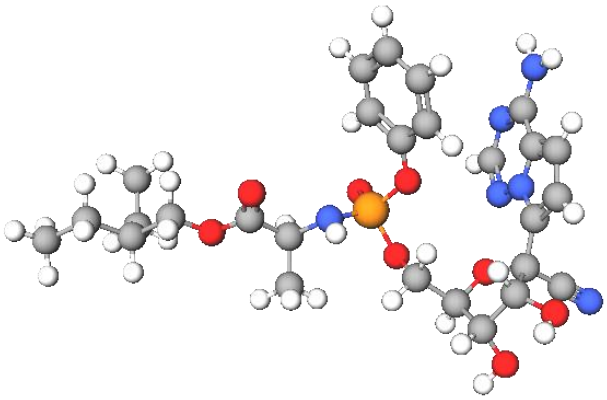

Fig. 1 shows the Remdesivir structure used in lungs infection medicine.

5.1.1 Remdesivir Graph

Let G be a graph of Remdesivir with edge partitions mentioned in Tab. 1.

5.1.2 Theorem 1

Let G be a graph of Remdesivir, then, KBSO and $KBSO_{red}$ indices are

$$KBSO\ (G) = 155.82 \quad (7)$$

$$KBSO_{red}\ (G) = 96.261 \quad (8)$$

Eq. 7 and Eq. 8 represents the proved results of graph of Remdesivir mentioned in the

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Fig. 1.

5.1.3 Investigation of Remdesivir Graphs by K-Banhatti Sombor Indices

Proof

$$KBSO(G) = \sum_{ue} \sqrt{d_u{}^2 + d_\varrho{}^2}$$

KBSO(G)=

$$\sqrt{1^2+1^2}\,(2) + \sqrt{1^2+2^2}\,(5) + \sqrt{1^2+3^2}\,(2) - \sqrt{2^2+2^2}\,(9) + \sqrt{2^2+3^2}\,(14) +$$
$$\sqrt{2^2+4^2}\,(4) + \sqrt{3^2+4^2}\,(6) - \sqrt{3^2+5^2}\,(2)$$

KBSO (G) = 155.82

$$KBSO_{red}(G) = \sum_{ue} \sqrt{(d_u - 1)^2 + (d_\varrho - 1)^2}$$

KBSO$_{red}$ (G) = $\sqrt{(1-1)^2+(1-1)^2}\,(2) + 5\sqrt{(1-1)^2+(2-1)^2}\,(5)$

$$+4\sqrt{(1-1)^2+(3-1)^2}\,(2) + \sqrt{(2-1)^2+(2-1)^2}(9) + \sqrt{(2-1)^2+(3-1)^2}\,(14) +$$
$$5\sqrt{(2-1)^2+(4-1)^2}\,(4)$$
$$+4\sqrt{(3-1)^2+(4-1)^2}\,(6) + \sqrt{(3-1)^2+(5-1)^2}(2)$$

KBSO$_{red}$ (G) =96.26

5.1.4 Theorem 2

Let G be a graph of Remdesivir, then, CQI and QCI indices are

$$CQI(G) = 45.544 \qquad (9)$$

$$QCI(G) = 42.587 \qquad (10)$$

Eq. 9 and Eq. 10 represents the proved results of graph of Remdesivir Structure mentioned in the Fig. 1

$$CQI(G) = \sum_{uv \in E(G)} \frac{\sqrt{2(d_G(u)^2 + d_G(v)^2)}}{d_G(u) + d_G(v)}$$

$$CQI(G) = \frac{\sqrt{2((1)^2+(1)^2)}}{1+1}(2) + \frac{\sqrt{2((1)^2+(2)^2)}}{1+2}(5) + \frac{\sqrt{2((1)^2+(3)^2)}}{1+3}(2) + \frac{\sqrt{2((2)^2+(2)^2)}}{2+2}(9) +$$
$$\frac{\sqrt{2((2)^2+(3)^2)}}{2+3}(14) + \frac{\sqrt{2((2)^2+(4)^2)}}{2+4}(4) + \frac{\sqrt{2((3)^2+(4)^2)}}{3+4}(6) + \frac{\sqrt{2((3)^2+(5)^2)}}{3+5}(2)$$

$$\boldsymbol{CQI(G) = 45.544}$$

$$QCI\ (G) = \sum_{uv \in E(G)} \frac{(d_G(u) + d_G(v))}{\sqrt{2(d_G(u)^2 + d_G(v)^2)}}$$

