Research Article

Treatment of COVID-19 Patients Using Some New Topological Indices

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Received 9 February 2022; Revised 9 March 2022; Accepted 25 March 2022; Published 9 May 2022

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COVID-19 is causing havoc to human health and the world economy right now. It is a single standard positive-sense RNA virus which is transferred by inhalation of a viral droplet. Its genome forms four structural proteins such as nucleocapsid protein, membrane protein, spike protein, and envelop protein. The capsid of coronavirus is a protein shell within which a positive strand of RNA is present which enables the virus to control the machinery of human cells. It has several variants, e.g., SARS, MERS, and now a new variant identified in 2019, which is a novel coronavirus that causes novel coronavirus disease (COVID-19). COVID-19 is a novel coronavirus disease that originally arose in Wuhan, China, and quickly spread around the world. Clinically, we identified the virus presence by a PCR-based test. Preventive measures and vaccination are the only treatment against coronavirus. Some of these include Remdesivir (GS-5734), Chloroquine, Hydroxychloroquine, and Theaflavin. A topological index (TI) is a mathematical function that assigns a numerical value to a (molecular) graph and predicts many physical, chemical, biological, thermodynamical, and structural features of that network. In this work, we will calculate a new topological index, namely, the first and second Gourava and Hyper-Gourava indices for the molecular graph of Remdesivir (GS-5734), Chloroquine, Hydroxychloroquine, and Theaflavin. We also plotted our computed results to examine how they were affected by the parameters involved. These findings could contribute in the development of new COVID-19 therapy options.

1. Introduction

Coronavirus is a family of viruses that cause upper respiratory infection in humans. Their incident rate is higher in winter or in moderate temperature. Historically, epidemics of various infectious diseases have killed millions of people in the last several centuries. The plague, flu, and cholera created the most frightening pandemics. It began in a seafood market in Wuhan and has been expanded throughout China and abroad [1]. There were 433,139,235 confirmed cases as of March 01, 2022, with 5,939,137 deaths globally (as per the WHO report). The new corona virus (COVID-19) is a beta coronavirus with the same genetic sequence and viral structure as the coronaviruses that cause SARS and MERS-CoV (Figure 1).

A useful drug discovery experiment is to see if existing antiviral drugs are effective in treating similar viral infections. In vitro testing revealed that certain existing antiviral medicines were successful in preventing infection of 2019-nCoV [2–6]. Remdesivir (GS5734), Chloroquine, Hydroxychloroquine, and Theaflavin are some of these antiviral drugs. Remdesivir is a broad-spectrum nucleotide analogue medication developed to prevent Ebola virus infection [7–9]. In vitro, it is also very effective at preventing 2019-nCoV [5]. The clinical trial is now taking place at many hospitals, and efficacy testing is pending. Chloroquine is a broad-spectrum antiviral medication that can be used to treat malaria and autoimmune diseases [10, 11]. A number of random controlled trials have looked into the usefulness
of chloroquine in the treatment of COVID-19. Positive therapy outcomes have included fever management, better CT imaging, and a postponement of disease progression [12, 13].

Hydroxychloroquine’s antiviral action is very similar to that of chloroquine. Both have immune-modifying features that may aid in their antiviral efficacy in vivo [14, 15]. The FDA has approved chloroquine and hydroxychloroquine for emergency coronavirus treatment, according to a Forbes report published on March 30, 2020. Hydroxychloroquine suppresses the cytokine storm by blocking T cell activation, which slows COVID-19’s acute progression. Theaflavin, a polyphenol molecule present in black tea, has been linked to the health benefits of the beverage [16]. Antiviral activity of Theaflavin has been demonstrated against a variety of viruses, including influenza A, B, and C [17, 18]. Wiener [19] discovered that theaflavin might be employed as a lead chemical for the development of a 2019-nCoV inhibitor. We refer to a molecular graph as a simple linked graph in which nodes and edges connecting them are atoms and chemical bonds, respectively [20, 21].

Topological indices are invariant under graph isomorphism mathematical measures of molecular graphs. It was founded in 1947, and since then, it has been on a journey [19]. There has been a lot of effort done on computing indices of various molecular graphs and networks, and a lot of topological indices have been produced. Mondal et al. [22] and Zheng et al. [23] developed topological indices of graphene and chemical compounds frequently employed in the manufacturing of anticancer medicines. The topological indices enable us explore the physiochemical properties and boiling activates of the linked chemical molecule, such as surface area, heat of formation, vapours pressure, surface tension, and boiling points. The various types of topological indices are based on distance, based on degree and based on surface [24–26].

