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Topological Invariants for the Chemical Structures Used in Treatment of COVID-19

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Abstract

A topological index is a quantity expressed as a number that help us to catch symmetry of chemical compounds. With the help of quantitative structure property relationship (QSPR), we can guess physical and chemical properties of several chemical compounds. Here, we will compute Shingali & Kanabour, Gourava and hype Gourava indices for the chemical compounds, used in treatment of COVID-19, namely Remdesivir, Chloroquine, Hydroxychloroquine Theaflavin.

Keywords: Topological indices, Gourava index, COVID-19.

1. Introduction

Historically, epidemics of multiple infectious diseases with millions dying have been recorded in the past few centuries. The most terrific was pandemics due to the plague, flu, cholera etc. Currently, the COVID-19 pandemic is disrupting human health and the economy around the world. It is originated in a Wuhan [1] seafood market but has rapidly spread in and beyond China. As of 3 April 2020, there were 1116643 confirmed cases, including 59158 deaths worldwide (as per world meter information). The novel corona virus (2019-nCoV) is a betacoronavirus and shares genetic sequence and viral structure with severe acute respiratory syndrome coronavirus (SARS-CoV), and Middle East respiratory syndrome coronavirus (MERS-CoV). No specific medication for the new disease is currently available. It is therefore urgent to identify appropriate antiviral agents to combat the pathogen. An effective experiment to drug discovery is to test whether existing antiviral drugs are efficient in the treatment of related viral diseases. Researchers tested some existing antiviral agents [2–6] and got positive results to inhibit the infection and transmission of the 2019-nCoV in vitro. Some of these antiviral compounds are remdesivir (GS5734), chloroquine, hydroxychloroquine, and theaflavin. Remdesivir is a nucleotide analog drug having broad spectrum activity developed to prevent Ebola virus infection [7]. It is also highly efficient to prevent 2019-nCoV in vitro [2]. The clinical trial is currently underway in several hospitals and tests on efficacy are awaited. Chloroquine is a broadspectrum antiviral drug [8, 9] effective for treating malaria and autoimmune disease. Many randomized controlled trials were performed to assess the impact of chloroquine in the treatment of COVID-19. Therapeutic results in terms of fever control, enhanced CT imaging and delayed disease progression have been reported. Hydroxychloroquine has antiviral activity very similar to that of chloroquine. Both exhibit immune modulating activity, which can improve their antiviral effect in vivo. As per Forbes report in 30 March 2020, FDA approves chloroquine and hydroxychloroquine for emergency coronavirus treatment. Hydroxychloroquine reduce the acute evolution of COVID-19 by suppressing the cytokine storm by inhibiting T cell activation. Theaflavin, a polyphenol chemical in black tea, is found liable for the medical benefit of black tea. Theaflavin has shown a wide range of antiviral activity against many viruses, including influenza A, B and hepatitis C viruses [10,11]. In [4], it is found that theaflavin may be used as a lead compound for the production of an inhibitor of 2019-nCoV. In pharmaceutical drug design, information related to physicochemical properties, biological activities of molecular graph of compounds is necessary. These properties can be predicted without using any weight lab by a well-known tool of chemical graph theory known as topological index.

A special number, in graph theoretical term, representing a molecular structure, is known as topological descriptor. A topological descriptor when correlates with a molecular property, it can be determine as graph-theoretic index or topological index. The First and second Zagreb indices are the oldest molecular descriptors invented in 1975 by Gutman [12] and their properties are extensively investigated. They are defined as:

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v).$$

$$M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v).$$

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Shingali & Kanabour in [13] introduce the following topological indices,

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}$$

$$R'(G) = \sum_{uv \in E(G)} \frac{1}{max\{d_u, d_v\}}$$

$$AG_1(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{2\sqrt{d_u \times d_v}}$$

$$SK(G) = \sum_{uv \in E(G)} \frac{d_2 + d_v}{2}$$

$$SK_1(G) = \sum_{uv \in E(G)} \frac{d_2 \times d_v}{2}$$

$$SK_2(G) = \sum_{uv \in E(G)} \left(\frac{d_2 + d_v}{2}\right)^2$$

In 2017, Kulli [15] introduce the the idea of Gourava indices as,

$$GO_1(G) = \sum_{uv \epsilon E(G)} [(d_u + d_v) + (d_u \times d_v)]$$

$$GO_1(G) = \sum_{uv \epsilon E(G)} [(d_u + d_v) \times (d_u \times d_v)]$$

In [16] Kulli introduce the idea of hyper Gourava indices as,

$$HGO_1(G) = \sum_{uv \epsilon E(G)} [(d_u + d_v) + (d_u \times d_v)]^2$$

$$HGO_1(G) = \sum_{uv \epsilon E(G)} [(d_u + d_v) \times (d_u \times d_v)]^2$$

For more about topological invariants one can find out detail [17–28].

