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EMPOWERMENT OF CHEMICAL STRUCTURE USED IN ANTI-CANCER AND CORONA MEDICINES

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Abstract:

Anti-cancer and Corona medications can be examined and improved by Cheminformatics which is a mix of chemistry, computer, and mathematics. Cheminformatics includes graph theory and its instruments. Any number that can be extraordinarily determined by a graph is known as a graph invariant. In chemical graph theory, chemical compounds are changed over into graphs with atoms as vertex and bonds as edges. Numerous topological lists have been produced for the assurance of actual properties of chemical structures of compounds. The review figured recently pre-arranged topological invariants, K-Banhatti Sombor Invariants, Dharwad Invariants, Quadratic-Contra harmonic Invariants and Irregularity Sombor Index of chemical structures utilized in crown medication to investigate their qualities, for example, hyaluronic corrosive. The determined outcomes are important and supportive in understanding the profound physical and chemical way of behaving of these chemical structures in the human body. These outcomes will likewise be helpful for analysts to understand how these chemical structures can be developed, and improved with various physical, and chemical properties and the viability of corona disease.

Keywords: Topological Invariants; K-banhatti sombor indices; maple; Dharwad invariants; molecular graph; Hyaluronic acid; contra harmonic-quadratic invariants; irregularity sombor index

1. Introduction

Corona viruses are the sort of infections that have crown-like spikes on their surfaces. Two significant types of corona viruses are found in serious intense respiratory conditions SARS and Middle East respiratory disorder MERS [1]. In December 2019 another type of SARS COV-2 was accounted for in Wuhan china [2]. The SARS Cov-2 that causes COVID-19 enters the human through the mouth, nose and eyes. It moves to the rear of nasal entries to the lungs where it duplicates and spreads to other body tissues [3]. Corona virus side effects are a hack, fever, windedness, cerebral pain, loss of taste, sore throat, blockage or runny nose, queasiness or regurgitation and lose bowels. Side effects normally seem 1 to 14 days after disease [4]. The most well-known drug utilized in the treatment of COVID-19

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is hyaluronic acid [5]. It has antiviral potential and a superior detailing against intestinal sickness and viral contaminations and is resistance supporting [6]. It has an expansive range of antiviral exercises against different infections like Influenza, hepatitis C, and in vitro against COVI-19. Nonetheless, it is given intravenously in medical clinics [7]. The pharmacological capability of medications can be examined through their sub-atomic structures. As of late topological indices or numerical graph has been involved by numerous scientists in the planning of engineered structures and working on factual highlights of medications [8]. As one more emerging science is created with the assistance of PC sciences, math and chemistry called cheminformatics, whose critical fragments consolidate Quantitative construction action relationship (QSAR) and Quantitative design property connections (QSPR) and the sections can add to the assessment of physicochemical attributes of manufactured combinations. QSAR is a modeling device used to tackle the geography of networks or construction of compounds and displayed the productive and best entertainer networks or structures. QSPR is likewise a modeling device that connects the properties of an organization's structures with the assistance of numerical conditions or articulation. It likewise gives the quantitative connection between properties of networks or chemical structures. Points of geography as the numeric worth can be depicted with the assistance of a graph on account of invariance.

In chemical graph theory, chemical compounds are changed over into graphs with atoms as vertex and bonds as edges [9]. Numerous topological indices have been created for the assurance of actual properties of chemical structures of compounds.

This paper initially presents the issue of articulation with hyaluronic acid Structure. This chemical construction is addressed by topological invariants like k-banhatti sombor indices presented by Gutman in 2021[10], Quadratic-Contra harmonic indices presented by V.R Kulli in 2022[11], Dharwad indices presented by V.R Kulli in 2021, Irregularity Sombor file presented by V. R. Kulli also[12]. Furthermore, audit the writing, thirdly examine the examination strategy area, in the fourth segment break down information and in the last area compose results and finish up the exploration. The review has suggestions in the fields of chemistry, and drug stores for modeling the motivation behind chemical structures, to work on the adequacy of prescriptions utilized against crown patients. K-Banhatti Sombor topological invariants and Quadratic-Contra harmonic invariants permit us to gather data about arithmetical design and numerically anticipate stowed away properties of different chemical construction, for example, hyaluronic acid utilized against crown patients.

