Research Article

Degree-Based Graph Invariants of some Chemical Structures for the Treatment of Corona Virus

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Coronavirus is a family of viruses that cause upper respiratory infections in humans. It has several variants, e.g., SARS and MERS, and now, a new variant has been identified in 2019 which is the novel coronavirus disease 2019 (COVID-19). The novel coronavirus disease 2019 (COVID-19) first appeared in Wuhan, China, and quickly spread throughout the world. Their incident rate is high in winter or in moderate temperature. Clinically, we identified the virus presence by PCR-based test. Preventive measures and vaccination are the only treatment against coronavirus. Some of them are remdesivir (GS-5734), chloroquine, hydroxychloroquine, theaflavin, ritonavir, and arbidol. 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, atom-bond connectivity (ABC) index, Geometrically Arithmetic (GA) index, Sombor index, Multiplicative Sambor index, and its reduced version for the molecular graph of remdesivir (GS-5734), chloroquine, hydroxychloroquine, theaflavin, ritonavir, and arbidol. We also plot our computed results to examine how they were affected by the parameters involved. The results obtained can aid in the design of new medicine for the treatment of COVID-19.

1. Introduction

Historically, in the last few centuries, epidemics of different infectious diseases have killed millions of people. Pandemics caused by the plague, flu, cholera, and other diseases were the most terrifying. The COVID-19 epidemic is currently wreaking havoc on human health and the global economy. It began in a seafood market in Wuhan and has since expanded throughout China and abroad [1]. There were 489,060,735 confirmed cases as of April 03, 2022 with 6,150,333 deaths globally (as per WHO report). The novel coronavirus (2019-nCoV) is a betacoronavirus with the same genetic sequence and viral structure as the coronaviruses that cause SARS and MERS, respectively (MERS-CoV) [2, 3].

Testing if existing antiviral medications are successful in the treatment of similar viral illnesses is an effective experiment in drug discovery. Researchers evaluated some existing antiviral drugs in vitro and found that they were effective in inhibiting infection and transmission of the 2019-nCoV [4–8]. Remdesivir (GS5734), chloroquine, hydroxychloroquine, theaflavin, ritonavir, and arbidol are some of these antiviral drugs. Remdesivir is a broad-spectrum nucleotide analogue medication developed to prevent Ebola virus infection [9, 10]. In vitro, it is also very effective at preventing 2019-nCoV [7, 11]. The clinical trial is now taking place at many hospitals, and efficacy testings are pending. Chloroquine is a broad-spectrum antiviral medication that can be used to treat malaria and autoimmune diseases [12, 13].
The effectiveness of chloroquine in the treatment of COVID-19 has been studied in a number of randomized controlled trials. Fever control, improved CT imaging, and a delay in disease development have all been reported as positive therapeutic outcomes [14].

The antiviral activity of hydroxychloroquine is remarkably comparable to that of chloroquine. Both have immune modifying properties, which can help them have a better antiviral effect in vivo. 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 [15, 16]. Theaflavin, a polyphenol molecule present in black tea, has been linked to the health benefits of the beverage. 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. Both ritonavir and arbidol act as inhibitor against virus and restrict the proliferation of virus. 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 to explore the physicochemical properties and boiling activities 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 is introduced by Milan Randic [27]. Zagreb indices is the oldest topological indices written by Gutman and Trinajstic [28]. In QSPRs, topological indices are utilized 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. The most popular connectivity topological index is “atom-bond connectivity (ABC) index” which is presented by Estrada et al. [29] as

\[
\text{ABC}(G) = \sum_{ij \in E(G)} \sqrt{d_i + d_j - 2} \quad (1)
\]

Another most popular topological descriptor of connectivity is “Geometrically Arithmetic (GA) index” that was presented by Vukicevic and Furtula [30] as

\[
\text{GA}(G) = \sum_{ij \in E(G)} 2 \sqrt{d_i d_j} \quad (2)
\]

Sambor indices and reduced Sambor indices have lately been characterized by Zheng et al. [23] as

\[
\text{SO}(G) = \sum_{ij \in E(G)} \sqrt{d_i^2 + d_j^2},
\]

\[
\text{SO}_{\text{red}}(G) = \sum_{ij \in E(G)} \sqrt{(d_i - 1)^2 + (d_j - 1)^2}.
\]

The Multiplicative Sambor index and multiplicative reduced Sambor index of a graph G is defined as

\[
\text{SOII}(G) = \prod_{ij \in E(G)} \sqrt{d_i^2 + d_j^2},
\]

\[
\text{SOII}_{\text{red}}(G) = \prod_{ij \in E(G)} \sqrt{(d_i - 1)^2 + (d_j - 1)^2}.
\]

We compute Sambor indices, multiplicative Sambor indices, and reduced Sambor indices for remdesivir (GS-5734), chloroquine, hydroxychloroquine, and theaflavin as well as their graphical representations, in this study [2, 31, 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 atom-bond connectivity (ABC) index, Geometrically Arithmetic (GA) index, and Sombor index definitions. We plotted 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, theaflavin, ritonavir, and arbidol.

3.1. Remdesivir (GS-5734). 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 is a prodrug that allows GS-441524 monophosphate to be delivered intracellularly and then bio-transformed into GS-441524 triphosphate, a ribonucleotide analogue inhibitor of viral RNA polymerase. Remdesivir
can be made from ribose derivatives in a number of ways. Figures 1–2 show the molecular structure and molecular graphs 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 ABC and GA indices for remdesivir (GS-5734) are as follows:

\[
ABC(G) = 55.8288, \\
GA(G) = 95.3680.
\]  