2. Main Results

Here, we will Shingali & Kanabour, Gourava and hyper Gourava indices for chemical structures used for the treatment of COVID-19 namely, Remdesivir, chloroquine, hydroxychloroquine and theaflavin in four different sections.

2.1 Shingali & Kanabour, Gourava and hyper Gourava indices for Remdesivir

The graph of Remdesivir given in Figure 1. There are eight type of edges are present in the graph of Remdesivir. The degree based edge partition is given in Table 1.

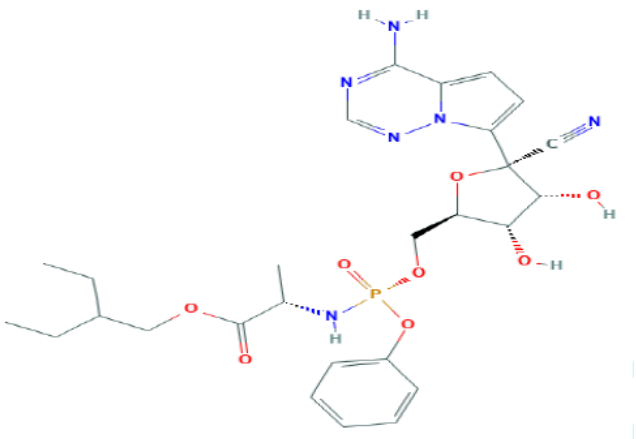

Figure 1: Graph of Remdesivir

(d_u, d_v)	Frequency
(1,2)	2
(1,3)	5
(1,4)	2
(2,2)	9
(2,3)	14
(2,4)	4
(3,3)	6
(3,4)	2

Table 1: Partition of $E(Remdesivir)$

Theorem 2.1. *Let G be the graph of Remdesivir. The Shingali & Kanabour indices for Remdesivir are.*

1. $\chi(G) = 20.12$.
2. $R'(G) = 15.82$.
3. $AG_1(G) = 46.58$.
4. $SK(G) = 108$.
5. $SK_1(G) = 128.5$.
6. $SK_2(G) = 275$.

Proof.

$$\begin{aligned}
1.\ \chi(G) &= \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}} \\
&= \left(\frac{1}{\sqrt{1+2}}\right)(2) + \left(\frac{1}{\sqrt{1+3}}\right)(5) + \left(\frac{1}{\sqrt{1+4}}\right)(2) \\
&\quad \left(\frac{1}{\sqrt{2+2}}\right)(9) + \left(\frac{1}{\sqrt{2+3}}\right)(14) + \left(\frac{1}{\sqrt{2+4}}\right)(4) \\
&\quad + \left(\frac{1}{\sqrt{3+3}}\right)(6) + \left(\frac{1}{\sqrt{3+4}}\right)(2) \\
&= 20.12.
\end{aligned}$$

$$\begin{aligned}
2.\ R'(G) &= \sum_{uv\in E(G)} \frac{1}{max\{d_u, d_v\}} \\
&= \left(\frac{1}{2}\right)(2) + \left(\frac{1}{3}\right)(5) + \left(\frac{1}{4}\right)(2) \\
&\quad + \left(\frac{1}{2}\right)(9) + \left(\frac{1}{3}\right)(14) + \left(\frac{1}{4}\right)(4) \\
&\quad + \left(\frac{1}{3}\right)(6) + \left(\frac{1}{4}\right)(2) \\
&= 15.82.
\end{aligned}$$