2. BACKGROUND

Curcumin is notable for its enemy of malignant growth viability, and its homegrown properties. The low water solvency that adds to diminished bioavailability is one of the huge impediments of Curcumin. Much accentuation has been centered around polymer-drug forms, basically to sidestep the lower dissolvability of medications and work on the steadiness of medications. This paper examines the topological exploration discoveries on the injury mending viability of Curcumin conjugated with hyaluronic acid (HA), a characteristic polysaccharide accepted to impact the recuperating system. Topological

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indices are basic devices for the examination of these chemical substances to think about the fundamental geography. Topological descriptors are the critical mathematical amounts or invariants in the fields of chemical graph theory. In this paper, we give unequivocal articulations of two as of late characterized novel ev-degrees and ve-degrees and recovered the quantitative shut details for the Zagreb, Randic, mathematical number juggling and particle bond network (ABC) indices for the Curcumin and hyaluronic acid conjugated sub-atomic construction graph in light of ev-degrees and ve-degrees. These sorts of examinations might help figure out the biological way of behaving medications [13].

The study fostered a few topological indices for the graphene and chemical compounds utilized for the therapy of malignant growth [14]. Kimrani detailed topological indices for eight antiviral medications including lopinavir, ritonavir, arbidol, and thalidomide through M-polynomial and NM-polynomials and performed QSPR and QSAR topological indices to anticipate the strength of these prescriptions utilized for the treatment of COVID-19 [15].

An episode of SARS-CoV-2 started in Wuhan china in December 2019. The infection spread universally and makes the huge number of death due to COVID-19 across the world and the World wellbeing association proclaimed this sickness a pandemic in March 2020 [16]. This pandemic made a financial weight on societies. WHO has prescribed preventive measures to control the spread of the pandemic, for example, quarantining suspects, the physical separation of no less than 3 ft, regular hand washing and the utilization of facial coverings [17].

In this paper, we examine the topological indices of Hyaluronic Acid. By building the graph of atomic construction and utilizing the edge apportioning strategy, we decide the overall Randi? index, first and second Zagreb polynomial indices, general total availability index, conventional geometric arithmetic index and general consonant index of Hyaluronic Acid [18].

Chloroquine is a quinoline that is subbed by a 5-diethylamino pentane-2-2yl amino gathering at 4 positions and by chlorine at 7 positions.[19] Hydroxychloroquine (HCQ) is a subsidiary of chloroquine (CQ) in which one of the ethyl bunches is hydroxylated at position 2. The two medications have solid antimalarial potential. These are frail bases and increment endosomal pH in intracellular organelles in this way hindering the autophagosome-lysosome combination and inactivating the proteins expected for infections' replication. More than 80 clinical preliminaries have been enrolled overall for Corona virus treatment [20].

Countless clinical trials have affirmed that the elements of medications have a nearby relationship with their sub-atomic design. Drug properties can be acquired by concentrating on the sub-atomic design of relating drugs. The computation of the topological index of a medication structure empowers researchers to have a superior comprehension of the actual chemistry and biological qualities of medications. In this paper, we center on Hyaluronic Acid-Paclitaxel forms which are generally utilized in the

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production of anticancer medications. A few topological still up in the air by temperance of the edge-parcel strategy, and our outcomes cure the absence of medication tests, in this way giving a hypothetical premise to drug designing [21].

3. LITERATURE REVIEW

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 [22].

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.

Quantitative construction action relationship (QSAR) addresses the quantitative connection of chemical underlying highlights called atomic descriptors and pharmacological movement as reaction endpoints. A topological file is a sub-atomic descriptor widely used to concentrate on the QSAR of drugs to evaluate their atomic qualities by mathematical calculation. Hypothetical appraisal of medication-like particles assists with speeding up the medication plan and disclosure process by justifying the lead distinguishing proof, leadership advancement and figuring out their instrument of activities [23]. Accordingly, in this article, the study has calculated the KBSO invariants, CQIs and Dharwad invariants of Hyaluronic acid-Curcumin forms by utilizing atomic design examination and edge apportioning method. Numerous standard topological indices are gotten as an exceptional instance. The study additionally figured the ISO index of Hyaluronic acid-Curcumin forms from which numerous inconsistencies are found.