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$$QCI(G) = \frac{1+1}{\sqrt{2((1)^2+(1)^2)}}(2) + \frac{1+2}{\sqrt{2((1)^2+(2)^2)}}(5) + \frac{1+3}{\sqrt{2((1)^2+(3)^2)}}(2) + \frac{2+2}{\sqrt{2((2)^2+(2)^2)}}(9) + \frac{2+3}{\sqrt{2((2)^2+(3)^2)}}(14) + \frac{2+4}{\sqrt{2((2)^2+(4)^2)}}(4) + \frac{3+4}{\sqrt{2((3)^2+(4)^2)}}(6) + \frac{3+5}{\sqrt{2((3)^2+(5)^2)}}(2)$$

$$\boldsymbol{QCI(G) = 42.587}$$

5.1.5Theorem 3

Let *G* be a graph of Remdesivir, then, *Dharwad* and *Dharwad*$_{red}$ indices are

$$D(G) = 264.52 \quad (11)$$

$$RD(G) = 206.43 \quad (12)$$

5.1.6 Investigation of Remdesivir Graphs by Dharwad Indices

Proof.

$$D(G) = \sum_{ue} \sqrt{du^3 + dv^3}$$

D(G)=

$$\sqrt{1^3+1^3}(2) + \sqrt{1^3+2^3}(5) + \sqrt{1^3+3^3}(2) - \sqrt{2^3+2^3}(9) + \sqrt{2^3+3^3}(14) + \sqrt{2^3+4^3}(4) + \sqrt{3^3+4^3}(6) - \sqrt{3^3+5^3}(2)$$

$$\boldsymbol{D\,(G) = 264.52}$$

$$RD\,(G) = \sum_{ue} \sqrt{(du-1)^3 + (dv-1)^3}$$

RD(G)=

$$\sqrt{(1-1)^3+(1-1)^3}(2) + \sqrt{(1-1)^3+(2-1)^3}(5) + \sqrt{(1-1)^3+(3-1)^3}(2) + \sqrt{(2-1)^3+(2-1)^3}(9) + \sqrt{(2-1)^3+(3-1)^3}(14) + \sqrt{(2-1)^3+(4-1)^3}(4) + \sqrt{(3-1)^3+(4-1)^3}(6) + \sqrt{(3-1)^3+(5-1)^3}(2)$$

$$\boldsymbol{RD\,(G) = 206.43}$$

Table 2: Edge Partition of Chloroquine Structure

ε	ε (du , dv)	De	ε(du , de)	Recurrence
ε_1	$\varepsilon_{(1,2)}$	1	$\varepsilon_{(1,1)}$	2
ε_2	$\varepsilon_{(1,3)}$	2	$\varepsilon_{(1,2)}$	2
ε_3	$\varepsilon_{(2,2)}$	2	$\varepsilon_{(2,2)}$	5
ε_4	$\varepsilon_{(2,3)}$	3	$\varepsilon_{(2,3)}$	12
ε_5	$\varepsilon_{(3,3)}$	4	$\varepsilon_{(3,4)}$	2

Tab. 2 describes the edge partitions of the graph of Chloroquine Structure

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5.2 Main Results of Chloroquine Structure

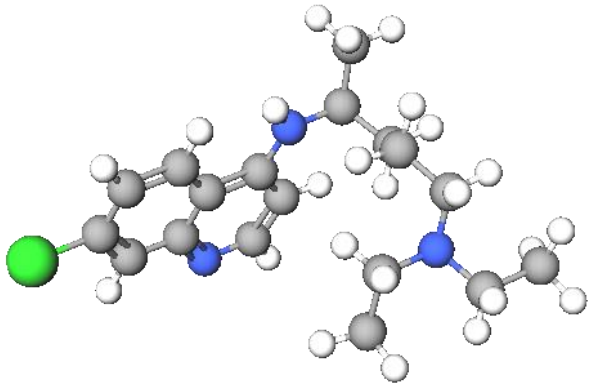

Figure 2: 3D Molecular Structure of Chloroquine

Fig. 2 shows Chloroquine Structure used in lungs infection Medicine.