$$\begin{aligned}
3.\ AG_1(G) &= \sum_{uv\in E(G)} \frac{d_u + d_v}{2\sqrt{d_u \times d_v}} \\
&= \left(\frac{1+2}{2\sqrt{1\times 2}}\right)(2) + \left(\frac{1+3}{2\sqrt{1\times 3}}\right)(5) + \left(\frac{1+4}{2\sqrt{1\times 4}}\right)(2) \\
&\quad + \left(\frac{2+2}{2\sqrt{2\times 2}}\right)(9) + \left(\frac{2+3}{2\sqrt{2\times 3}}\right)(14) + \left(\frac{2+4}{2\sqrt{2\times 4}}\right)(4) \\
&\quad + \left(\frac{3+3}{2\sqrt{3\times 3}}\right)(6) + \left(\frac{3+4}{2\sqrt{3\times 4}}\right)(2) \\
&= 46.58.
\end{aligned}$$

$$4.\ SK(G) = \sum_{uv\in E(G)} \frac{d_u + d_v}{2}$$

$$
\begin{aligned}
&= \left(\frac{1+2}{2}\right)(2) + \left(\frac{1+3}{2}\right)(5) + \left(\frac{1+4}{2}\right)(2) \\
&\quad + \left(\frac{2+2}{2}\right)(9) + \left(\frac{2+3}{2}\right)(14) + \left(\frac{2+4}{2}\right)(4) \\
&\quad + \left(\frac{3+3}{2}\right)(6) + \left(\frac{3+4}{2}\right)(2) \\
&= 108.
\end{aligned}
$$

$$
\begin{aligned}
5.\ SK_1(G) &= \sum_{uv \in E(G} \frac{d_u \times d_v}{2} \\
&= \left(\frac{1\times 2}{2}\right)(2) + \left(\frac{1\times 3}{2}\right)(5) + \left(\frac{1\times 4}{2}\right)(2) \\
&\quad + \left(\frac{2\times 2}{2}\right)(9) + \left(\frac{2\times 3}{2}\right)(14) + \left(\frac{2\times 4}{2}\right)(4) \\
&\quad + \left(\frac{3\times 3}{2}\right)(6) + \left(\frac{3\times 4}{2}\right)(2) \\
&= 128.5.
\end{aligned}
$$

$$
\begin{aligned}
6.\ SK_2(G) &= \sum_{uv \in E(G)} \left(\frac{d_u + d_v}{2}\right)^2 \\
&= \left(\frac{1+2}{2}\right)^2(2) + \left(\frac{1+3}{2}\right)^2(5) + \left(\frac{1+4}{2}\right)^2(2) \\
&\quad + \left(\frac{2+2}{2}\right)^2(9) + \left(\frac{2+3}{2}\right)^2(14) + \left(\frac{2+4}{2}\right)^2(4) \\
&\quad + \left(\frac{3+3}{2}\right)^2(6) + \left(\frac{3+4}{2}\right)^2(2) \\
&= 275.
\end{aligned}
$$

□

Theorem 2.2. *Let G be the graph of Remdesivir. Then the Gourava and hyper Gourava indices for Remdesivir are*

1. $GO_1(G) = 473$.
2. $GO_2(G) = 1360$.
3. $HGO_1(G) = 5583$.
4. $HGO_2(G) = 57320$.

Proof.

$$
\begin{aligned}
1.\ GO_1(G) &= \sum_{uv \epsilon E(G)} [(d_u + d_v) + (d_u \times d_v)] \\
&= [(1+2)+(1\times 2)](2) + [(1+3)+(1\times 3)](5) + [(1+4)+(1\times 4)](2) \\
&\quad + [(2+2)+(2\times 2)](9) + [(2+3)+(2\times 3)](14) + [(2+4)+(2\times 4)](4) \\
&\quad + [(3+3)+(3\times 3)](6) + [(3+4)+(3\times 4)](2) \\
&= 473.
\end{aligned}
$$

$$
\begin{aligned}
2.\ GO_2(G) &= \sum_{uv \in E(G)} [(d_u + d_v) \times (d_u \times d_v)] \\
&= [(1+2)\times(1\times 2)](2) + [(1+3)\times(1\times 3)](5) + [(1+4)\times(1\times 4)](2) \\
&\quad + [(2+2)\times(2\times 2)](9) + [(2+3)\times(2\times 3)](14) + [(2+4)\times(2\times 4)](4) \\
&\quad + [(3+3)\times(3\times 3)](6) + [(3+4)\times(3\times 4)](2) \\
&= 1360.
\end{aligned}
$$

$$
3.\ HGO_1(G) = \sum_{uv \in E(G)} [(d_u + d_v) + (d_u \times d_v)]^2
$$

$$
\begin{aligned}
&= [(1+2)+(1\times 2)]^2(2)+[(1+3)+(1\times 3)]^2(5)+[(1+4)+(1\times 4)]^2(2)\\
&\quad +[(2+2)+(2\times 2)]^2(9)+[(2+3)+(2\times 3)]^2(14)+[(2+4)+(2\times 4)]^2(4)\\
&\quad +[(3+3)+(3\times 3)]^2(6)+[(3+4)+(3\times 4)]^2(2)\\
&= 5583.
\end{aligned}
$$