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 is commonly employed in catalysis to separate and purify gases, as well as conduct 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 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

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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[24].

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[25].

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 have been cited in diverse settings. The approaches can also be used in a variety of autocatalytic processes that are important in chemical engineering [26].

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4. RESEARCH METHODOLOGY

This systematic study will take the existing hyaluronic acid Structure associate it with a graph and solve the topology of the graph with the help of k-banhatti Sombor indices, Quadratic- Contra harmonic index, Dharwad index,its reduced forms and Irregularity Sombor index. 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 anti-cancer and corona medicine. This model is very concerning as it solved the topology of hyaluronic acid Curcumin structure in numeric and graphical form and gives accurate results. After analysis, a simulation tool maple is used for the verification and validation of results [27].

5. EXPERIMENTAL RESULTS

Hyaluronic acid Curcumin Structure is associated with the graph. This is solved through K-Banhatti sombor index, Contra harmonics-Quadratic index, Dharwad index, their other forms and Irregularity Sombor index.

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

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

Eq. (1) and Eq. (2) show the k-banhatti sombor index and its reduced form which will be used for the solution of hyaluronic acid curcumin structure.

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

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

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

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

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

Eq. (5) and Eq. (6) show the Dharwad index and its reduced form will also be used for the solution of hyaluronic acid curcumin structure.

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$$ISO(G) = \sum_{ue} \sqrt{|du^2 - dv^2|} \qquad (6A)$$

Eq. (6A) shows the Irregularity sombor indexwhich will be used for the solution of hyaluronic acid Curcumin structure and also finds irregularities in the topology of the structure.

Table 1: Edge partition of hyaluronic acid curcumin structure Network

E	ε (du , dv)	De	ε(du , de)	Recurrence
ε_1	ε(1, 2)	1	ε(1, 1)	3n+1
ε_2	ε(1, 3)	2	ε(1, 2)	9n
ε_3	ε(2, 2)	2	ε(2, 2)	5n
ε_4	ε(2, 3)	3	ε(2, 3)	28n
	ε(3, 3)	4	ε(3, 4)	11n-1

de = du + dv – 2

Tab. 1 describes the edge partitions of graph hyaluronic acid curcumin structure given in Fig.1.

5.1 Main Results of Hyaluronic Acid Curcumin Structure Network

Figure1: 3D Molecular Structure of hyaluronic acid curcumin

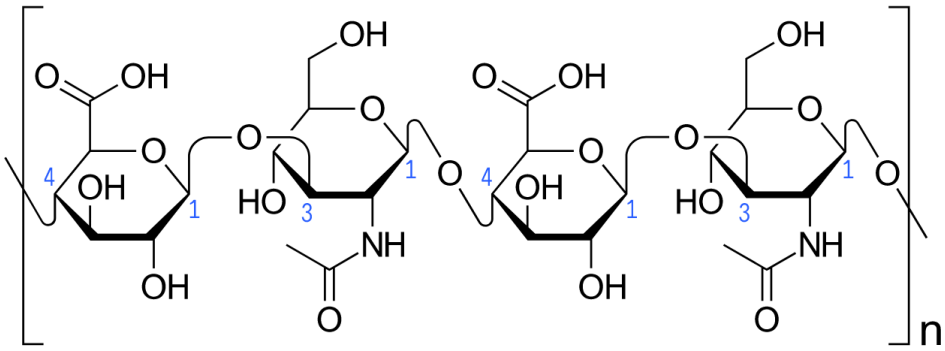

Fig. 1shows the hyaluronic acid curcumin structure used in coronavirus medicine.

5.1.1 Hyaluronic Acid Graph

Let G be a graph of hyaluronic acid curcumin structurewith edge partitions mentioned in Tab. 1.

5.1.2 Theorem 1

Let G be a graph of hyaluronic acid curcumin structure, then, KBSO and $KBSO_{red}$ indices are

$$KBSO\ (G) = \sqrt{2}(3n + 1) + 9\sqrt{5}\ n + 10\sqrt{2}\ n + 28\sqrt{13}\ n + 55n - 5 \qquad (7)$$

$$KBSO_{red}\ (G) = 9n + 28\sqrt{5}\ n + 5\sqrt{2}\ n + \sqrt{13}\ (11n - 1) \qquad (8)$$

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Eq.7 and Eq. 8 represent the proven results of the graph of the hyaluronic acid curcumin structure mentioned in Fig.1 for KBSO indices.