5.2.1 Chloroquine Structure

Let G be a graph of Chloroquine with edge partitions mentioned in Tab. 2 which provides a detailed description of the edge set.

5.2.2 Theorem 4

Let G be a graph of Cloroquine Structure Then *KBSO* and KB*SO*$_{red}$ are

$$KBSO\ (G)\ = 74.709$$

(13)

$$KBSO_{red}\ (G) = 43.115$$

(14)

Eq. 13 and Eq. 14 represent the proved results of structure of Cloroquine mentioned in the Fig. 3.

5.2.3 Investigation of Cloroquine Structure by K-Banhatti Sombor Indices

Proof

$$KBSO(G) = \sum_{ue} \sqrt{d_u{}^2 + d_\varrho{}^2}$$

$$KBSO\ (G) = \sqrt{1^2 + 1^2}(2) + \sqrt{1^2 + 2^2}(2) + \sqrt{2^2 + 2^2}(5) + \sqrt{2^2 + 3^2}(12) + \sqrt{3^2 + 4^2}(2)$$

$$\boldsymbol{KBSO\ (G) = 74.709}$$

$$KBSO_{r\varrho\underline{d}}\ (G) = \sum_{ue} \sqrt{(d_u - 1)^2 + (d_\varrho - 1)^2}$$

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$KBSO_{red}$ (G) = $\sqrt{(1-1)^2+(1-1)^2}(2)+\sqrt{(1-1)^2+(2-1)^2}(2)+\sqrt{(2-1)^2+(2-1)^2}(5)+\sqrt{(2-1)^2+(3-1)^2}(12)+\sqrt{(3-1)^2+(4-1)^2}(2)$

$$\boldsymbol{KBSO_{red}\,(G)=43.115}$$

5.2.4 Theorem 5

Let G be a graph of Cloroquine Structure then *CQI and QCI* are

$$CQI(G)=23.582 \quad (15)$$

$$QCI(G)=22.453 \quad (16)$$

Eq. 15 and Eq. 16 represent the proven results of the graph of Chloroquine mentioned in Fig. 3

5.2.5 Investigation of Cloroquine Structure by Contrharmonic-Quadratic Indices

Proof

$$CQI(G)=\sum_{uv\in E(G)}\frac{\sqrt{2(d_G(u)^2+d_G(v)^2)}}{d_G(u)+d_G(v)}$$

$$CQI(G)=\frac{\sqrt{2((1)^2+(2)^2)}}{1+2}(2)+\frac{\sqrt{2((1)^2+(3)^2)}}{1+3}(2)+\frac{\sqrt{2((2)^2+(2)^2)}}{2+2}(5)+\frac{\sqrt{2((2)^2+(3)^2)}}{2+3}(12)+\frac{\sqrt{2((3)^2+(3)^2)}}{3+3}(2)$$

$$\boldsymbol{CQI(G)=23.582}$$

$$QCI\ (G)=\sum_{uv\in E(G)}\frac{(d_G(u)+d_G(v))}{\sqrt{2(d_G(u)^2+d_G(v)^2)}}$$

$$CQI(G)=\frac{1+2}{\sqrt{2((1)^2+(2)^2)}}(2)+\frac{1+3}{\sqrt{2((1)^2+(3)^2)}}(2)+\frac{2+2}{\sqrt{2((2)^2+(2)^2)}}(5)\frac{2+3}{\sqrt{2((2)^2+(3)^2)}}(12)+\frac{3+3}{\sqrt{2((3)^2+(3)^2)}}(2)$$

$$\boldsymbol{QCI(G)=22.453}$$

5.2.6 Theorem 6

Let *G* be a graph of Cloroquine, then, *Dharwad* and $Dharwad_{red}$ indices are

$$D\,(G)=264.52 \quad (17)$$

$$RD\,(G)=206.43 \quad (18)$$

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5.2.7 Investigation of Cloroquine Graphs by Dharwad Indices