4. $$
\begin{aligned}
HGO_2(G) &= \sum_{uv\in E(G)} [(d_u+d_v)\times(d_u\times d_v)]^2\\
&= [(1+2)\times(1\times 2)]^2(2)+[(1+3)\times(1\times 3)]^2(5)+[(1+4)\times(1\times 4)]^2(2)\\
&\quad +[(2+2)\times(2\times 2)]^2(9)+[(2+3)\times(2\times 3)]^2(14)+[(2+4)\times(2\times 4)]^2(4)\\
&\quad +[(3+3)\times(3\times 3)]^2(6)+[(3+4)\times(3\times 4)]^2(2)\\
&= 57320.
\end{aligned}
$$

□

2.2 Shingali & Kanabour, Gourava and hyper Gourava indices for Chloroquine

The graph of Chloroquine given in Figure 2. There are five type of edges are present in the graph of Chloroquine. The degree based edge partition is given in Table 2.

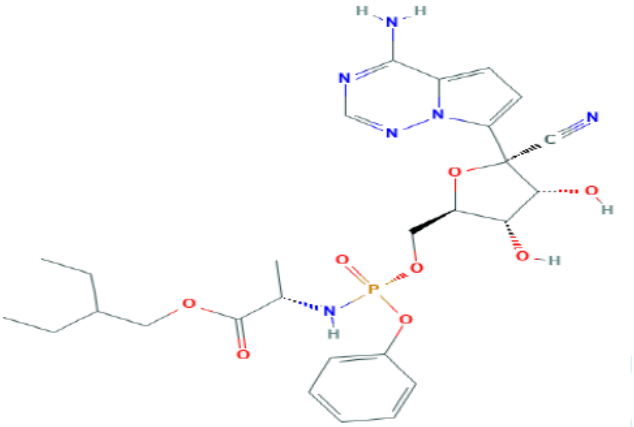

Figure 2: Graph of Chloroquine

(d_u, d_v)	Frequency
(1,2)	2
(1,3)	2
(2,2)	5
(2,3)	12
(3,3)	2

Table 2: Partition of $E(Chloroquine)$

Theorem 2.3. *Let G be the graph of Chloroquine. The Shingali & Kanabour indices for Chloroquine are.*

1. $\chi(G) = 10.83$.
2. $R'(G) = 5.66$.
3. $AG_1(G) = 23.67$.
4. $SK(G) = 53$.
5. $SK_1(G) = 60$.
6. $SK_2(G) = 125.5$.

Proof.

$$
\begin{aligned}
1.\ \chi(G) &= \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}} \\
&= \left(\frac{1}{\sqrt{1+2}}\right)(2) + \left(\frac{1}{\sqrt{1+3}}\right)(2) + \left(\frac{1}{\sqrt{2+2}}\right)(5) \\
&\quad + \left(\frac{1}{\sqrt{2+3}}\right)(12) + \left(\frac{1}{\sqrt{3+2}}\right)(2) \\
&= 10.83.
\end{aligned}
$$

$$
\begin{aligned}
2.\ R'(G) &= \sum_{uv\in E(G)} \frac{1}{max\{d_u, d_v\}} \\
&= \left(\frac{1}{2}\right)(2) + \left(\frac{1}{3}\right)(2) + \left(\frac{1}{2}\right)(5) \\
&\quad + \left(\frac{1}{12}\right)(6) + \left(\frac{1}{2}\right)(2) \\
&= 5.66.
\end{aligned}
$$