The first topological index, known as the Wiener index, was developed by Wiener while examining the boiling point of alkanes [19]. Randic index is a simple topological index which are introduced by Milan randic [27]. Zagreb indices is the oldest topological indices written by Gutman and Trinajstic [28, 29]. In QSPRs, topological indices are utilised to guess the properties of the concerned compound. There are no such type of topological index exist which give us an idea of all the properties of the concerned compound. As a result, there is constantly a need for new topological indices to be defined. First and second Gourava indices have lately been characterised as

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

\[
GO_2(G) = \sum_{uv \in E(G)} [(d_u + d_v) \times (d_u \times d_v)].
\]

The first and second hyper-Gourava indices of a graph G are defined as

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

\[
HGO_2(G) = \sum_{uv \in E(G)} [(d_u + d_v) \times (d_u \times d_v)]^2.
\]

We compute Gourava and Hyper-Gourava indices for Remdesivir (GS-5734), Chloroquine, Hydroxychloroquine, and Theaflavin as well as their graphical representations in this study [30–32].

2. Methodology

Our main findings include topological indices of some antiviral drug structures. We first built a graph of the molecular compounds and counted the total number of vertices and edges to arrive at our conclusions. Second, based on the degrees of the end vertices, we classified the graphs’ edge set into several types. We arrived at our desired findings by using Gourava indices definitions. We plot our computed findings to examine how they were affected by the parameters involved.

3. Results and Discussion

The main computational results are presented in this section. We present results about Remdesivir (GS-5734), Chloroquine, Hydroxychloroquine, and Theaflavin.

3.1. Remdesivir (GS-5734). Remdesivir is a prodrug that allows GS-441524 monophosphate to be delivered intracellularly and then biotransformed into GS-441524 triphosphate, a ribonucleotide analogue inhibitor of viral RNA polymerase. Remdesivir is a broad spectrum antiviral medicine originally developed to treat hepatitis C and is now being administrated for after-treatment of COVID 19. Remdesivir can be made from ribose derivatives in a number of ways. Figures 2 and 3 show the molecular structure and molecular graph of Remdesivir (GS-5734). Table 1 shows the edge partition of the Remdesivir (GS-5734) based on the degree and neighborhood degree sum of vertices.
Theorem 1. The $GO_1$ and $GO_2$ indices for Remdesivir (GS-5734) are as follows:

$$GO_1(G) = 2647,$$
$$GO_2(G) = 21123.$$  

Proof. From the edge partitioning based on degree of Remdesivir (GS-5734), we have the following computations for $GO_1$ and $GO_2$ indices:

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

$$= [(1+2) \times (1\times2)](5) + [(1+3) \times (1\times3)](5) + [(1+4) \times (1\times4)](2) + [(2+2) \times (2\times2)](9) + [(2+3) \times (2\times3)](14) + [(2+4) \times (2\times4)](6) + [(3+3) \times (3\times3)](3) + [(3+3) \times (3\times3)](6) + [(3+6) \times (3\times6)](1) + [(3+6) \times (3\times6)](2) + [(4+4) \times (4\times4)](2) + [(4+7) \times (4\times7)](1) + [(4+9) \times (4\times9)](1) + [(5+5) \times (5\times5)](2) + [(5+6) \times (5\times6)](6) + [(5+7) \times (5\times7)](1) + [(5+8) \times (5\times8)](2) + [(5+9) \times (5\times9)](1) + [(6+6) \times (6\times6)](1) + [(6+7) \times (6\times7)](3) + [(6+8) \times (6\times8)](1) + [(7+7) \times (7\times7)](4) + [(7+8) \times (7\times8)](1) + [(7+9) \times (7\times9)](1) + [(8+8) \times (8\times8)](1) + [(8+9) \times (8\times9)](2) + [(9+9) \times (9\times9)](1) = 2647.$$  