**Proof.** From the edge partitioning based on degree of remdesivir (GS-5734), we have the following computations for ABC and GA indices:

\[
ABC(G) = \sum_{ij \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}} = \sqrt{\frac{1 + 2 - 2}{1 \times 2}} + \sqrt{\frac{1 + 3 - 2}{1 \times 3}} (5)
\]

\[
+ \sqrt{\frac{9 + 9 - 2}{9 \times 9}} = 55.8288,
\]

\[
GA(G) = \sum_{ij \in E(G)} \sqrt{\frac{d_i d_j}{d_i + d_j}} = 2 \sqrt{\frac{1 \times 2}{1 + 2}} (2) + 2 \sqrt{\frac{1 \times 3}{1 + 3}} (5)
\]

\[
+ 2 \sqrt{\frac{2 \times 2}{2 + 2}} (2) + 2 \sqrt{\frac{2 \times 3}{2 + 3}} (14)
\]

\[
+ 2 \sqrt{\frac{3 \times 3}{3 + 3}} (6) + 2 \sqrt{\frac{3 \times 4}{3 + 4}} (2)
\]

\[
+ 2 \sqrt{\frac{4 \times 4}{4 + 4}} (2) + 2 \sqrt{\frac{4 \times 5}{4 + 5}} (4) + 2 \sqrt{\frac{4 \times 6}{4 + 6}} (2)
\]

\[
+ 2 \sqrt{\frac{5 \times 7}{5 + 7}} (1) + 2 \sqrt{\frac{5 \times 8}{5 + 8}} (2)
\]

\[
+ 2 \sqrt{\frac{6 \times 8}{6 + 8}} (1) + 2 \sqrt{\frac{7 \times 7}{7 + 7}} (4) + 2 \sqrt{\frac{7 \times 8}{7 + 8}} (1)
\]

\[
+ 2 \sqrt{\frac{8 \times 9}{8 + 9}} (1) + 2 \sqrt{\frac{9 \times 9}{9 + 9}} (1) = 95.3680.
\]

**Theorem 2.** The SO and SO\(_{\text{red}}\) indices for remdesivir (GS-5734) are as follows:

\[
SO(G) = 526.9637,
\]

\[
SO_{\text{red}}(G) = 406.4166.
\]

**Proof.** From the edge partitioning based on degree of remdesivir (GS-5734), we have the following computations for SO and SO\(_{\text{red}}\) indices:

\[
SO(G) = \sum_{ij \in E(G)} d_i^2 + d_j^2 = \sqrt{1^2 + 2^2 (2)} + \sqrt{1^2 + 3^2 (5)}
\]

\[
+ \sqrt{2^2 + 4^2 (2)} + \sqrt{2^2 + 2^2 (9)} + \sqrt{2^2 + 3^2 (14)}
\]

\[
+ \sqrt{3^2 + 4^2 (6)} + \sqrt{3^2 + 3^2 (6)} + \sqrt{3^2 + 4^2 (2)}
\]

\[
+ \sqrt{4^2 + 4^2 (2)} + \sqrt{4^2 + 5^2 (4)} + \sqrt{4^2 + 6^2 (2)}
\]

\[
+ \sqrt{5^2 + 5^2 (1)} + \sqrt{4^2 + 9^2 (1)} + \sqrt{5^2 + 5^2 (2)}
\]

\[
+ \sqrt{5^2 + 6^2 (6)} + \sqrt{5^2 + 7^2 (1)} + \sqrt{5^2 + 8^2 (2)}
\]

\[
+ \sqrt{6^2 + 6^2 (2)} + \sqrt{6^2 + 7^2 (1)} + \sqrt{6^2 + 8^2 (3)}
\]

\[
+ \sqrt{7^2 + 7^2 (4)} + \sqrt{7^2 + 8^2 (1)}
\]

\[
+ \sqrt{7^2 + 9^2 (1)} + \sqrt{8^2 + 8^2 (1)} + \sqrt{8^2 + 9^2 (2)} + \sqrt{9^2 + 9^2 (1)} = 526.9637,
\]
\[
SOI_{\text{red}}(G) = \sum_{(i,j) \in E(G)} \sqrt{(d_i - 1)^2 + (d_j - 1)^2} = \sqrt{(1 - 1)^2 + (2 - 1)^2} + 2 + 3 + \cdots + 8.
\]

\[SOI_{\text{red}}(G) = \prod_{(i,j) \in E(G)} \sqrt{(d_i - 1)^2 + (d_j - 1)^2} = \sqrt{(1 - 1)^2 + (2 - 1)^2} + \sqrt{(2 - 1)^2 + (3 - 1)^2} + \cdots + \sqrt{(8 - 1)^2 + (9 - 1)^2} = 2.2789 \times 10^{31}.
\]

\[\text{Theorem 3.} \quad \text{The SOII and SOI}_{\text{red}} \text{ indices for remdesivir (GS-5734) are as follows:}
\]
\[SOII(G) = 9.6196 \times 10^{34}, \quad SOI_{\text{red}}(G) = 2.2789 \times 10^{31}.
\]

**Proof.** From the edge partitioning based on degree of remdesivir (GS-5734), we have the following computations for SOII and SOI_{\text{red}} indices:

\[SOII(G) = \sum_{(i,j) \in E(G)} \sqrt{d_i^2 + d_j^2} = \sqrt{1^2 + 2^2} \times \sqrt{2^2 + 3^2} \times \cdots \times \sqrt{8^2 + 9^2}.
\]

\[SOI_{\text{red}}(G) = \prod_{(i,j) \in E(G)} \sqrt{d_i^2 + d_j^2} = \sqrt{1^2 + 2^2} \times \sqrt{2^2 + 3^2} \times \cdots \times \sqrt{8^2 + 9^2}.
\]

3.2 Chloroquine. Chloroquine or chlorine phosphate is used to cure malaria. It was studied to treat COVID-19 early in the pandemic, but research was mainly abandoned in the summer of 2020 and it is no longer recommended for this use. It is taken orally. Muscle pain, loss of appetite, diarrhea, and a rash are all common adverse effects. Chloroquine’s lysosomotropic property is thought to be responsible for much of its antimalarial effect; the drug accumulates in the parasite’s acidic feeding vacuole and disrupts critical activities.

Figures 3–4 show the molecular structure and molecular graphs of chloroquine. Table 2 shows the edge partition of the chloroquine based on the degree and neighborhood degree sum of vertices.

**Theorem 4.** The ABC and GA indices for chloroquine are as follows:

\[ABC(G) = 25.5223, \quad GA(G) = 45.0542.
\]

**Proof.** From the edge partitioning based on degree of chloroquine, we have the following computations for ABC and GA indices:
Figure 2: Molecular graph of remdesivir (GS-5734).