5.1.3 Investigation of Hyaluronic Acid Curcumin Structure Graphs by K-Banhatti Sombor Indices

Proof

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

$$KBSO(G) = \sqrt{1^2 + 1^2}\,(3n+1) + \sqrt{1^2 + 2^2}\,(9n) + \sqrt{2^2 + 2^2}\,(5n) + \sqrt{2^2 + 3^2}\,(28n) + \sqrt{3^2 + 4^2}\,(11n-1)$$

$$\boldsymbol{KBSO\,(G) =} \sqrt{2}\,(3n+1) + 9\sqrt{5}\,n + 10\sqrt{2}\,n + 28\sqrt{13}\,n + 55n - 5$$

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

$$KBSO_{red}(G) = \sqrt{(1-1)^2 + (1-1)^2}\,(3n+1) + 5\sqrt{(1-1)^2 + (2-1)^2}\,(9n)$$

$$+\sqrt{(2-1)^2 + (2-1)^2}(5n) + \sqrt{(2-1)^2 + (3-1)^2}\,(28n) + 4\sqrt{(3-1)^2 + (4-1)^2}\,(11n-1)$$

$$\boldsymbol{KBSO_{red}\,(G) =} 9n + 28\sqrt{5}\,n + 5\sqrt{2}\,n + \sqrt{13}\,(11n-1)$$

Figure 2: KBSO and $KBSO_{red}$ for Hyaluronic Acid Curcumin Structure

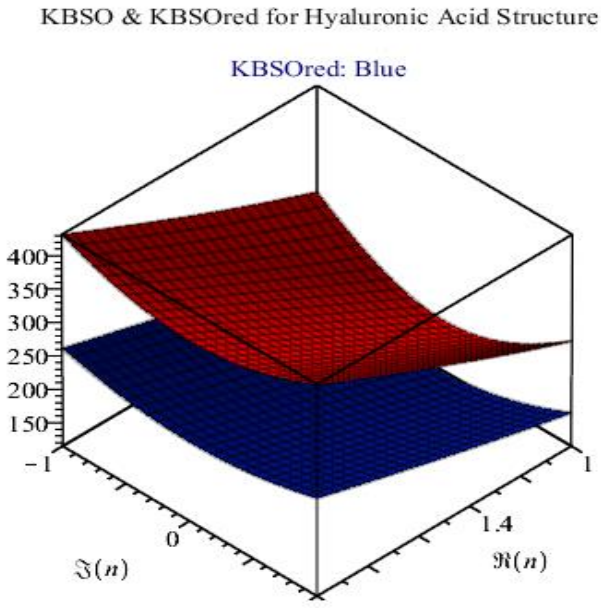

Fig. 2 results show little sharp lower and upper bounds Eq. 7 and Eq. 8 of the KBSO index and its reduced form in red and blue respectively

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5.1.4 Theorem 2

Let G be a graph of hyaluronic acid curcumin structure, then, CQI and QCI indices are

$$\mathrm{CQI(G)} = \frac{\sqrt{10}}{3}(3\mathrm{n}+1) + \frac{\sqrt{5}}{2}(9\mathrm{n}) + 16\mathrm{n} - 1 + \frac{28\sqrt{26}}{5}\mathrm{n} \qquad (9)$$

$$\mathrm{QCI(G)} = \mathbf{3}\frac{\sqrt{10}}{10}(3\mathrm{n}+1) + \frac{18\sqrt{5}}{5}\mathrm{n} + 16\mathrm{n} - 1 + \frac{70\sqrt{26}}{13}\mathrm{n} \qquad (10)$$

Eq. (9) and Eq. (10) represent the proven results of the graph of the hyaluronic acid curcumin structure mentioned in Fig. 1 for the Contra harmonic-quadratic index and its other form.