$$GO_2(G) = \sum_{uv \in E(G)} [(d_u + d_v) \times (d_u d_v)]$$

$$= [(1+2) \times (1\times2)](5) + [(1+3) \times (1\times3)](5) + [(1+4) \times (1\times4)](2) + [(2+2) \times (2\times2)](9) + [(2+3) \times (2\times3)](14) + [(2+4) \times (2\times4)](6) + [(3+4) \times (3\times4)](2) + [(3+5) \times (3\times5)](6) + [(3+6) \times (3\times6)](3) + [(3+7) \times (3\times7)](1) + [(3+8) \times (3\times8)](1) + [(4+4) \times (4\times4)](2) + [(4+5) \times (4\times5)](4) + [(4+6) \times (4\times6)](2) + [(4+7) \times (4\times7)](1) + [(4+9) \times (4\times9)](1) + [(5+5) \times (5\times5)](2) + [(5+6) \times (5\times6)](6) + [(5+7) \times (5\times7)](1) + [(5+8) \times (5\times8)](2) + [(5+9) \times (5\times9)](1) + [(6+6) \times (6\times6)](1) + [(6+7) \times (6\times7)](3) + [(6+8) \times (6\times8)](1) + [(7+7) \times (7\times7)](4) + [(7+8) \times (7\times8)](1) + [(7+9) \times (7\times9)](1) + [(8+8) \times (8\times8)](1) + [(8+9) \times (8\times9)](2) + [(9+9) \times (9\times9)](1) = 21123.$$  

Theorem 2. The $HGO_1$ and $HGO_2$ indices for Remdesivir (GS-5734) are as follows:

$$HGO_1(G) = 117740,$$
$$HGO_2(G) = 14045816.$$  

Proof. From the edge partitioning based on degree of Remdesivir (GS-5734), we have the following computations for $HGO_1$ and $HGO_2$ indices:

$$HGO_1(G) = \sum_{uv \in E(G)} [(d_u + d_v) + (d_u d_v)]$$

$$= [(1+2) \times (1\times2)](5) + [(1+3) \times (1\times3)](5) + [(1+4) \times (1\times4)](2) + [(2+2) \times (2\times2)](9) + [(2+3) \times (2\times3)](14) + [(2+4) \times (2\times4)](6) + [(3+4) \times (3\times4)](2) + [(3+5) \times (3\times5)](6) + [(3+6) \times (3\times6)](3) + [(3+7) \times (3\times7)](1) + [(3+8) \times (3\times8)](1) + [(4+4) \times (4\times4)](2) + [(4+5) \times (4\times5)](4) + [(4+6) \times (4\times6)](2) + [(4+7) \times (4\times7)](1) + [(4+9) \times (4\times9)](1) + [(5+5) \times (5\times5)](2) + [(5+6) \times (5\times6)](6) + [(5+7) \times (5\times7)](1) + [(5+8) \times (5\times8)](2) + [(5+9) \times (5\times9)](1) + [(6+6) \times (6\times6)](1) + [(6+7) \times (6\times7)](3) + [(6+8) \times (6\times8)](1) + [(7+7) \times (7\times7)](4) + [(7+8) \times (7\times8)](1) + [(7+9) \times (7\times9)](1) + [(8+8) \times (8\times8)](1) + [(8+9) \times (8\times9)](2) + [(9+9) \times (9\times9)](1) = 117740.$$  

$$HGO_2(G) = \sum_{uv \in E(G)} [(d_u + d_v) \times (d_u d_v)]$$

$$= [(1+2) \times (1\times2)](5) + [(1+3) \times (1\times3)](5) + [(1+4) \times (1\times4)](2) + [(2+2) \times (2\times2)](9) + [(2+3) \times (2\times3)](14) + [(2+4) \times (2\times4)](6) + [(3+4) \times (3\times4)](2) + [(3+5) \times (3\times5)](6) + [(3+6) \times (3\times6)](3) + [(3+7) \times (3\times7)](1) + [(3+8) \times (3\times8)](1) + [(4+4) \times (4\times4)](2) + [(4+5) \times (4\times5)](4) + [(4+6) \times (4\times6)](2) + [(4+7) \times (4\times7)](1) + [(4+9) \times (4\times9)](1) + [(5+5) \times (5\times5)](2) + [(5+6) \times (5\times6)](6) + [(5+7) \times (5\times7)](1) + [(5+8) \times (5\times8)](2) + [(5+9) \times (5\times9)](1) + [(6+6) \times (6\times6)](1) + [(6+7) \times (6\times7)](3) + [(6+8) \times (6\times8)](1) + [(7+7) \times (7\times7)](4) + [(7+8) \times (7\times8)](1) + [(7+9) \times (7\times9)](1) + [(8+8) \times (8\times8)](1) + [(8+9) \times (8\times9)](2) + [(9+9) \times (9\times9)](1) = 14045816.$$
Table 1: Edge partitioning based on degree of Remdesivir (GS-5734).