Proof.

$$D(G) = \sum_{ue} \sqrt{du^3 + dv^3}$$

$$D\ (G) = \sqrt{1^3 + 2^3}\ (2) + \sqrt{1^3 + 3^3}\ (2) + \sqrt{2^3 + 2^3}\ (5) - \sqrt{2^3 + 3^3}\ (12) + \sqrt{3^3 + 3^3}\ (2)$$

$$\boldsymbol{D\ (G) = 122.28}$$

$$RD\ (G) = \sum_{ue} \sqrt{(du - 1)^3 + (dv - 1)^3}$$

$$RD(G) = \sqrt{(1-1)^3 + (2-1)^3}\ (2) + \sqrt{(1-1)^3 + (3-1)^3}\ (2) + \sqrt{(2-1)^3 + (2-1)^3}\ (5) + \sqrt{(2-1)^3 + (3-1)^3}(12) + \sqrt{(3-1)^3 + (3-1)^3}\ (2)$$

$$\boldsymbol{RD\ (G) = 58.728}$$

Table 3: Edge partition of HydroxyChloroquine Structure

ε	ε (du , dv)	de	ε(du , de)	Recurrence
ε_1	$\varepsilon_{(1,2)}$	1	$\varepsilon_{(1,1)}$	2
ε_2	$\varepsilon_{(1,3)}$	2	$\varepsilon_{(1,2)}$	2
ε_3	$\varepsilon_{(2,2)}$	2	$\varepsilon_{(2,2)}$	6
ε_4	$\varepsilon_{(2,3)}$	3	$\varepsilon_{(2,3)}$	12
ε_5	$\varepsilon_{(3,3)}$	4	$\varepsilon_{(3,4)}$	2

Tab. 3 describes the edge partitions of the graph of Hydroxychloroquine Structure given in Fig. 4

5.3 Main Results of Hydroxychloroquine Structure

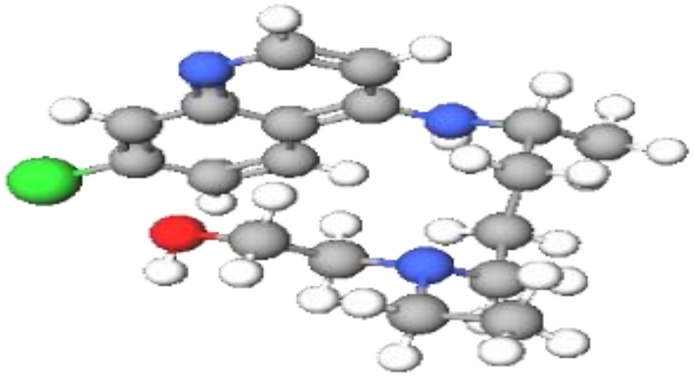

Figure 3: 3D Molecular Structure of HydroxyChloroquine

Fig. 3 shows Hydroxychloroquine Structure used in lungs infection Medicine

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5.3.1 Theorem 7

Let G be a graph of Hydroxychloroquine Structure Then *KBSO* and KB*SO*$_{red}$ are

$$KBSO\ (G)\ = 77.538 \quad (19)$$

$$KBSO_{red}\ (G) = 44.529 \quad (20)$$

Eq. 19 and Eq. 20 represent the proven results of the graph of Hydroxychloroquine Structure mentioned in Fig. 5.

5.3.2 Investigation of Hydroxychloroquine Structure by K-Banhatti Sombor Indices

Proof

$$KBSO(G) = \sum_{ue} \sqrt{{d_u}^2 + {d_\varrho}^2}$$

$$KBSO\ (G) = \sqrt{1^2 + 1^2}(2) + \sqrt{1^2 + 2^2}(2) + \sqrt{2^2 + 2^2}(6) + \sqrt{2^2 + 3^2}(12) + \sqrt{3^2 + 4^2}(2)$$