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

$$CQI(G) = \frac{\sqrt{2((1)^2+(2)^2)}}{1+2}(3\mathrm{n}+1) + \frac{\sqrt{2((1)^2+(3)^2)}}{1+3}(9\mathrm{n}) + \frac{\sqrt{2((2)^2+(2)^2)}}{2+2}(5\mathrm{n}) + \frac{\sqrt{2((2)^2+(3)^2)}}{2+3}(28\mathrm{n}) + \frac{\sqrt{2((3)^2+(4)^2)}}{3+4}(11\mathrm{n}-1)$$

$$\boldsymbol{CQI(G)} = \frac{\sqrt{10}}{3}(3\mathrm{n}+1) + \frac{\sqrt{5}}{2}(9\mathrm{n}) + 16n - 1 + \frac{28\sqrt{26}}{5}\mathrm{n}$$

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

$$QCI(G) = \frac{1+2}{\sqrt{2((1)^2+(2)^2)}}(3\mathrm{n}+1) + \frac{1+3}{\sqrt{2((1)^2+(3)^2)}}(9\mathrm{n}) + \frac{2+2}{\sqrt{2((2)^2+(2)^2)}}(5\mathrm{n}) + \frac{2+3}{\sqrt{2((2)^2+(3)^2)}}(28\mathrm{n}) + \frac{3+4}{\sqrt{2((3)^2+(4)^2)}}(11\mathrm{n}-1)$$

$$\boldsymbol{QCI(G)} = \mathbf{3}\frac{\sqrt{10}}{10}(3\mathrm{n}+1) + \frac{18\sqrt{5}}{5}\mathrm{n} + 16n - 1 + \frac{70\sqrt{26}}{13}\mathrm{n}$$

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Figure 3: CQI and QCI for Hyaluronic Acid Curcumin Structure

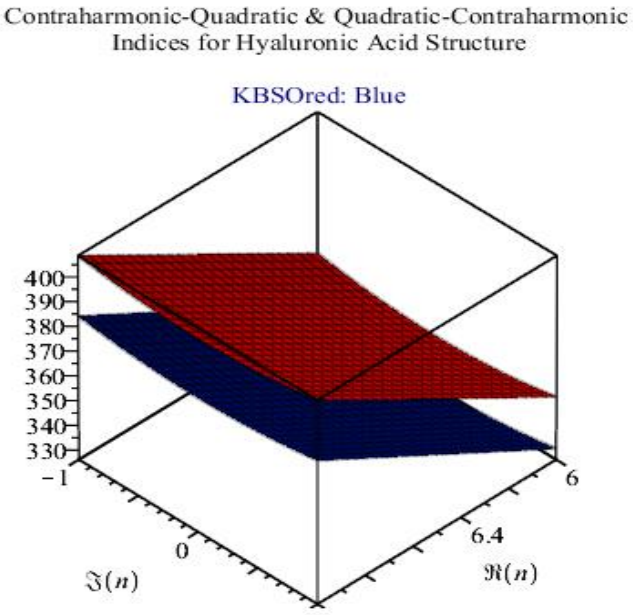

Fig. 3 results show little sharp lower and upper bounds Eq. 9 and Eq. 10 of the KBSO index and its reduced form in red and blue respectively

5.1.5Theorem 3

Let G be a graph of hyaluronic acid structure, then Dharwad and Dharwad$_{red}$ indices are

$$D(G) = 29n + 3 + 18\sqrt{7}\,n + 28\sqrt{35}\,n + 3\sqrt{6}\,(11n - 1) \quad (11)$$

$$RD(G) = 131n - 3 + 23\sqrt{2}n \quad (12)$$

Eq. (11) and Eq. (12) represent the proven results of the graph of the hyaluronic acid curcumin structure mentioned in Fig. 1 for dhrarwad indices

5.1.6 Investigation of Hyaluronic Acid Curcumin Structure Graphs by Dharwad Indices

Proof.