$$
\begin{aligned}
3.\ AG_1(G) &= \sum_{uv\in E(G)} \frac{d_u + d_v}{2\sqrt{d_u \times d_v}} \\
&= \left(\frac{1+2}{2\sqrt{1\times 2}}\right)(2) + \left(\frac{1+3}{2\sqrt{1\times 3}}\right)(2) + \left(\frac{2+2}{2\sqrt{2\times 2}}\right)(5) \\
&\quad + \left(\frac{2+3}{2\sqrt{2\times 3}}\right)(12) + \left(\frac{3+3}{2\sqrt{3\times 3}}\right)(2) \\
&= 23.67.
\end{aligned}
$$

$$
\begin{aligned}
4.\ SK(G) &= \sum_{uv\in E(G)} \frac{d_u + d_v}{2} \\
&= \left(\frac{1+2}{2}\right)(2) + \left(\frac{1+3}{2}\right)(2) + \left(\frac{2+2}{2}\right)(5) \\
&\quad + \left(\frac{2+3}{2}\right)(12) + \left(\frac{3+3}{2}\right)(2) \\
&= 53.
\end{aligned}
$$

$$
\begin{aligned}
5.\ SK_1(G) &= \sum_{uv\in E(G} \frac{d_u \times d_v}{2} \\
&= \left(\frac{1\times 2}{2}\right)(2) + \left(\frac{1\times 3}{2}\right)(2) + \left(\frac{2\times 2}{2}\right)(5) \\
&\quad + \left(\frac{2\times 3}{2}\right)(12) + \left(\frac{3\times 3}{2}\right)(2) \\
&= 60.
\end{aligned}
$$

$$
\begin{aligned}
6.\ SK_2(G) &= \sum_{uv\in E(G)} \left(\frac{d_u + d_v}{2}\right)^2 \\
&= \left(\frac{1+2}{2}\right)^2(2) + \left(\frac{1+3}{2}\right)^2(2) + \left(\frac{2+2}{2}\right)^2(5) \\
&\quad + \left(\frac{2+3}{2}\right)^2(12) + \left(\frac{3+3}{2}\right)^2(2) \\
&= 125.5.
\end{aligned}
$$

□

Theorem 2.4. *Let G be the graph of Chloroquine. Then the Gourava and hyper Gourava indices for Chloroquine are*

1. $GO_1(G) = 454$.
2. $GO_2(G) = 584$.

3. $HGO_1(G) = 2370$.

4. $HGO_2(G) = 18272$.

Proof.

$$
\begin{aligned}
1.\ GO_1(G) &= \sum_{uv \epsilon E(G)} [(d_u + d_v) + (d_u \times d_v)] \\
&= [(1+2)+(1\times 2)](2) + [(1+3)+(1\times 3)](2) + [(2+2)+(2\times 2)](5) \\
&\quad +[(2+3)+(2\times 3)](12) + [(3+3)+(3\times 3)](2) \\
&= 454.
\end{aligned}
$$

$$
\begin{aligned}
2.\ GO_2(G) &= \sum_{uv \in E(G)} [(d_u + d_v) \times (d_u \times d_v)] \\
&= [(1+2)\times(1\times 2)](2) + [(1+3)\times(1\times 3)](2) + [(2+2)\times(2\times 2)](5) \\
&\quad +[(2+3)\times(2\times 3)](12) + [(3+3)\times(3\times 3)](2) \\
&= 584.
\end{aligned}
$$

$$
\begin{aligned}
3.\ HGO_1(G) &= \sum_{uv \in E(G)} [(d_u + d_v) + (d_u \times d_v)]^2 \\
&= [(1+2)+(1\times 2)]^2(2) + [(1+3)+(1\times 3)]^2(2) + [(2+2)+(2\times 2)]^2(5) \\
&\quad +[(2+3)+(2\times 3)]^2(12) + [(3+3)+(3\times 3)]^2(2) \\
&= 2370.
\end{aligned}
$$

$$
\begin{aligned}
4.\ HGO_2(G) &= \sum_{uv \in E(G)} [(d_u + d_v) \times (d_u \times d_v)]^2 \\
&= [(1+2)\times(1\times 2)]^2(2) + [(1+3)\times(1\times 3)]^2(2) + [(2+2)\times(2\times 2)]^2(5) \\
&\quad +[(2+3)\times(2\times 3)]^2(12) + [(3+3)\times(3\times 3)]^2(2) \\
&= 18272.
\end{aligned}
$$

□

2.3 Shingali & Kanabour, Gourava and hyper Gourava indices for Hydroxychloroquine

The graph of Hydroxychloroquine given in Figure 3. There are five type of edges are present in the graph of Hydroxychloroquine. The degree based edge partition is given in Table 3.