| $d$ | $d(d,d_d)$ | Frequency |
|-----|------------|-----------|
| $e_1$ | $e_{(1,2)}$ | 2         |
| $e_2$ | $e_{(1,3)}$ | 5         |
| $e_3$ | $e_{(1,4)}$ | 2         |
| $e_4$ | $e_{(2,2)}$ | 9         |
| $e_5$ | $e_{(2,3)}$ | 14        |
| $e_6$ | $e_{(2,4)}$ | 6         |
| $e_7$ | $e_{(3,3)}$ | 6         |
| $e_8$ | $e_{(3,4)}$ | 2         |
| $e_9$ | $e_{(4,5)}$ | 3         |
| $e_{10}$ | $e_{(4,6)}$ | 1         |
| $e_{11}$ | $e_{(5,5)}$ | 2         |
| $e_{12}$ | $e_{(5,6)}$ | 6         |
| $e_{13}$ | $e_{(5,7)}$ | 1         |
| $e_{14}$ | $e_{(6,6)}$ | 1         |
| $e_{15}$ | $e_{(6,7)}$ | 1         |
| $e_{16}$ | $e_{(6,8)}$ | 2         |
| $e_{17}$ | $e_{(6,9)}$ | 1         |
| $e_{18}$ | $e_{(7,7)}$ | 3         |
| $e_{19}$ | $e_{(7,8)}$ | 4         |
| $e_{20}$ | $e_{(7,9)}$ | 1         |
| $e_{21}$ | $e_{(8,8)}$ | 2         |
| $e_{22}$ | $e_{(8,9)}$ | 1         |

Proof. From the edge partitioning based on degree of Chloroquine, we have the following computations for $GO_1$ and $GO_2$ indices:

\[
GO_1(G) = 1111,
\]

\[
GO_2(G) = 7992.
\]

\[
GO_2(G) = \sum_{\{d = d, d_d\} \in \{d = d, d_d\}} [(d = d, d_d) \times (d = d, d_d)]
\]

3.2. Chloroquine. It was studied to treat COVID-19 early in the pandemic, but research was mainly abandoned in summer of 2020, and it is no longer recommended for this use. Chloroquine or chlorine phosphate is used to cure malaria. It is taken orally. Muscle pain, loss of appetite, diarrhea, and a rash are all common adverse effects. Chloroquine lysosomotropic property is thought to be responsible for much of its antimalarial effect the drug accumulates in the parasites acidic feeding vacuole and disrupts critical activities. Figures 4 and 5 show the molecular structure and molecular graph of chloroquine. Table 2 shows the edge partition of the chloroquine based on the degree and neighborhood degree sum of vertices.

Theorem 3. The $GO_1$ and $GO_2$ indices for Chloroquine are as follows:

\[
GO_1(G) = 1111,
\]

\[
GO_2(G) = 7992.
\]

HGO$_2$(G) = \sum_{u \in V(G)} [(d = d, d_d) \times (d = d, d_d)]
\]

\[
= [(1 + 1) \times (1 \times 2)](5) + [(1 + 3) \times (1 \times 3)](5) + [(2 + 2) \times (2 \times 2)](9) + [(2 + 3) \times (2 \times 3)](14) + [(2 + 4) \times (2 \times 4)](6) + [(3 + 3) \times (3 \times 3)](9) + [(3 + 6) \times (3 \times 6)](3) + [(3 + 7) \times (3 \times 7)](6) + [(4 + 4) \times (4 \times 4)](2) + [(4 + 5) \times (4 \times 5)](4) + [(4 + 6) \times (4 \times 6)](2) + [(5 + 5) \times (5 \times 5)](1) + [(5 + 6) \times (5 \times 6)](6) + [(5 + 7) \times (5 \times 7)](1) + [(5 + 8) \times (5 \times 8)](2) + [(5 + 9) \times (5 \times 9)](1) + [(6 + 6) \times (6 \times 6)](1) + [(6 + 7) \times (6 \times 7)](3) + [(6 + 8) \times (6 \times 8)](1) + [(7 + 7) \times (7 \times 7)](4) + [(7 + 8) \times (7 \times 8)](1) + [(7 + 9) \times (7 \times 9)](1) + [(8 + 8) \times (8 \times 8)](1) + [(8 + 9) \times (8 \times 9)](2) + [(9 + 9) \times (9 \times 9)](1)
\]

\[
= 14045816.
\]
Theorem 4. The HGO\textsubscript{1} and HGO\textsubscript{2} indices for Chloroquine are as follows:

\begin{align*}
HGO_1(G) &= 41573, \\
HGO_2(G) &= 3441312.
\end{align*}

Proof. From the edge partitioning based on degree of Chloroquine, we have the following computations for HGO\textsubscript{1} and HGO\textsubscript{2} indices:

\begin{align*}
HGO_1(G) &= \sum_{uv \in E(G)} [(d_u + d_v) + (d_u + d_v)]^2 \\
&= [(1 + 2) + (1 \times 2)]^2(2) + [(1 + 3) + (1 \times 3)]^2(2) \\
&\quad + [(2 + 2) + (2 \times 2)]^2(5) + [(2 + 3) + (2 \times 3)]^2(12) \\
&\quad + [(3 + 3) + (3 \times 3)]^2(2) + [(2 + 4) + (2 \times 4)]^2(2) \\
&\quad + [(3 + 5) + (3 \times 5)]^2(2) + [(4 + 5) + (4 \times 5)]^2(4) \\
&\quad + [(4 + 6) + (4 \times 6)]^2(2) + [(5 + 5) + (5 \times 5)]^2(3) \\
&\quad + [(5 + 6) + (5 \times 6)]^2(3) + [(5 + 7) + (5 \times 7)]^2(2) \\
&\quad + [(5 + 8) + (5 \times 8)]^2(1) + [(6 + 7) + (6 \times 7)]^2(2) \\
&\quad + [(7 + 8) + (7 \times 8)]^2(2) = 41573,
\end{align*}

\begin{align*}
HGO_2(G) &= \sum_{uv \in E(G)} [(d_u + d_v) \times (d_u + d_v)]^2 \\
&= [(1 + 2) \times (1 \times 2)]^2(2) + [(1 + 3) \times (1 \times 3)]^2(2) \\
&\quad + [(2 + 2) \times (2 \times 2)]^2(5) + [(2 + 3) \times (2 \times 3)]^2(12) \\
&\quad + [(3 + 3) \times (3 \times 3)]^2(2) + [(2 + 4) \times (2 \times 4)]^2(2) \\
&\quad + [(3 + 5) \times (3 \times 5)]^2(2) + [(4 + 5) \times (4 \times 5)]^2(4) \\
&\quad + [(4 + 6) \times (4 \times 6)]^2(2) + [(5 + 5) \times (5 \times 5)]^2(3) \\
&\quad + [(5 + 6) \times (5 \times 6)]^2(3) + [(5 + 7) \times (5 \times 7)]^2(2) \\
&\quad + [(5 + 8) \times (5 \times 8)]^2(1) + [(6 + 7) \times (6 \times 7)]^2(2) \\
&\quad + [(7 + 8) \times (7 \times 8)]^2(2) = 3441312.
\end{align*}
Hydroxychloroquine, we have the following computations from the edge partitioning based on degree of disease 2019 (COVID 19). However, clinical trials have researched for its capacity to prevent and treat coronavirus.

3.3. Hydroxychloroquine. Hydroxychloroquine has been researched for its capacity to prevent and treat coronavirus. It is an antimalarial drug administrated to those areas where malaria remains sensitive to chloroquine. Rheumatoid arthritis, lupus, and porphyria cutanea tarda are among the conditions for which it has been used. It is usually taken as hydroxychloroquine sulphate, and it is taken by mouth.

Figures 6 and 7 show the molecular structure and molecular graph of hydroxychloroquine. Table 3 shows the edge partition of the hydroxychloroquine based on the degree and neighborhood degree sum of vertices.

| $E$ | $E_{(d_i,d_j)}$ | Frequency |
|-----|---------------|-----------|
| $E_1$ | $E_{(1,2)}$ | 2 |
| $E_2$ | $E_{(1,3)}$ | 2 |
| $E_3$ | $E_{(2,2)}$ | 6 |
| $E_4$ | $E_{(2,3)}$ | 13 |
| $E_5$ | $E_{(3,3)}$ | 2 |
| $E_6$ | $E_{(2,4)}$ | 1 |
| $E_7$ | $E_{(3,5)}$ | 3 |
| $E_8$ | $E_{(4,5)}$ | 4 |
| $E_9$ | $E_{(4,6)}$ | 1 |
| $E_{10}$ | $E_{(5,5)}$ | 3 |
| $E_{11}$ | $E_{(5,6)}$ | 4 |
| $E_{12}$ | $E_{(5,7)}$ | 2 |
| $E_{13}$ | $E_{(5,8)}$ | 1 |
| $E_{14}$ | $E_{(6,7)}$ | 2 |
| $E_{15}$ | $E_{(7,8)}$ | 2 |

3.3. Hydroxychloroquine. Hydroxychloroquine has been researched for its capacity to prevent and treat coronavirus disease 2019 (COVID 19). However, clinical trials have shown it ineffective and with a risk of significant side effects. It is an antimalarial drug administrated to those areas where malaria remains sensitive to chloroquine. Rheumatoid arthritis, lupus, and porphyria cutanea tarda are among the conditions for which it has been used. It is usually taken as hydroxychloroquine sulphate, and it is taken by mouth.