Table 1: Edge partitioning based on degree of remdesivir (GS-5734).

| $\mathcal{E}$ | $\mathcal{E}'_{(d,j)}$ | Frequency |
|---------------|-------------------------|-----------|
| $\mathcal{E}_1$ | $\mathcal{E}_{(1,2)}$ | 2         |
| $\mathcal{E}_2$ | $\mathcal{E}_{(1,3)}$ | 5         |
| $\mathcal{E}_3$ | $\mathcal{E}_{(1,4)}$ | 2         |
| $\mathcal{E}_4$ | $\mathcal{E}_{(2,2)}$ | 9         |
| $\mathcal{E}_5$ | $\mathcal{E}_{(2,3)}$ | 14        |
| $\mathcal{E}_6$ | $\mathcal{E}_{(2,4)}$ | 6         |
| $\mathcal{E}_7$ | $\mathcal{E}_{(3,3)}$ | 6         |
| $\mathcal{E}_8$ | $\mathcal{E}_{(3,4)}$ | 2         |
| $\mathcal{E}_9$ | $\mathcal{E}_{(3,6)}$ | 3         |
| $\mathcal{E}_{10}$ | $\mathcal{E}_{(3,7)}$ | 1         |
| $\mathcal{E}_{11}$ | $\mathcal{E}_{(3,8)}$ | 1         |
| $\mathcal{E}_{12}$ | $\mathcal{E}_{(4,4)}$ | 2         |
| $\mathcal{E}_{13}$ | $\mathcal{E}_{(4,5)}$ | 4         |
| $\mathcal{E}_{14}$ | $\mathcal{E}_{(4,6)}$ | 2         |
| $\mathcal{E}_{15}$ | $\mathcal{E}_{(4,7)}$ | 1         |
| $\mathcal{E}_{16}$ | $\mathcal{E}_{(4,9)}$ | 1         |
| $\mathcal{E}_{17}$ | $\mathcal{E}_{(5,5)}$ | 2         |
| $\mathcal{E}_{18}$ | $\mathcal{E}_{(5,6)}$ | 6         |
| $\mathcal{E}_{19}$ | $\mathcal{E}_{(5,7)}$ | 1         |
| $\mathcal{E}_{20}$ | $\mathcal{E}_{(5,8)}$ | 2         |
| $\mathcal{E}_{21}$ | $\mathcal{E}_{(5,9)}$ | 1         |
| $\mathcal{E}_{22}$ | $\mathcal{E}_{(6,6)}$ | 1         |
| $\mathcal{E}_{23}$ | $\mathcal{E}_{(6,7)}$ | 3         |
| $\mathcal{E}_{24}$ | $\mathcal{E}_{(6,8)}$ | 1         |
| $\mathcal{E}_{25}$ | $\mathcal{E}_{(7,7)}$ | 4         |
| $\mathcal{E}_{26}$ | $\mathcal{E}_{(7,8)}$ | 1         |
| $\mathcal{E}_{27}$ | $\mathcal{E}_{(7,9)}$ | 1         |
| $\mathcal{E}_{28}$ | $\mathcal{E}_{(8,8)}$ | 1         |
| $\mathcal{E}_{29}$ | $\mathcal{E}_{(8,9)}$ | 2         |
| $\mathcal{E}_{30}$ | $\mathcal{E}_{(9,9)}$ | 1         |

Figure 3: Molecular structure of chloroquine.

Table 2: Edge partitioning based on degree of chloroquine.

| $\mathcal{E}$ | $\mathcal{E}'_{(d,j)}$ | Frequency |
|---------------|-------------------------|-----------|
| $\mathcal{E}_1$ | $\mathcal{E}_{(1,2)}$ | 2         |
| $\mathcal{E}_2$ | $\mathcal{E}_{(1,3)}$ | 2         |
| $\mathcal{E}_3$ | $\mathcal{E}_{(2,2)}$ | 5         |
| $\mathcal{E}_4$ | $\mathcal{E}_{(2,3)}$ | 12        |
| $\mathcal{E}_5$ | $\mathcal{E}_{(3,3)}$ | 2         |
| $\mathcal{E}_6$ | $\mathcal{E}_{(3,4)}$ | 2         |
| $\mathcal{E}_7$ | $\mathcal{E}_{(4,5)}$ | 4         |
| $\mathcal{E}_8$ | $\mathcal{E}_{(4,6)}$ | 2         |
| $\mathcal{E}_9$ | $\mathcal{E}_{(4,7)}$ | 2         |
| $\mathcal{E}_{10}$ | $\mathcal{E}_{(5,5)}$ | 3         |
| $\mathcal{E}_{11}$ | $\mathcal{E}_{(5,6)}$ | 3         |
| $\mathcal{E}_{12}$ | $\mathcal{E}_{(5,7)}$ | 2         |
| $\mathcal{E}_{13}$ | $\mathcal{E}_{(5,8)}$ | 1         |
| $\mathcal{E}_{14}$ | $\mathcal{E}_{(6,7)}$ | 2         |
| $\mathcal{E}_{15}$ | $\mathcal{E}_{(7,8)}$ | 2         |
Theorem 5. The SO and SO_red indices for are as follows:

\[ SO(G) = 248.313, \]
\[ SO_{\text{red}}(G) = 169.56. \]  

Proof. From the edge partitioning based on degree of chloroquine, we have the following computations for SO and SO_red indices:

\[
\text{SO}(G) = \sum_{j \in \mathcal{E}(G)} \sqrt{d_i + d_j - 2} = \sqrt{1 + 2 - 2 \cdot 1 \cdot 2} + \sqrt{1 + 3 - 2 \cdot 1 \cdot 3} \\
+ \sqrt{2 + 2 - 2 \cdot 2 \cdot (5)} + \sqrt{2 + 3 - 2 \cdot 2 \cdot 3} + \sqrt{3 + 3 - 2 \cdot 3 \cdot 3} \\
+ \sqrt{4 + 2 - 2 \cdot 2 \cdot 4} + \sqrt{3 + 5 - 2 \cdot 3 \cdot 5} + \sqrt{4 + 5 - 2 \cdot 4 \cdot 5} \\
+ \sqrt{4 + 4 - 2 \cdot 4 \cdot 6} + \sqrt{5 + 5 - 2 \cdot 5 \cdot 5} + \sqrt{4 + 6 - 2 \cdot 4 \cdot 6} \\
+ \sqrt{5 + 7 - 2 \cdot 5 \cdot 7} + \sqrt{5 + 8 - 2 \cdot 5 \cdot 8} + \sqrt{6 + 7 - 2 \cdot 6 \cdot 7} \\
+ \sqrt{7 + 8 - 2 \cdot 7 \cdot 8} = 248.313,
\]