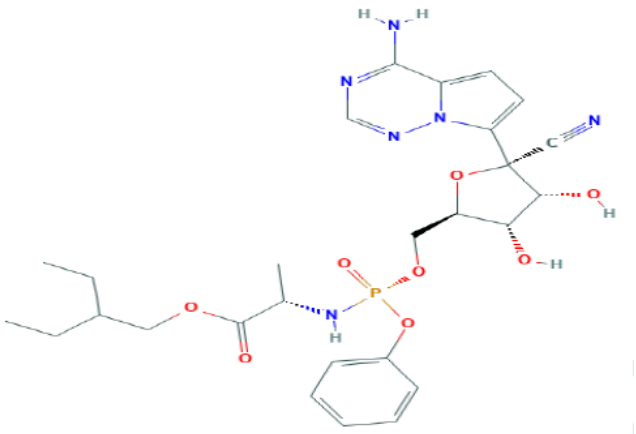

Figure 3: Graph of Hydroxychloroquine

Theorem 2.5. *Let G be the graph of Hydroxychloroquine. The Shingali & Kanabour indices for Hydroxychloroquine are.*

1. $\chi(G) = 11.33$.

(d_u, d_v)	Frequency
(1,2)	2
(1,3)	2
(2,2)	6
(2,3)	12
(3,3)	2

Table 3: Partition of $E(Hydroxychloroquine)$

2. $R'(G) = 6.16$.

3. $AG_1(G) = 24.67$.

4. $SK(G) = 55$.

5. $SK_1(G) = 62$.

6. $SK_2(G) = 129.5$.

Proof.

$$\begin{aligned} 1.\ \chi(G) &= \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}} \\ &= \left(\frac{1}{\sqrt{1+2}}\right)(2) + \left(\frac{1}{\sqrt{1+3}}\right)(2) + \left(\frac{1}{\sqrt{2+2}}\right)(6) \\ &\quad + \left(\frac{1}{\sqrt{2+3}}\right)(12) + \left(\frac{1}{\sqrt{3+2}}\right)(2) \\ &= 11.33. \end{aligned}$$

$$\begin{aligned} 2.\ R'(G) &= \sum_{uv\in E(G)} \frac{1}{max\{d_u, d_v\}} \\ &= \left(\frac{1}{2}\right)(2) + \left(\frac{1}{3}\right)(2) + \left(\frac{1}{2}\right)(6) \\ &\quad + \left(\frac{1}{12}\right)(6) + \left(\frac{1}{2}\right)(2) \\ &= 6.16. \end{aligned}$$

$$\begin{aligned} 3.\ AG_1(G) &= \sum_{uv\in E(G)} \frac{d_u + d_v}{2\sqrt{d_u \times d_v}} \\ &= \left(\frac{1+2}{2\sqrt{1\times 2}}\right)(2) + \left(\frac{1+3}{2\sqrt{1\times 3}}\right)(2) + \left(\frac{2+2}{2\sqrt{2\times 2}}\right)(6) \\ &\quad + \left(\frac{2+3}{2\sqrt{2\times 3}}\right)(12) + \left(\frac{3+3}{2\sqrt{3\times 3}}\right)(2) \\ &= 24.67. \end{aligned}$$

$$\begin{aligned} 4.\ SK(G) &= \sum_{uv\in E(G)} \frac{d_u + d_v}{2} \\ &= \left(\frac{1+2}{2}\right)(2) + \left(\frac{1+3}{2}\right)(2) + \left(\frac{2+2}{2}\right)(6) \\ &\quad + \left(\frac{2+3}{2}\right)(12) + \left(\frac{3+3}{2}\right)(2) \\ &= 55. \end{aligned}$$

$$\begin{aligned} 5.\ SK_1(G) &= \sum_{uv\in E(G} \frac{d_u \times d_v}{2} \\ &= \left(\frac{1\times 2}{2}\right)(2) + \left(\frac{1\times 3}{2}\right)(2) + \left(\frac{2\times 2}{2}\right)(6) \end{aligned}$$

$$+\left(\frac{2\times 3}{2}\right)(12)+\left(\frac{3\times 3}{2}\right)(2)$$
$$= 62.$$