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

$D(G) = \sqrt{1^3 + 2^3}\,(3n+1) + \sqrt{1^3 + 3^3}\,(9n) - \sqrt{2^3 + 2^3}\,(5n) + \sqrt{2^3 + 3^3}\,(28n) + \sqrt{3^3 + 4^3}\,(11n - 1)$

$\boldsymbol{D\,(G) =}\ 29n + 3 + 18\sqrt{7}\,n + 28\sqrt{35}\,n + 3\sqrt{6}\,(11n - 1)$

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

$RD(G) = \sqrt{(1-1)^3 + (2-1)^3}\,(3n+1) + \sqrt{(1-1)^3 + (3-1)^3}\,(9n) + \sqrt{(2-1)^3 + (2-1)^3}(5n) +$

$\sqrt{(2-1)^3 + (3-1)^3}\,(28n) + \sqrt{(3-1)^3 + (4-1)^3}\,(11n - 1)$

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RD (G) = $131n - 3 + 23\sqrt{2}n$

Figure 4: Dharwad and Dharwad$_{red}$ for Hyaluronic Acid Curcumin Structure

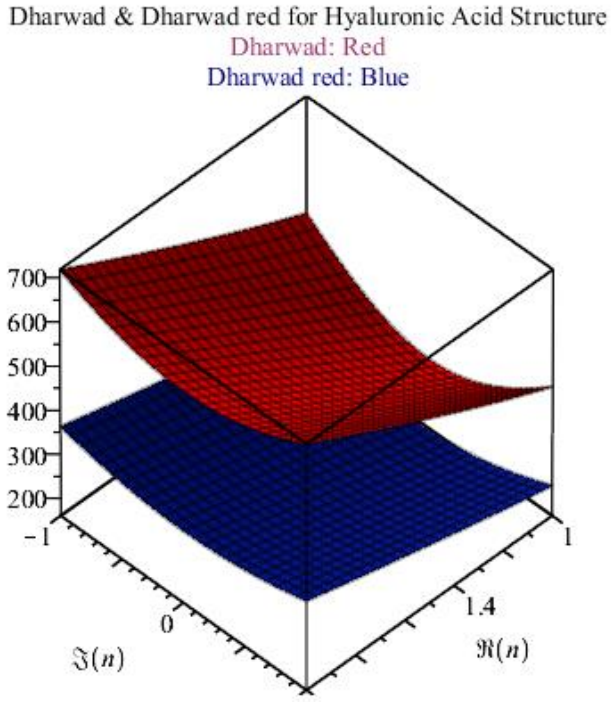

Fig. 4 results show little sharp lower and upper bounds Eq. 11 and Eq. 12 of Dharwad and Dharwad$_{red}$ in red and blue respectively

5.1.6Theorem 4

Let G be a graph of hyaluronic acid curcumin structure, then the Irregularity Sombor index is

ISO (G) = $\sqrt{3}(3n + 1) + 18\sqrt{2}\,n + 28\sqrt{5}\,n$
(13)

Eq. (13) represents the proven result of the graph of the hyaluronic acid curcumin structure mentioned in Fig. 1 for the ISO index.

5.1.7 Investigation of Hyaluronic Acid Curcumin Structure Graphs by Irregularity Sombor Index [28]

Proof.

$ISO(G) = \sum_{ue} \sqrt{|du^2 - dv^2|}$

$ISO(G) = \sqrt{|1^2 - 2^2|}\,(3n + 1) + \sqrt{|1^2 - 3^2|}\,(9n) + \sqrt{|2^2 - 2^2|}\,(5n) + \sqrt{|2^2 - 3^2|}\,(28n) + \sqrt{|3^2 - 4^2|}\,(11n - 1)$

ISO(G) = $\sqrt{3}\,(3n + 1) + 18\sqrt{2}\,n + 28\sqrt{5}\,n$

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Figure 5: Dharwad and Dharwad$_{red}$ for Hyaluronic Acid Curcumin Structure [29]

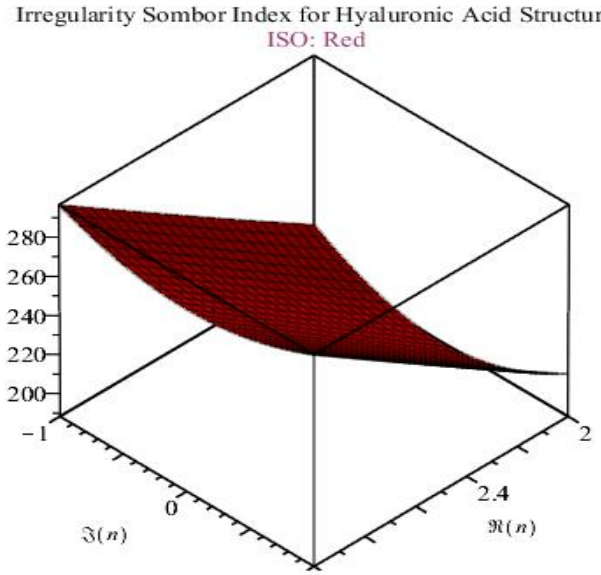

Fig. 5 result shows sharp lower and upper bounds Eq. 13 of ISO index in red color.