Figures 6 and 7 show the molecular structure and molecular graph of hydroxychloroquine. Table 3 shows the edge partition of the hydroxychloroquine based on the degree and neighborhood degree sum of vertices.

Theorem 5. The $G_{O1}$ and $G_{O2}$ indices for Hydroxychloroquine are as follows:

$$G_{O1}(G) = 1146,$$

$$G_{O2}(G) = 8200.$$  

Proof. From the edge partitioning based on degree of Hydroxychloroquine, we have the following computations for $G_{O1}$ and $G_{O2}$ indices:

$$G_{O1}(G) = \sum_{uv \in E(G)} [(d_u + d_v) + (d_u, d_v)]$$

$$= [(1 + 2) + (1 \times 2)](2) + [(1 + 3) + (1 \times 3)](2)$$
$$+ [(2 + 2) + (2 \times 2)](6) + [(2 + 3) + (2 \times 3)](13)$$
$$+ [(3 + 3) + (3 \times 3)](2) + [(2 + 4) + (2 \times 4)](1)$$
$$+ [(3 + 5) + (3 \times 5)](3) + [(4 + 5) + (4 \times 5)](4)$$
$$+ [(4 + 6) + (4 \times 6)](1) + [(5 + 5) + (5 \times 5)](3)$$
$$+ [(5 + 6) + (5 \times 6)](4) + [(5 + 7) + (5 \times 7)](2)$$
$$+ [(5 + 8) + (5 \times 8)](1) + [(6 + 7) + (6 \times 7)](2)$$
$$+ [(7 + 8) + (7 \times 8)](2) = 1146,$$

$$G_{O2}(G) = \sum_{uv \in E(G)} [(d_u + d_v) \times (d_u, d_v)]$$

$$= [(1 + 2) \times (1 \times 2)](2) + [(1 + 3) \times (1 \times 3)](2)$$
$$+ [(2 + 2) \times (2 \times 2)](6) + [(2 + 3) \times (2 \times 3)](13)$$
$$+ [(3 + 3) \times (3 \times 3)](2) + [(2 + 4) \times (2 \times 4)](1)$$
$$+ [(3 + 5) \times (3 \times 5)](3) + [(4 + 5) \times (4 \times 5)](4)$$
$$+ [(4 + 6) \times (4 \times 6)](1) + [(5 + 5) \times (5 \times 5)](3)$$
$$+ [(5 + 6) \times (5 \times 6)](4) + [(5 + 7) \times (5 \times 7)](2)$$
$$+ [(5 + 8) \times (5 \times 8)](1) + [(6 + 7) \times (6 \times 7)](2)$$
$$+ [(7 + 8) \times (7 \times 8)](2) = 8200.$$  

Proof. From the edge partitioning based on degree of Hydroxychloroquine, we have the following computations for $G_{O1}$ and $G_{O2}$ indices:

$$H_{G_{O1}}(G) = 42616,$$

$$H_{G_{O2}}(G) = 3605864.$$  

Proof. From the edge partitioning based on degree of Hydroxychloroquine, we have the following computations for $G_{O1}$ and $G_{O2}$ indices:

$$H_{G_{O1}}(G) = \sum_{uv \in E(G)} [(d_u + d_v)]^2$$

$$= [(1 + 2) + (1 \times 2)]^2(2) + [(1 + 3) + (1 \times 3)]^2(2)$$
$$+ [(2 + 2) + (2 \times 2)]^2(6) + [(2 + 3) + (2 \times 3)]^2(13)$$
$$+ [(3 + 3) + (3 \times 3)]^2(2) + [(2 + 4) + (2 \times 4)]^2(1)$$
$$+ [(3 + 5) + (3 \times 5)]^2(3) + [(4 + 5) + (4 \times 5)]^2(4)$$
$$+ [(4 + 6) + (4 \times 6)]^2(1) + [(5 + 5) + (5 \times 5)]^2(3)$$
$$+ [(5 + 6) + (5 \times 6)]^2(4) + [(5 + 7) + (5 \times 7)]^2(2)$$
$$+ [(5 + 8) + (5 \times 8)]^2(1) + [(6 + 7) + (6 \times 7)]^2(2)$$
$$+ [(7 + 8) + (7 \times 8)]^2(2) = 42616.$$
Proof. From the edge partitioning based on degree of Thea- 
flavin, we have the following computations for GO1 and G O2 indices:

\[ \begin{align*}
\text{GO1}(G) &= \sum_{uv \in E(G)} [(d_u + d_v) \times (d_u, d_v)] \\
&= [(1 + 3) \times (1 + 3)](10) + [(2 + 3) \times (2 + 3)](12) \\
&+ [(3 + 3) \times (3 + 3)](14) + [(3 + 3) \times (3 + 3)](2) \\
&+ [(3 + 3) \times (3 + 3)](6) + [(3 + 3) \times (3 + 3)](12) \\
&+ [(5 + 6) \times (5 + 6)](4) + [(6 + 6) \times (6 + 6)](6) \\
&+ [(6 + 7) \times (6 + 7)](8) + [(6 + 8) \times (6 + 8)](10) \\
&+ [(7 + 8) \times (7 + 8)](3) + [(7 + 9) \times (7 + 9)](2) \\
&+ [(8 + 8) \times (8 + 8)](2) + [(8 + 9) \times (8 + 9)](1) = 2924. 
\end{align*} \]

\[ \begin{align*}
\text{GO2}(G) &= \sum_{uv \in E(G)} [(d_u + d_v) \times (d_u, d_v)] \\
&= [(1 + 3) \times (1 + 3)](10) + [(2 + 3) \times (2 + 3)](22) \\
&+ [(3 + 3) \times (3 + 3)](14) + [(3 + 5) \times (3 + 5)](2) \\
&+ [(3 + 6) \times (3 + 6)](6) + [(3 + 7) \times (3 + 7)](2) \\
&+ [(5 + 6) \times (5 + 6)](4) + [(6 + 6) \times (6 + 6)](6) \\
&+ [(6 + 7) \times (6 + 7)](8) + [(6 + 8) \times (6 + 8)](10) \\
&+ [(7 + 8) \times (7 + 8)](3) + [(7 + 9) \times (7 + 9)](2) \\
&+ [(8 + 8) \times (8 + 8)](2) + [(8 + 9) \times (8 + 9)](1) = 25976. 
\end{align*} \]

3.4. Theaflavin. Theaflavins are antioxidant polyphenols that are generated when flavan-3-ols in tea leaves are condensed during enzymatic oxidation. All theaflavin and gallate derivatives were found to exhibit inactivation action against bovine rotavirus (in vitro). The yield of each extraction was quantified by measuring the crude theaflavin extract, with the Indian source of tea giving the crudest extract.

Figures 8 and 9 show the molecular structure and molecular graph of theaflavin. Table 4 shows the edge partition of the theaflavin based on the degree and neighborhood degree sum of vertices.

**Theorem 7.** The GO1 and GO2 indices for Theaflavin are as follows:

\[ \begin{align*}
\text{GO1}(G) &= 2924, \\
\text{GO2}(G) &= 25976. 
\end{align*} \]

**Proof.** From the edge partitioning based on degree of Thea- 
flavin, we have the following computations for GO1 and G O2 indices:

\[ \begin{align*}
\text{GO1}(G) &= \sum_{uv \in E(G)} [(d_u + d_v) \times (d_u, d_v)] \\
&= [(1 + 3) \times (1 + 3)](10) + [(2 + 3) \times (2 + 3)](22) \\
&+ [(3 + 3) \times (3 + 3)](14) + [(3 + 5) \times (3 + 5)](2) \\
&+ [(3 + 6) \times (3 + 6)](6) + [(3 + 7) \times (3 + 7)](2) \\
&+ [(5 + 6) \times (5 + 6)](4) + [(6 + 6) \times (6 + 6)](6) \\
&+ [(6 + 7) \times (6 + 7)](8) + [(6 + 8) \times (6 + 8)](10) \\
&+ [(7 + 8) \times (7 + 8)](3) + [(7 + 9) \times (7 + 9)](2) \\
&+ [(8 + 8) \times (8 + 8)](2) + [(8 + 9) \times (8 + 9)](1) = 2924. 
\end{align*} \]