$$\boldsymbol{KBSO\ (G) = 77.538}$$

$$KBSO_{red}\ (G) = \sum_{ue} \sqrt{(d_u - 1)^2 + (d_\varrho - 1)^2}$$

$$KBSO_{red}\ (G) = \sqrt{(1-1)^2 + (1-1)^2}(2) + \sqrt{(1-1)^2 + (2-1)^2}\ (2) + \sqrt{(2-1)^2 + (2-1)^2}(6) + \sqrt{(2-1)^2 + (3-1)^2}(12) + \sqrt{(3-1)^2 + (4-1)^2}\ (2)$$

$$\boldsymbol{KBSO_{red}\ (G) = 44.529}$$

5.3.3 Theorem 8

Let G be a graph of Hydroxychloroquine Structure Then *Contrharmonic-Quadratic and Quadratic-Contraharmonic Indices* are

$$CQI(G) = 24.582 \quad (21)$$

$$QCI(G) = 23.453 \quad (22)$$

Eq. 21 and Eq. 22 represent the proven results of the graph of Hydroxychloroquine mentioned in Fig. 4

$$CQI(G) = \sum_{uv \in E(G)} \frac{\sqrt{2(d_G(u)^2 + d_G(v)^2)}}{d_G(u) + d_G(v)}$$

$$CQI(G) = \frac{\sqrt{2((1)^2+(2)^2)}}{1+2}(2) + \frac{\sqrt{2((1)^2+(3)^2)}}{1+3}(2) + \frac{\sqrt{2((2)^2+(2)^2)}}{2+2}(6) + \frac{\sqrt{2((2)^2+(3)^2)}}{2+3}(12) + \frac{\sqrt{2((3)^2+(3)^2)}}{3+3}(2)$$

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$$\boldsymbol{CQI(G) = 24.582}$$

$$QCI\ (G) = \sum_{uv \in E(G)} \frac{(d_G(u)+d_G(v))}{\sqrt{2(d_G(u)^2+d_G(v)^2)}}$$

$$CQI(G) = \frac{1+2}{\sqrt{2((1)^2+(2)^2)}}(2) + \frac{1+3}{\sqrt{2((1)^2+(3)^2)}}(2) + \frac{2+2}{\sqrt{2((2)^2+(2)^2)}}(6)\frac{2+3}{\sqrt{2((2)^2+(3)^2)}}(12) + \frac{3+3}{\sqrt{2((3)^2+(3)^2)}}(2)$$

$$\boldsymbol{QCI(G) = 23.453}$$

5.3.4 Theorem 9

Let *G* be a graph of Hydroxychloroquine, then, *Dharwad* and *Dharwad*$_{red}$ indices are

$$D\ (G) = 126.28 \qquad (23)$$

$$RD\ (G) = 60.142 \qquad (24)$$

5.3.5 Investigation of Hydroxychloroquine Graphs by Dharwad Indices

Proof.

$$D(G) = \sum_{ue} \sqrt{du^3 + dv^3}$$

$$D\ (G) = \sqrt{1^3 + 2^3}\ (2) + \sqrt{1^3 + 3^3}\ (2) + \sqrt{2^3 + 2^3}\ (6) - \sqrt{2^3 + 3^3}\ (12) + \sqrt{3^3 + 3^3}\ (2)$$

$$\boldsymbol{D\ (G) = 126.28}$$

$$RD\ (G) = \sum_{ue} \sqrt{(du-1)^3 + (dv-1)^3}$$

$$RD(G) = \sqrt{(1-1)^3 + (2-1)^3}\ (2) + \sqrt{(1-1)^3 + (3-1)^3}\ (2) + \sqrt{(2-1)^3 + (2-1)^3}\ (6) + \sqrt{(2-1)^3 + (3-1)^3}(12) + \sqrt{(3-1)^3 + (3-1)^3}\ (2)$$

$$\boldsymbol{RD\ (G) = 60.142}$$

Table 4: Edge partition of Theaflavin Structures

ε	ε (du , dv)	de	ε(du , de)	Recurrence
ε_1	$\varepsilon_{(1, 3)}$	2	$\varepsilon_{(1, 2)}$	10
ε_2	$\varepsilon_{(2, 3)}$	3	$\varepsilon_{(2, 3)}$	22
ε_3	$\varepsilon_{(3, 3)}$	4	$\varepsilon_{(3, 4)}$	14

Tab. 4 describes the edge partitions of the graph of theaflavin structures given in Fig. 4 with frequencies.