6. 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 anti-cancer medicines and corona medicine. The study, discusses the k-banhatti sombor invariants, Contra harmonic-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. hyaluronic acid. In addition, the study also calculated the irregularities found in the structure of hyaluronic acid curcumin with the help of the irregularity sombor index. These deduced results from Eq. 7 to Eq. 11will be used for the modeling and improvements of chemical structures used in anti-cancer and corona medicine with different properties also.

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REFERENCES

1. F. Levi-Schaffer and A. Marco, “Coronavirus disease 2019 and the revival of passive immunization: Antibody therapy for inhibiting severe acute respiratory syndrome coronavirus 2 and preventing host cell infection: IUPHAR review 31,” Br J Pharmacol, vol. 178, no. 17, pp. 3359–3372, Sep. 2021, doi: 10.1111/bph.15359.

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2. “Academic Journals.” https://journals.tubitak.gov.tr/medical/abstract.htm?id=27222 (accessed Apr. 30, 2022).
3. D. Kumar, “Corona Virus: A Review of COVID-19,” EJMO, 2020, doi: 10.14744/ejmo.2020.51418.
4. “Attributes and predictors of Long-COVID: analysis of COVID cases and their symptoms collected by the Covid Symptoms Study App - UCL Discovery.” https://discovery.ucl.ac.uk/id/eprint/10113906/ (accessed Apr. 30, 2022).
5. “Full article: Old and re-purposed drugs for the treatment of COVID-19.” https://www.tandfonline.com/doi/full/10.1080/14787210.2020.1771181 (accessed Apr. 30, 2022).
6. “Efficacy of chloroquine and hydroxychloroquine in the treatment of COVID-19. | Eur Rev Med Pharmacol Sci;24(8): 4539-4547, 2020 04. | MEDLINE.” https://search.bvsalud.org/global-literature-on-novel-coronavirus-2019-ncov/resource/es/covidwho-202585 (accessed Apr. 30, 2022).
7. “Remdesivir for Treatment of COVID-19: Combination of Pulmonary and IV Administration May Offer Aditional Benefit | SpringerLink.” https://link.springer.com/article/10.1208/s12248-020-00459-8 (accessed Apr. 30, 2022).
8. “Predicting potential drug-drug interactions on topological and semantic similarity features using statistical learning.” https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0196865 (accessed Apr. 30, 2022).
9. “Chemical Graph Theory | Nenad Trinajstic | Taylor & Francis Group.” https://www.taylorfrancis.com/books/mono/10.1201/9781315139111/chemical-graph-theory-nenad-trinajstic (accessed Apr. 30, 2022).
10. Faculty of Science, University of Kragujevac, Kragujevac, Serbia and I. Gutman, “Some basic properties of Sombor indices,” Open J. Discret. Appl. Math., vol. 4, no. 1, pp. 1–3, Dec. 2021, doi: 10.30538/psrp-odam2021.0047.
11. V. Kulli, “CONTRAHARMONIC QUADRATIC INDEX OF CERTAIN NANOSTAR DENDRIMERS,” vol. 13, pp. 1–7, Jan. 2022.
12. V. R. Kulli, “Dharwad index,” International Journal of Engineering Sciences and Research Technology, vol. 10, no. 4, pp. 17–21, 2021.
13. A. Rauf, B. Akram, M. Ishtiaq, and M. K. Siddiqui, “Topological Properties of Curcumin and Hyaluronic Acid Conjugated Molecular Structure: An Anti-Cancer Drug,” Polycyclic Aromatic Compounds, vol. 0, no. 0, pp. 1–14, Dec. 2021, doi: 10.1080/10406638.2021.2014530.
14. W. Gao, W. Wang, and M. R. Farahani, “Topological Indices Study of Molecular Structure in Anticancer Drugs,” Journal of Chemistry, vol. 2016, p. e3216327, Mar. 2016, doi: 10.1155/2016/3216327.
15. S. A. K. Kirmani, P. Ali, and F. Azam, “Topological indices and QSPR/QSAR analysis of some antiviral drugs being investigated for the treatment of COVID-19 patients,” International Journal of Quantum Chemistry, vol. 121, no. 9, p. e26594, 2021, doi: 10.1002/qua.26594.
16. A. L. García-Basteiro et al., “Monitoring the COVID-19 epidemic in the context of widespread local transmission,” The Lancet Respiratory Medicine, vol. 8, no. 5, pp. 440–442, May 2020, doi: 10.1016/S2213-2600(20)30162-4.
17. K. McIntosh, “Coronavirus disease 2019 (COVID-19): Epidemiology, virology, and prevention,” p. 31, 2019.
18. P. Ali, S. A. K. Kirmani, O. Al Rugaie, and F. Azam, “Degree-based topological indices and polynomials of hyaluronic acid-curcumin conjugates,” Saudi Pharmaceutical Journal, vol. 28, no. 9, pp. 1093–1100, Sep. 2020, doi: 10.1016/j.jsps.2020.07.010.