6. $SK_2(G) = \sum_{uv\in E(G)}\left(\frac{d_u+d_v}{2}\right)^2$
$$= \left(\frac{1+2}{2}\right)^2(2)+\left(\frac{1+3}{2}\right)^2(2)+\left(\frac{2+2}{2}\right)^2(6)$$
$$+\left(\frac{2+3}{2}\right)^2(12)+\left(\frac{3+3}{2}\right)^2(2)$$
$$= 129.5.$$

□

Theorem 2.6. *Let G be the graph of Hydroxychloroquine. Then the Gourava and hyper Gourava indices for Hydroxychloroquine are*

1. $GO_1(G) = 462$.
2. $GO_2(G) = 600$.
3. $HGO_1(G) = 2434$.
4. $HGO_2(G) = 18528$.

Proof.

1. $GO_1(G) = \sum_{uv\in E(G)}[(d_u+d_v)+(d_u\times d_v)]$
$$= [(1+2)+(1\times 2)](2)+[(1+3)+(1\times 3)](2)+[(2+2)+(2\times 2)](6)$$
$$+[(2+3)+(2\times 3)](12)+[(3+3)+(3\times 3)](2)$$
$$= 462.$$

2. $GO_2(G) = \sum_{uv\in E(G)}[(d_u+d_v)\times(d_u\times d_v)]$
$$= [(1+2)\times(1\times 2)](2)+[(1+3)\times(1\times 3)](2)+[(2+2)\times(2\times 2)](6)$$
$$+[(2+3)\times(2\times 3)](12)+[(3+3)\times(3\times 3)](2)$$
$$= 600.$$

3. $HGO_1(G) = \sum_{uv\in E(G)}[(d_u+d_v)+(d_u\times d_v)]^2$
$$= [(1+2)+(1\times 2)]^2(2)+[(1+3)+(1\times 3)]^2(2)+[(2+2)+(2\times 2)]^2(6)$$
$$+[(2+3)+(2\times 3)]^2(12)+[(3+3)+(3\times 3)]^2(2)$$
$$= 2434.$$

4. $HGO_2(G) = \sum_{uv\in E(G)}[(d_u+d_v)\times(d_u\times d_v)]^2$
$$= [(1+2)\times(1\times 2)]^2(2)+[(1+3)\times(1\times 3)]^2(2)+[(2+2)\times(2\times 2)]^2(6)$$
$$+[(2+3)\times(2\times 3)]^2(12)+[(3+3)\times(3\times 3)]^2(2)$$
$$= 18528.$$

□

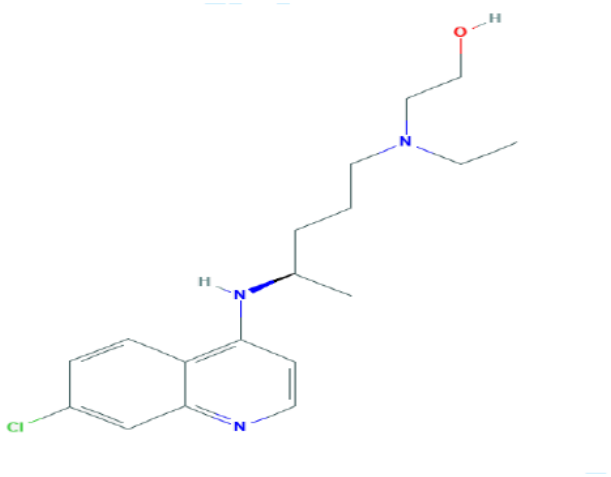

Figure 4: Graph of Theaflavin

(d_u, d_v)	Frequency
(1,3)	10
(2,3)	22
(3,3)	14

Table 4: Partition of $E(Theaflavin)$

2.4 Shingali & Kanabour, Gourava and hyper Gourava indices for Theaflavin

The graph of Theaflavin given in Figure 4. There are three type of edges are present in the graph of Theaflavin. The degree based edge partition is given in Table 4.

Theorem 2.7. *Let G be the graph of Theaflavin. The Shingali & Kanabour indices for Theaflavin are.*

1. $\chi(G) = 19.50$.
2. $R'(G) = 15.33$.
3. $AG_1(G) = 48$.
4. $SK(G) = 117$.
5. $SK_1(G) = 144$.
6. $SK_2(G) = 303.5$.