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5.4 Main Results of Theaflavin Structures

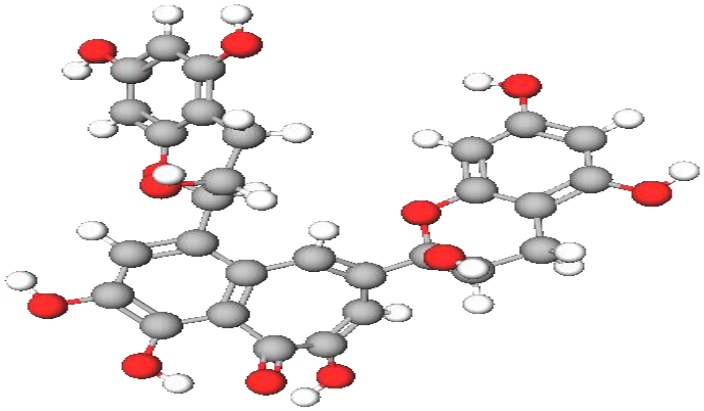

Figure 4: 3D Molecular Structure of Theaflavin

Fig. 4 shows Theaflavin Structures used in lungs infection curing medicine

5.4.1 Theorem 10

Let G be a graph of Theaflavin Structures Then *KBSO* and KB*SO*$_{red}$ are

$$KBSO\,(G) = 171.68 \quad (25)$$

$$KBSO_{red}\,(G) = 109.67 \quad (26)$$

Eq. 25 and Eq. 26 represent the proven results of the graph of Theaflavin Structures mentioned in Fig. 7.

5.4.2 Investigation of Theaflavin Structure by K-Banhatti Sombor Indices

Proof

$$KBSO(G) = \sum_{ue} \sqrt{d_u{}^2 + d_\varrho{}^2}$$

$$KBSO\,(G) = \sqrt{1^2 + 2^2}(10) + \sqrt{2^2 + 3^2}(22) + \sqrt{3^2 + 4^2}(14)$$

$$\boldsymbol{KBSO\,(G) = 171.68}$$

$$KBSO_{r\varrho\underline{d}}\,(G) = \sum_{ue} \sqrt{(d_u - 1)^2 + (d_\varrho - 1)^2}$$

$$KBSO_{red}\,(G) = \sqrt{(1-1)^2 + (2-1)^2}(10) + \sqrt{(2-1)^2 + (3-1)^2}(22) + \sqrt{(3-1)^2 + (4-1)^2}\,(14)$$

$$\boldsymbol{KBSO_{red}\,(G) = 109.67}$$

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5.4.3 Theorem 11

Let G be a graph of Theaflavin Structure Then *Contrharmonic-Quadratic and Quadratic-Contraharmonic Indices* are

$$CQI(G) = 47.616 \quad (27)$$

$$QCI(G) = 44.517 \quad (28)$$

Eq. 27 and Eq. 28 represent the proven results of the graph of Theaflavin mentioned in Fig. 7

$$CQI(G) = \sum_{uv \in E(G)} \frac{\sqrt{2(d_G(u)^2 + d_G(v)^2)}}{d_G(u) + d_G(v)}$$

$$CQI(G) = \frac{\sqrt{2((1)^2+(3)^2)}}{1+3}(10) + \frac{\sqrt{2((2)^2+(3)^2)}}{2+3}(22) + \frac{\sqrt{2((3)^2+(3)^2)}}{3+3}(14)$$

$$\boldsymbol{CQI(G) = 47.616}$$

$$QCI\ (G) = \sum_{uv \in E(G)} \frac{(d_G(u) + d_G(v))}{\sqrt{2(d_G(u)^2 + d_G(v)^2)}}$$

$$CQI(G) = \frac{1+3}{\sqrt{2((1)^2+(3)^2)}}(10) + \frac{2+3}{\sqrt{2((2)^2+(3)^2)}}(22) + \frac{3+3}{\sqrt{2((3)^2+(3)^2)}}(14)$$

$$\boldsymbol{QCI(G) = 44.517}$$

5.4.4 Theorem 12

Let *G* be a graph of Theaflavin, then, *Dharwad* and *Dharwad*$_{red}$ indices are

$$D\ (G) = 285.95 \quad (29)$$

$$RD\ (G) = 150.28 \quad (30)$$

5.4.5 Investigation of Theaflavin Graphs by Dharwad Indices

Proof.