\[
\text{SO}_{\text{red}}(G) = \sum_{j \in \mathcal{E}(G)} \sqrt{(d_i - 1)^2 + (d_j - 1)^2} \\
= \sqrt{(1 - 1)^2 + (2 - 1)^2} + \sqrt{(1 - 1)^2 + (3 - 1)^2} \\
+ \sqrt{(2 - 1)^2 + (2 - 1)^2} + \sqrt{(2 - 1)^2 + (3 - 1)^2} \\
+ \sqrt{(3 - 1)^2 + (3 - 1)^2} + \sqrt{(2 - 1)^2 + (4 - 1)^2} \\
+ \sqrt{(3 - 1)^2 + (5 - 1)^2} + \sqrt{(4 - 1)^2 + (5 - 1)^2} \\
+ \sqrt{(4 - 1)^2 + (6 - 1)^2} + \sqrt{(5 - 1)^2 + (5 - 1)^2} \\
+ \sqrt{(5 - 1)^2 + (6 - 1)^2} + \sqrt{(6 - 1)^2 + (7 - 1)^2} \\
+ \sqrt{(7 - 1)^2 + (8 - 1)^2} = 169.56.
\]
3.3. Hydroxychloroquine. It is an antimalarial drug administered to those areas where malaria remains sensitive to chloroquine. Rheumatoid arthritis, lupus, and porphyria cutanea tarda are among the conditions for which it is used. It is usually taken as hydroxychloroquine sulphate, and it is taken by mouth. 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.

Figures 5–6 show the molecular structure and molecular graphs of hydroxychloroquine. Table 3 shows the edge partition of the hydroxychloroquine based on the degree and neighborhood degree sum of vertices.

**Theorem 7.** The ABC and GA indices for hydroxychloroquine are as follows:

\[
\begin{align*}
ABC(G) &= 30.8323, \\
GA(G) &= 47.3676.
\end{align*}
\]

**Proof.** From the edge partitioning based on degree of hydroxychloroquine, we have the following computations for ABC and GA indices:

\[
\begin{align*}
ABC(G) &= \sum_{i,j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}} = \sqrt{\frac{1 + 2 - 2}{1 \times 2}} (2) + \sqrt{\frac{1 + 3 - 2}{1 \times 3}} (2) \\
&\quad + \sqrt{\frac{2 + 2 - 2}{2 \times 2}} (6) + \sqrt{\frac{2 + 3 - 2}{2 \times 3}} (13) + \sqrt{\frac{3 + 3 - 2}{3 \times 3}} (2) \\
&\quad + \sqrt{\frac{2 + 4 - 2}{2 \times 4}} (1) + \sqrt{\frac{3 + 5 - 2}{3 \times 5}} (3) + \sqrt{\frac{4 + 5 - 2}{4 \times 5}} (4) \\
&\quad + \sqrt{\frac{4 + 6 - 2}{4 \times 6}} (1) + \sqrt{\frac{5 + 5 - 2}{5 \times 5}} (3) + \sqrt{\frac{5 + 6 - 2}{5 \times 6}} (4) \\
&\quad + \sqrt{\frac{5 + 7 - 2}{5 \times 7}} (2) + \sqrt{\frac{5 + 8 - 2}{5 \times 8}} (1) + \sqrt{\frac{6 + 7 - 2}{6 \times 7}} (2) \\
&\quad + \sqrt{\frac{7 + 8 - 2}{7 \times 8}} (2) = 30.8323, \\
\end{align*}
\]

\[
\begin{align*}
GA(G) &= \sum_{i,j \in E(G)} 2 \sqrt{\frac{d_i d_j}{d_i + d_j}} = 2 \sqrt{\frac{1 \times 2}{1 + 2}} (2) + 2 \sqrt{\frac{1 \times 3}{1 + 3}} (2) \\
&\quad + 2 \sqrt{\frac{2 \times 2}{2 + 2}} (6) + 2 \sqrt{\frac{2 \times 3}{2 + 3}} (13) + 2 \sqrt{\frac{3 \times 3}{3 + 3}} (2) \\
&\quad + 2 \sqrt{\frac{2 \times 4}{2 + 4}} (1) + 2 \sqrt{\frac{3 \times 5}{3 + 5}} (3) + 2 \sqrt{\frac{4 \times 5}{4 + 5}} (4) \\
&\quad + 2 \sqrt{\frac{4 \times 6}{4 + 6}} (1) + 2 \sqrt{\frac{5 \times 5}{5 + 5}} (3) + 2 \sqrt{\frac{5 \times 6}{5 + 6}} (4) \\
&\quad + 2 \sqrt{\frac{5 \times 7}{5 + 7}} (2) + 2 \sqrt{\frac{5 \times 8}{5 + 8}} (1) + 2 \sqrt{\frac{6 \times 7}{6 + 7}} (2) \\
&\quad + 2 \sqrt{\frac{7 \times 8}{7 + 8}} (2) = 47.3676.
\end{align*}
\]

\[
\begin{align*}
\text{Figure 5: Molecular structure of hydroxychloroquine.}
\end{align*}
\]

\[
\begin{align*}
\text{Figure 6: Molecular graph of hydroxychloroquine.}
\end{align*}
\]

**Theorem 8.** The SO and \( SO_{\text{red}} \) indices for hydroxychloroquine are as follows:

\[
\begin{align*}
SO(G) &= 256.706, \\
SO_{\text{red}}(G) &= 190.746.
\end{align*}
\]

**Proof.** From the edge partitioning based on degree of hydroxychloroquine, we have the following computations for SO and \( SO_{\text{red}} \) indices:

\[
\begin{align*}
SO(G) &= \sum_{i,j \in E(G)} \sqrt{d_i^2 + d_j^2} = \sqrt{1^2 + 2^2} (2) + \sqrt{1^2 + 3^2} (2) \\
&\quad + \sqrt{2^2 + 2^2} (6) + \sqrt{2^2 + 3^2} (13) + \sqrt{3^2 + 3^2} (2) \\
&\quad + \sqrt{2^2 + 4^2} (1) + \sqrt{3^2 + 5^2} (3) + \sqrt{4^2 + 5^2} (4) \\
&\quad + \sqrt{4^2 + 6^2} (1) + \sqrt{5^2 + 5^2} (3) + \sqrt{5^2 + 6^2} (4) \\
&\quad + \sqrt{5^2 + 7^2} (2) + \sqrt{5^2 + 8^2} (1) + \sqrt{6^2 + 7^2} (2) \\
&\quad + \sqrt{7^2 + 8^2} (2) = 256.706,
\end{align*}
\]
SOII(G) = \sum_{i \in V(G)} \sqrt{(d_i - 1)^2 + (d_j - 1)^2} = \sqrt{(1 - 1)^2 + (2 - 1)^2(2)}
+ \sqrt{(1 - 1)^2 + (3 - 1)^2(2)} + \sqrt{(2 - 1)^2 + (2 - 1)^2(6)}
+ \sqrt{(2 - 1)^2 + (3 - 1)^2(12)} + \sqrt{(3 - 1)^2 + (3 - 1)^2(2)}
+ \sqrt{(2 - 1)^2 + (3 - 1)^2(1)} + \sqrt{(2 - 1)^2 + (4 - 1)^2(1)}
+ \sqrt{(3 - 1)^2 + (5 - 1)^2(3)} + \sqrt{(4 - 1)^2 + (6 - 1)^2(1)}
+ \sqrt{(4 - 1)^2 + (5 - 1)^2(4)} + \sqrt{(5 - 1)^2 + (5 - 1)^2(3)}
+ \sqrt{(5 - 1)^2 + (6 - 1)^2(4)} + \sqrt{(5 - 1)^2 + (7 - 1)^2(2)}
+ \sqrt{(5 - 1)^2 + (8 - 1)^2(1)} + \sqrt{(6 - 1)^2 + (7 - 1)^2(2)}
+ \sqrt{(7 - 1)^2 + (8 - 1)^2(2)} = 190.746.

Theorem 9. The SOII and SOII_{red} indices for hydroxychloroquine are as follows:

SOII(G) = 3.8716 \times 10^{17},

SOII_{red}(G) = 1.6591 \times 10^{15}.

Proof. From the edge partitioning based on degree of hydroxychloroquine, we have the following computations for SOII and SOII_{red} indices:

SOII(G) = \prod_{i \in V(G)} \sqrt{d_i^2 + d_j^2} = \sqrt{1^2 + 2^2(2)} \times \sqrt{1^2 + 3^2(2)}
\times \sqrt{2^2 + 3^2(6)} \times \sqrt{2^2 + 3^2(12)} \times \sqrt{3^2 + 3^2(2)}
\times \sqrt{2^2 + 3^2(1)} \times \sqrt{2^2 + 4^2(1)} \times \sqrt{3^2 + 5^2(3)}
\times \sqrt{4^2 + 6^2(1)} \times \sqrt{4^2 + 5^2(4)} \times \sqrt{5^2 + 5^2(3)}
\times \sqrt{5^2 + 6^2(4)} \times \sqrt{5^2 + 7^2(2)} \times \sqrt{5^2 + 8^2(1)}
\times \sqrt{6^2 + 7^2(2)} \times \sqrt{6^2 + 8^2(2)} = 3.8716 \times 10^{17}.

SOII_{red}(G) = \prod_{i \in V(G)} \sqrt{(d_i - 1)^2 + (d_j - 1)^2} = \sqrt{(1 - 1)^2 + (2 - 1)^2(2)}
\times \sqrt{(1 - 1)^2 + (3 - 1)^2(2)} \times \sqrt{(2 - 1)^2 + (2 - 1)^2(6)}
\times \sqrt{(2 - 1)^2 + (3 - 1)^2(12)} \times \sqrt{(3 - 1)^2 + (3 - 1)^2(2)}
\times \sqrt{(2 - 1)^2 + (3 - 1)^2(1)} \times \sqrt{(2 - 1)^2 + (4 - 1)^2(1)}
\times \sqrt{(3 - 1)^2 + (5 - 1)^2(3)} \times \sqrt{(4 - 1)^2 + (6 - 1)^2(1)}
\times \sqrt{(4 - 1)^2 + (5 - 1)^2(4)} \times \sqrt{(5 - 1)^2 + (5 - 1)^2(3)}
\times \sqrt{(5 - 1)^2 + (6 - 1)^2(4)} \times \sqrt{(5 - 1)^2 + (7 - 1)^2(2)}
\times \sqrt{(5 - 1)^2 + (8 - 1)^2(1)} \times \sqrt{(6 - 1)^2 + (7 - 1)^2(2)}
\times \sqrt{(7 - 1)^2 + (8 - 1)^2(2)} = 1.6591 \times 10^{15}.

Table 3: Edge partitioning based on degree of hydroxychloroquine.

| \(E\)  | \(E_{(d,j)}\) | 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         |

3.4. 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 7–8 show the molecular structure and molecular graphs of theaflavin. Table 4 shows the edge partition of the theaflavin based on the degree and neighborhood degree sum of vertices.
Theorem 10. The ABC and GA indices for theaflavin are as follows:

\[
ABC(G) = 62.3821, \\
\text{GA}(G) = 89.4750.
\]  

Proof. From the edge partitioning based on degree of theaflavin, we have the following computations for ABC and GA indices:

\[
\begin{align*}
ABC(G) &= \sum_{i,j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}} = \sqrt{\frac{1 + 3 - 2}{1 \times 3}} + \sqrt{\frac{2 + 3 - 2}{2 \times 3}} + \sqrt{\frac{3 + 3 - 2}{3 \times 3}} + \sqrt{\frac{5 + 5 - 2}{3 \times 5}} + \sqrt{\frac{6 + 6 - 2}{3 \times 6}} + \sqrt{\frac{6 + 7 - 2}{6 \times 7}} + \sqrt{\frac{7 + 9 - 2}{7 \times 9}} + \sqrt{\frac{8 + 9 - 2}{8 \times 9}} = 62.3821, \\
\text{GA}(G) &= \sum_{i,j \in E(G)} 2 \sqrt{\frac{d_i d_j}{d_i + d_j}} = 2 \sqrt{\frac{1 \times 3}{1 + 3}} + 2 \sqrt{\frac{2 \times 3}{2 + 3}} + 2 \sqrt{\frac{3 \times 5}{3 + 5}} + 2 \sqrt{\frac{3 \times 6}{3 + 6}} + 2 \sqrt{\frac{5 \times 6}{5 + 6}} + 2 \sqrt{\frac{6 \times 8}{6 + 8}} + 2 \sqrt{\frac{7 \times 8}{7 + 8}} + 2 \sqrt{\frac{8 \times 9}{8 + 9}} = 89.4750.
\end{align*}
\]

\[]