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19. PubChem, “Hydroxychloroquine.” https://pubchem.ncbi.nlm.nih.gov/compound/3652 (accessed Apr. 30, 2022).
20. R. E. Ferner and J. K. Aronson, “Chloroquine and hydroxychloroquine in covid-19,” BMJ, vol. 369, p. m1432, Apr. 2020, doi: 10.1136/bmj.m1432.
21. L. Zheng, Y. Wang, and W. Gao, “Topological Indices of Hyaluronic Acid-Paclitaxel Conjugates’ Molecular Structure in Cancer Treatment,” Open Chemistry, vol. 17, no. 1, pp. 81–87, Jan. 2019, doi: 10.1515/chem-2019-0009.
22. C.-C. Wei et al., “Some Topological Invariants of Graphs Associated with the Group of Symmetries,” Journal of Chemistry, vol. 2020, pp. 1–13, Mar. 2020, doi: 10.1155/2020/6289518.
23. S. A. K. Kirmani, P. Ali, F. Azam, and P. A. Alvi, “On Ve-Degree and Ev-Degree Topological Properties of Hyaluronic Acid-Anticancer Drug Conjugates with QSPR,” Journal of Chemistry, vol. 2021, p. e3860856, Jul. 2021, doi: 10.1155/2021/386085
24. G. Hong, Z. Gu, M. Javaid, H. M. Awais, and M. K. Siddiqui, “Degree-Based Topological Invariants of Metal-Organic Networks,” IEEE Access, vol. 8, pp. 68288–68300, 2020, doi: 10.1109/ACCESS.2020.2985729.
25. M. C. Shanmukha, N. S. Basavarajappa, K. C. Shilpa, and A. Usha, “Degree-based topological indices on anticancer drugs with QSPR analysis,” Heliyon, vol. 6, no. 6, p. e04235, Jun. 2020, doi: 10.1016/j.heliyon.2020.e04235.
26. J. C. Xavier, W. Hordijk, S. Kauffman, M. Steel, and W. F. Martin, “Autocatalytic chemical networks at the origin of metabolism,” Proceedings of the Royal Society B: Biological Sciences, vol. 287, no. 1922, p. 20192377, Mar. 2020, doi: 10.1098/rspb.2019.2377.
27. H. Khalid, M. W. Iqbal, A. U. R. Virk, M. U. Ashraf, A. M. Alghamdi et al., “K-Banhatti sombor invariants of certain computer networks,” Computer. Materials and Continua., vol. 73, no. 1, pp. 15, 2022.
28. A. Virk, shamas Bilal, and K. Hamid, “Irregularity invariants for chemical structures used in the treatment of COVID-19,” SIR, vol. 4, no. 1, pp. 38-60, 2020.
29. K. Hamid, M. W. Iqbal, H. A. B. Muhammad, Z. Fuzail, Z. T. Ghafoor, et al., “Detection of Brain Tumor from Brain MRI Images with the Help of Machine Learning & Deep Learning,” International Journal of Computer Science and Network Security,vol. 22 no. 5 pp. 709-721, 2022.