$$D(G) = \sum_{ue} \sqrt{du^3 + dv^3}$$

$$D\ (G) = \sqrt{1^3 + 3^3}\ (10) + \sqrt{2^3 + 2^3}\ (22) + \sqrt{3^3 + 3^3}\ (14)$$

$$\boldsymbol{D\ (G) = 285.95}$$

$$RD\ (G) = \sum_{ue} \sqrt{(du - 1)^3 + (dv - 1)^3}$$

$$RD\ (G) = \sqrt{(1-1)^3 + (3-1)^3}\ (10) + \sqrt{(2-1)^3 + (3-1)^3}(22) + \sqrt{(3-1)^3 + (3-1)^3}\ (14)$$

$$\boldsymbol{RD\ (G) = 150.28}$$

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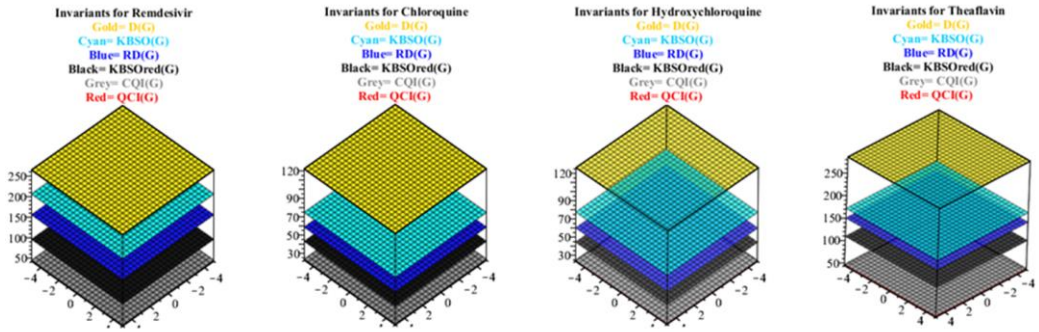

Figure 5: Comparison of Invariants in Context with Coronavirus Medicinal Structures

Fig. 5 shows the contrast between topological invariants dharwad, reduced dharwad, k-banhatti sombor, reduced k-banhatti sombor, Contraharmonic-quadratic and quadratic-contraharmonic when applied to corona medicinal structures.

Table 5: Comparison of Topological Invariants for Corona Medicinal Structures

Lungs Infection medicines / TI's	KBSO	$KBSO_{red}$	CQI	QCI	Dharwad	$Dharwad_{red}$
Remdesivir	155.82	96.261	45.544	42.587	264.52	206.43
Chloroquine	74.709	43.115	23.582	22.453	122.28	58.728
HydroxyChloroquine	77.536	44.529	24.582	23.453	126.28	60.142
Theaflavin	171.68	109.67	47.616	44.517	285.95	150.28

Tab. 5 describes the comparison of topological invariants for medicinal graphs for investigation of different properties like bond strength, sharp upper bounds, lower bounds, boiling, melting points and chemical reactivity, etc**.**

CONCLUSION

TIs have lots of uses and implementations in many fields of computer science, chemistry, biology, informatics, arithmetic, material sciences, and many more. But the utmost significant application is in the non-exact QSPR and QSAR. TIs are associated with the structure of chemical compounds used in lungs infections and corona curing medicines. The study, discusses the k-banhatti sombor invariants, Contraharmonic-Quadratic invariants, Dharwad invariants and their reduced forms which are freshly presented and have numerous prediction qualities for different variants of chemical structures, i.e. Remdesivir, Chloroquine, Hydroxychloroquine and Theaflavin. These deduced results from Eq. 7 to Eq. 30 will be used for the modeling and improvements of chemical structures used in lungs infections and corona curing medicines with different properties also.

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