Table 4: Edge partitioning based on degree of theaflavin.

| \(\varepsilon\) | \(\varepsilon_{(d_i, d_j)}\) | Frequency |
|----------------|-----------------|-----------|
| \(\varepsilon_1\) | \(\varepsilon_{(1,3)}\) | 10        |
| \(\varepsilon_2\) | \(\varepsilon_{(2,3)}\) | 22        |
| \(\varepsilon_3\) | \(\varepsilon_{(3,3)}\) | 14        |
| \(\varepsilon_4\) | \(\varepsilon_{(3,5)}\) | 2         |
| \(\varepsilon_5\) | \(\varepsilon_{(3,6)}\) | 6         |
| \(\varepsilon_6\) | \(\varepsilon_{(3,7)}\) | 2         |
| \(\varepsilon_7\) | \(\varepsilon_{(5,6)}\) | 4         |
| \(\varepsilon_8\) | \(\varepsilon_{(6,6)}\) | 6         |
| \(\varepsilon_9\) | \(\varepsilon_{(6,7)}\) | 8         |
| \(\varepsilon_{10}\) | \(\varepsilon_{(6,8)}\) | 10        |
| \(\varepsilon_{11}\) | \(\varepsilon_{(7,8)}\) | 3         |
| \(\varepsilon_{12}\) | \(\varepsilon_{(7,9)}\) | 2         |
| \(\varepsilon_{13}\) | \(\varepsilon_{(8,8)}\) | 2         |
| \(\varepsilon_{14}\) | \(\varepsilon_{(8,9)}\) | 1         |

Theorem 11. The SO and SO\(_{\text{red}}\) indices for theaflavin are as follows:

\[
\text{SO}(G) = 582.751, \\
\text{SO}_{\text{red}}(G) = 410.37.
\]

Proof. From the edge partitioning based on degree of theaflavin, we have the following computations for SO and SO\(_{\text{red}}\) indices:

\[
\begin{align*}
\text{SO}(G) &= \sum_{i,j \in E(G)} \sqrt{d_i^2 + d_j^2} = \sqrt{1^2 + 3^2} + \sqrt{2^2 + 3^2} + \sqrt{3^2 + 5^2} + \sqrt{3^2 + 6^2} + \sqrt{5^2 + 6^2} + \sqrt{6^2 + 8^2} + \sqrt{7^2 + 8^2} + \sqrt{8^2 + 9^2} = 582.751, \\
\text{SO}_{\text{red}}(G) &= \sum_{i,j \in E(G)} \sqrt{(d_i - 1)^2 + (d_j - 1)^2} = \sqrt{(1 - 1)^2 + (3 - 1)^2} + \sqrt{(2 - 1)^2 + (3 - 1)^2} + \sqrt{(3 - 1)^2 + (5 - 1)^2} + \sqrt{(6 - 1)^2 + (6 - 1)^2} + \sqrt{(5 - 1)^2 + (7 - 1)^2} + \sqrt{(6 - 1)^2 + (7 - 1)^2} + \sqrt{(7 - 1)^2 + (8 - 1)^2} + \sqrt{(8 - 1)^2 + (9 - 1)^2} = 410.37.
\end{align*}
\]

\[]
Theorem 12. The SOII and SOII\textsubscript{red} indices for theaflavin are as follows:
\[
\begin{aligned}
\text{SOII}(G) &= 2.4755 \times 10^{24}, \\
\text{SOII}_{\text{red}}(G) &= 4.4016 \times 10^{18}.
\end{aligned}
\]  
(27)

Proof. From the edge partitioning based on degree of theaflavin, we have the following computations for SOII and SOI\textsubscript{red} indices:
\[
\begin{aligned}
\text{SOII}(G) &= \prod_{(ij) \in G} \sqrt{d_i^2 + d_j^2} = \sqrt{1^2 + 3^2} \times (10) \times \sqrt{2^2 + 3^2} \times 22, \\
&\quad \times \sqrt{3^2 + 2^2} \times (14) \times \sqrt{3^2 + 5^2} \times (2) \times \sqrt{3^2 + 6^2} \times (6), \\
&\quad \times \sqrt{3^2 + 7^2} \times (2) \times \sqrt{5^2 + 6^2} \times (4) \times \sqrt{6^2 + 6^2} \times (6), \\
&\quad \times \sqrt{6^2 + 7^2} \times (8) \times \sqrt{6^2 + 8^2} \times (10) \times \sqrt{7^2 + 8^2} \times (3), \\
&\quad \times \sqrt{7^2 + 9^2} \times (2) \times \sqrt{8^2 + 8^2} \times (2), \\
&\quad \times \sqrt{8^2 + 9^2} \times (1) = 2.4755 \times 10^{24}, \\
\text{SOII}_{\text{red}}(G) &= \prod_{(ij) \in G} \sqrt{(d_i - 1)^2 + (d_j - 1)^2} = \sqrt{(1 - 1)^2 + (3 - 1)^2} \times (10), \\
&\quad \times \sqrt{(2 - 1)^2 + (3 - 1)^2} \times (22) \times \sqrt{(3 - 1)^2 + (3 - 1)^2} \times (14), \\
&\quad \times \sqrt{(3 - 1)^2 + (5 - 1)^2} \times (2) \times \sqrt{(3 - 1)^2 + (6 - 1)^2} \times (6), \\
&\quad \times \sqrt{(3 - 1)^2 + (7 - 1)^2} \times (2) \times \sqrt{(5 - 1)^2 + (6 - 1)^2} \times (4), \\
&\quad \times \sqrt{(6 - 1)^2 + (6 - 1)^2} \times (6) \times \sqrt{(6 - 1)^2 + (7 - 1)^2} \times (8), \\
&\quad \times \sqrt{(6 - 1)^2 + (8 - 1)^2} \times (10) \times \sqrt{(7 - 1)^2 + (8 - 1)^2} \times (3), \\
&\quad \times \sqrt{(7 - 1)^2 + (9 - 1)^2} \times (2) \times \sqrt{(8 - 1)^2 + (8 - 1)^2} \times (2), \\
&\quad \times \sqrt{(8 - 1)^2 + (9 - 1)^2} \times (1) = 4.4016 \times 10^{18}. \\
\end{aligned}
\]  
(28)

3.5. Ritonavir. Ritonavir (a bioactive protein inhibitor drug) is used against virus. It creates deregulation in structural and functional protein of virus and produces noninfectious virus. It showed antiviral activity against major types of coronavirus which cause respiratory infection in human. Ritonavir is commonly used for mild and moderate COVID-19.