Proof.

$$\begin{aligned} 1.\ \chi(G) &= \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}} \\ &= \left(\frac{1}{\sqrt{1+3}}\right)(10) + \left(\frac{1}{\sqrt{2+3}}\right)(22) + \left(\frac{1}{\sqrt{3+3}}\right)(14) \\ &= 19.50. \end{aligned}$$

$$\begin{aligned} 2.\ R'(G) &= \sum_{uv\in E(G)} \frac{1}{max\{d_u, d_v\}} \\ &= \left(\frac{1}{3}\right)(10) + \left(\frac{1}{3}\right)(22) + \left(\frac{1}{3}\right)(14) \\ &= 15.33. \end{aligned}$$

$$\begin{aligned} 3.\ AG_1(G) &= \sum_{uv\in E(G)} \frac{d_u + d_v}{2\sqrt{d_u \times d_v}} \\ &= \left(\frac{1+3}{2\sqrt{1\times 3}}\right)(10) + \left(\frac{2+3}{2\sqrt{2\times 3}}\right)(22) + \left(\frac{3+3}{2\sqrt{3\times 3}}\right)(14) \end{aligned}$$

$$= 48.$$

4. $$SK(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{2}$$
$$= \left(\frac{1+3}{2}\right)(10) + \left(\frac{2+3}{2}\right)(22) + \left(\frac{3+3}{2}\right)(14)$$
$$= 117.$$

5. $$SK_1(G) = \sum_{uv \in E(G} \frac{d_u \times d_v}{2}$$
$$= \left(\frac{1\times 3}{2}\right)(10) + \left(\frac{2\times 3}{2}\right)(22) + \left(\frac{3\times 3}{2}\right)(14)$$
$$= 144.$$

6. $$SK_2(G) = \sum_{uv \in E(G)} \left(\frac{d_u + d_v}{2}\right)^2$$
$$= \left(\frac{1+3}{2}\right)^2(10) + \left(\frac{2+3}{2}\right)^2(22) + \left(\frac{3+3}{2}\right)^2(14)$$
$$= 303.5.$$

□

Theorem 2.8. *Let G be the graph of Theaflavin. Then the Gourava and hyper Gourava indices for Theaflavin are*

1. $GO_1(G) = 522$.
2. $GO_2(G) = 1536$.
3. $HGO_1(G) = 6302$.
4. $HGO_2(G) = 62064$.

Proof.

1. $$GO_1(G) = \sum_{uv \epsilon E(G)} [(d_u + d_v) + (d_u \times d_v)]$$
$$= [(1+3) + (1\times 3)](10) + [(2+3) + (2\times 3)](22) + [(3+3) + (3\times 3)](14)$$
$$= 522.$$

2. $$GO_2(G) = \sum_{uv \in E(G)} [(d_u + d_v) \times (d_u \times d_v)]$$
$$= [(1+3) \times (1\times 3)](10) + [(2+3) \times (2\times 3)](22) + [(3+3) \times (3\times 3)](14)$$
$$= 1536.$$

3. $$HGO_1(G) = \sum_{uv \in E(G)} [(d_u + d_v) + (d_u \times d_v)]^2$$
$$= [(1+3) + (1\times 3)]^2(10) + [(2+3) + (2\times 3)]^2(22) + [(3+3) + (3\times 3)]^2(14)$$
$$= 6302.$$

4. $$HGO_2(G) = \sum_{uv \in E(G)} [(d_u + d_v) \times (d_u \times d_v)]^2$$
$$= [(1+3) \times (1\times 3)]^2(10) + [(2+3) \times (2\times 3)]^2(22) + [(3+3) \times (3\times 3)]^2(14)$$
$$= 62064.$$

□

Conclusion

In this article, we have calculated Shingali & Kanabour, Gourava and hype Gourava indices for the chemical compounds used in the treatment of COVID-19. The application of topological invariants to analyze chemical structures crucial in COVID-19 treatment offers valuable insights into their molecular properties. Topological indices approach enhances our understanding of structure-activity relationships, guiding the rational design of more effective antiviral drugs. The interdisciplinary nature of this research underscores the significance of collaboration between chemistry and medicine. Leveraging topological principles provides a promising framework for navigating chemical space and optimizing drug discovery processes. As we advance, incorporating advanced computational techniques will further refine these analyses, contributing to the development of targeted and potent therapeutic interventions.

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