\[ \begin{align*}
\text{GO2}(G) &= \sum_{uv \in E(G)} [(d_u + d_v) \times (d_u, d_v)] \\
&= [(1 + 3) \times (1 + 3)](10) + [(2 + 3) \times (2 + 3)](22) \\
&+ [(3 + 3) \times (3 + 3)](14) + [(3 + 5) \times (3 + 5)](2) \\
&+ [(3 + 6) \times (3 + 6)](6) + [(3 + 7) \times (3 + 7)](2) \\
&+ [(5 + 6) \times (5 + 6)](4) + [(6 + 6) \times (6 + 6)](6) \\
&+ [(6 + 7) \times (6 + 7)](8) + [(6 + 8) \times (6 + 8)](10) \\
&+ [(7 + 8) \times (7 + 8)](3) + [(7 + 9) \times (7 + 9)](2) \\
&+ [(8 + 8) \times (8 + 8)](2) + [(8 + 9) \times (8 + 9)](1) = 25976. 
\end{align*} \]
Figure 10: 2D graphical comparison and 3D graphical comparison of Remdesivir (GS-5734), Chloroquine, Hydroxychloroquine, and Theaflavin.
Theorem 8. The $HGO_1$ and $HGO_2$ indices for Theaflavin are as follows:

$$HGO_1(G) = 145170,$$
$$HGO_2(G) = 14439744. \quad (18)$$

Proof. From the edge partitioning based on degree of Theaflavin, we have the following computations for $HGO_1$ and $HGO_2$ indices:

$$HGO_1(G) = \sum_{u \in V(G)} \left[ (d_u + d_v) + (d_u, d_v) \right]^2$$

$$= [(1 + 3) + (1 \times 3)]^2(10) + [(2 + 3) + (2 \times 3)]^2(22)$$
$$+ [(3 + 3) + (3 \times 3)]^2(14) + [(3 + 5) + (3 \times 5)]^2(2)$$
$$+ [(3 + 6) + (3 \times 6)]^2(6) + [(3 + 7) + (3 \times 7)]^2(2)$$
$$+ [(5 + 6) + (5 \times 6)]^2(4) + [(6 + 6) + (6 \times 6)]^2(6)$$
$$+ [(6 + 7) + (6 \times 7)]^2(8) + [(6 + 8) + (6 \times 8)]^2(10)$$
$$+ [(7 + 8) + (7 \times 8)]^2(3) + [(7 + 9) + (7 \times 9)]^2(2)$$
$$+ [(8 + 8) + (8 \times 8)]^2(2) + [(8 + 9) + (8 \times 9)]^2(1)$$
$$= 145170,$$

$$HGO_2(G) = \sum_{u \in V(G)} \left[ (d_u + d_v) \times (d_u, d_v) \right]^2$$

$$= [(1 + 3) \times (1 \times 3)]^2(10) + [(2 + 3) \times (2 \times 3)]^2(22)$$
$$+ [(3 + 3) \times (3 \times 3)]^2(14) + [(3 + 5) \times (3 \times 5)]^2(2)$$
$$+ [(3 + 6) \times (3 \times 6)]^2(6) + [(3 + 7) \times (3 \times 7)]^2(2)$$
$$+ [(5 + 6) \times (5 \times 6)]^2(4) + [(6 + 6) \times (6 \times 6)]^2(6)$$
$$+ [(6 + 7) \times (6 \times 7)]^2(8) + [(6 + 8) \times (6 \times 8)]^2(10)$$
$$+ [(7 + 8) \times (7 \times 8)]^2(3) + [(7 + 9) \times (7 \times 9)]^2(2)$$
$$+ [(8 + 8) \times (8 \times 8)]^2(2) + [(8 + 9) \times (8 \times 9)]^2(1)$$
$$= 14439744. \quad (19)$$

4. Conclusion

Using degree-based indices, we investigated the topological features of various chemical substances used to suppress COVID-19 outbreaks and transmission in this article. Polygonal shapes, trees, graphs, and other geometrical shapes are widely used to depict drugs and other chemical compounds. We discuss the newly introduced Gourava indices for the molecular graph of Remdesivir (GS-5734), Chloroquine, Hydroxymchloroquine, and Theaflavin. The Gourava indices are a step in the right direction, and they are very similar to the Zagreb indices. Chemists and mathematicians are highly interested in Zagreb indices because of their numerous uses in chemistry. Figure 10 gives the graphical comparison of computed results for the above-mentioned chemical structures. Because topological indices can predict several qualities and activities such as boiling point, entropy, enthalpy, acentric factor, and critical pressure. Our findings can aid in the development of new medications and vaccines for COVID-19 treatment.

Data Availability

All data required for this paper are included within this paper.

Conflicts of Interest

The authors do not have any conflicts.

Authors’ Contributions

All authors contributed equally to this paper.

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