Figures 9–10 show the molecular structure and molecular graphs of ritonavir. Table 5 shows the degree partition of the ritonavir based on the degree and neighborhood degree sum of vertices.

Theorem 13. The ABC and GA indices for ritonavir are as follows:
\[
\begin{aligned}
\text{ABC}(G) &= 68.0157, \\
\text{GA}(G) &= 103.7042.
\end{aligned}
\]  
(29)

Proof. From the edge partitioning based on degree of ritonavir, we have the following computations for ABC and GA indices:
\[
\begin{aligned}
\text{ABC}(G) &= \sum_{(ij) \in G} \frac{d_i + d_j - 2}{d_i d_j} = \sqrt{1 + \frac{3 - 2}{1 \times 3}} + \sqrt{2 + \frac{2 - 2}{2 \times 2} (26) + \sqrt{3 + \frac{3 - 2}{3 \times 3}} + \sqrt{5 + \frac{5 - 2}{5 \times 5} (5) + \sqrt{3 + \frac{3 - 2}{3 \times 3}} + \sqrt{5 + \frac{5 - 2}{5 \times 5} (6), \\
&\quad + \sqrt{4 + \frac{4 - 2}{4 \times 4} (5) + \sqrt{3 + \frac{3 - 2}{3 \times 3}} + \sqrt{5 + \frac{5 - 2}{5 \times 5} (6), \\
&\quad + \sqrt{5 + \frac{5 - 2}{5 \times 5} (3) + \sqrt{3 + \frac{3 - 2}{3 \times 3}} + \sqrt{5 + \frac{5 - 2}{5 \times 5} (10), \\
&\quad + \sqrt{5 + \frac{5 - 2}{5 \times 5} (3) + \sqrt{3 + \frac{3 - 2}{3 \times 3}} + \sqrt{5 + \frac{5 - 2}{5 \times 5} (6), \\
&\quad + \sqrt{6 + \frac{6 - 2}{6 \times 6} (11) + \sqrt{5 + \frac{5 - 2}{5 \times 5} (1) + \sqrt{6 + \frac{6 - 2}{6 \times 6} (3}, \\
&\quad + \sqrt{6 + \frac{6 - 2}{6 \times 6} (2) = 68.0157, \\
\text{GA}(G) &= \sum_{(ij) \in G} \frac{2}{d_i d_j} = \frac{2}{d_i d_j} \sqrt{1 + \frac{3}{1 \times 3}} (9) + \frac{2}{d_i d_j} \sqrt{2 + \frac{2}{2 \times 2} (13), \\
&\quad + \frac{2}{d_i d_j} \frac{3}{2 \times 3} (26) + \frac{2}{d_i d_j} \frac{3}{3 \times 3} (5) + \frac{2}{d_i d_j} \frac{5}{5 \times 5} (5), \\
&\quad + \frac{2}{d_i d_j} \frac{4}{4 \times 4} (5) + \frac{2}{d_i d_j} \frac{3}{3 \times 3} (4) + \frac{2}{d_i d_j} \frac{5}{5 \times 5} (6), \\
&\quad + \frac{2}{d_i d_j} \frac{5}{5 \times 5} (3) + \frac{2}{d_i d_j} \frac{5}{5 \times 5} (10) + \frac{2}{d_i d_j} \frac{5}{5 \times 5} (3), \\
&\quad + \frac{2}{d_i d_j} \frac{6}{6 \times 6} (11) + \frac{2}{d_i d_j} \frac{5}{5 \times 5} (1) + \frac{2}{d_i d_j} \frac{6}{6 \times 6} (3), \\
&\quad + \frac{2}{d_i d_j} \frac{6}{6 \times 6} (2) = 103.7042. \\
\end{aligned}
\]  
(30)

Theorem 14. The SO and SO\textsubscript{red} indices for ritonavir are as follows:
\[
\begin{aligned}
\text{SO}(G) &= 578.4316, \\
\text{SO}_{\text{red}}(G) &= 432.8938.
\end{aligned}
\]  
(31)

Proof. From the edge partitioning based on degree of ritonavir, we have the following computations for SO and SO\textsubscript{red} indices:
Theorem 15. The SOII and SOII\textsubscript{red} indices for ritonavir are as follows:

\[
\begin{align*}
\text{SOII}(G) & = 3.684 \times 10^{22}, \\
\text{SOII}_{\text{red}}(G) & = 4.956 \times 10^{20}.
\end{align*}
\]

Proof. From the edge partitioning based on degree of ritonavir, we have the following computations for SOII and SOII\textsubscript{red} indices:
SOII(G) = \prod_{ij \in \mathcal{E}(G)} \sqrt{d_i^2 + d_j^2} = \sqrt{1^2 + 3^2} \times \sqrt{2^2 + 5^2} \times \sqrt{3^2 + 2^2} \times \sqrt{3^2 + 2^2} \times \sqrt{3^2 + 5^2} \times \sqrt{5^2 + 5^2} \times \sqrt{5^2 + 6^2} \times \sqrt{2^2 + 4^2} \\
= 3.684 \times 10^{22}.

\text{SOII}_\text{red}(G) = \prod_{ij \in \mathcal{E}(G)} \sqrt{(d_i - 1)^2 + (d_j - 1)^2} = \sqrt{(1 - 1)^2 + (3 - 1)^2} \times \sqrt{(2 - 1)^2 + (2 - 1)^2} \times \sqrt{(3 - 1)^2 + (3 - 1)^2} \times \sqrt{(4 - 1)^2 + (4 - 1)^2} \\
= 4.956 \times 10^{32}.

3.6. Arbidol. Arbidol acts as a viral inhibitor which inhibits the process of replication for virus for SARS coronavirus. It blocks the lipid membranous site of virus which make them bind with the host cell by blocking virus replication. It lowers the incidence of SARS-CoV-2 infection and selected for high risk population.

Figures 11–12 show the chemical structure and molecular graphs of arbidol. Table 6 shows the edge partition of the arbidol based on the degree and neighborhood degree sum of vertices.

Table 6: Edge partitioning based on degree of arbidol.

| \(\mathcal{E}\) | \(\mathcal{E}(d, d_i)\) | Frequency |
|------------------|--------------------------|-----------|
| \(\mathcal{E}_1\) | \(\mathcal{E}_{(1,1)}\)  | 1         |
| \(\mathcal{E}_2\) | \(\mathcal{E}_{(1,3)}\)  | 6         |
| \(\mathcal{E}_3\) | \(\mathcal{E}_{(2,2)}\)  | 6         |
| \(\mathcal{E}_4\) | \(\mathcal{E}_{(2,3)}\)  | 10        |
| \(\mathcal{E}_5\) | \(\mathcal{E}_{(3,3)}\)  | 9         |
| \(\mathcal{E}_6\) | \(\mathcal{E}_{(3,4)}\)  | 2         |
| \(\mathcal{E}_7\) | \(\mathcal{E}_{(3,5)}\)  | 1         |
| \(\mathcal{E}_8\) | \(\mathcal{E}_{(4,4)}\)  | 2         |
| \(\mathcal{E}_9\) | \(\mathcal{E}_{(5,5)}\)  | 4         |
| \(\mathcal{E}_{10}\) | \(\mathcal{E}_{(6,6)}\)  | 1         |
| \(\mathcal{E}_{11}\) | \(\mathcal{E}_{(6,8)}\)  | 2         |
| \(\mathcal{E}_{12}\) | \(\mathcal{E}_{(7,8)}\)  | 3         |
| \(\mathcal{E}_{13}\) | \(\mathcal{E}_{(7,9)}\)  | 1         |
| \(\mathcal{E}_{14}\) | \(\mathcal{E}_{(8,9)}\)  | 3         |
| \(\mathcal{E}_{15}\) | \(\mathcal{E}_{(9,9)}\)  | 1         |

Proof. From the edge partitioning based on degree of arbidol, we have the following computations for ABC and GA indices:

\[\text{ABC}(G) = \sum_{ij \in \mathcal{E}(G)} \sqrt{d_i + d_j} = \sqrt{1 + 2} + \sqrt{2 + 3} + \sqrt{3 + 5} + \sqrt{4 + 4} \]
\[+ \sqrt{5 + 7} + \sqrt{6 + 8} + \sqrt{8 + 9} = 39.3796,\]

\[\text{GA}(G) = 60.4714.\]
GA(G) = \sum_{ij \in E(G)} 2 \sqrt{d_i d_j} = 2 \sqrt{1 \times 2 1 + 2} + 2 \sqrt{1 \times 3 1 + 3} \\
+ 2 \sqrt{2 \times 2 2 + 2} + 2 \sqrt{2 \times 3 2 + 3} + 2 \sqrt{3 \times 3 3 + 3} \\
+ 2 \sqrt{3 \times 4 3 + 4} + 2 \sqrt{3 \times 5 3 + 5} + 2 \sqrt{4 \times 4 4 + 4} \\
+ 2 \sqrt{3 \times 6 3 + 6} + 2 \sqrt{5 \times 5 5 + 5} + 2 \sqrt{6 \times 6 6 + 6} \\
+ 2 \sqrt{6 \times 8 6 + 8} + 2 \sqrt{7 \times 7 7 + 7} + 2 \sqrt{9 \times 9 9 + 9} (36)

\textbf{Theorem 17.} The SO and SO_{\text{red}} indices for arbidol are as follows:

\[ \text{SO}(G) = 365.2403, \]
\[ \text{SO}_{\text{red}}(G) = 327.6648. \] (37)

\textbf{Proof.} From the edge partitioning based on degree of arbidol, we have the following computations for SO and SO_{\text{red}} indices:

\[ \text{SO}(G) = \sum_{ij \in E(G)} \sqrt{d_i^2 + d_j^2} = \sqrt{1^2 + 2^2(1)} + \sqrt{1^2 + 3^2(6)} \\
+ \sqrt{2^2 + 2^2(6)} + \sqrt{2^2 + 3^2(10)} + \sqrt{3^2 + 3^2(9)} \\
+ \sqrt{3^2 + 4^2(2)} + \sqrt{3^2 + 5^2(1)} + \sqrt{4^2 + 4^2(2)} \\
+ \sqrt{3^2 + 6^2(2)} + \sqrt{4^2 + 5^2(2)} + \sqrt{5^2 + 7^2(2)} \\
+ \sqrt{4^2 + 6^2(1)} + \sqrt{5^2 + 5^2(1)} + \sqrt{5^2 + 6^2(4)} \\
+ \sqrt{6^2 + 6^2(1)} + \sqrt{5^2 + 8^2(1)} + \sqrt{6^2 + 7^2(1)} \\
+ \sqrt{6^2 + 8^2(2)} + \sqrt{7^2 + 8^2(3)} + \sqrt{6^2 + 9^2(1)} \\
+ \sqrt{8^2 + 9^2(3)} + \sqrt{9^2 + 9^2(1)} = 365.2403, \]

\[ \text{SO}_{\text{red}}(G) = \sum_{ij \in E(G)} \sqrt{(d_i - 1)^2 + (d_j - 1)^2} = \sqrt{(1 - 1)^2 + (2 - 2)^2(1)} \\
+ \sqrt{(1 - 1)^2 + (3 - 1)^2(6)} + \sqrt{(2 - 1)^2 + (2 - 1)^2(6)} \\
+ \sqrt{(2 - 1)^2 + (3 - 1)^2(10)} + \sqrt{(3 - 1)^2 + (3 - 1)^2(9)} \\
+ \sqrt{(3 - 1)^2 + (4 - 1)^2(2)} + \sqrt{(3 - 1)^2 + (5 - 1)^2(1)} \\
+ \sqrt{(4 - 1)^2 + (6 - 1)^2(2)} + \sqrt{(3 - 1)^2 + (7 - 1)^2(2)} \\
+ \sqrt{(4 - 1)^2 + (5 - 1)^2(2)} + \sqrt{(3 - 1)^2 + (7 - 1)^2(2)} \\
+ \sqrt{(4 - 1)^2 + (5 - 1)^2(2)} + \sqrt{(3 - 1)^2 + (7 - 1)^2(2)} + \sqrt{(5 - 1)^2 + (5 - 1)^2(1)} \\
+ \sqrt{(5 - 1)^2 + (6 - 1)^2(4)} + \sqrt{(6 - 1)^2 + (6 - 1)^2(1)} \\
+ \sqrt{(5 - 1)^2 + (8 - 1)^2(2)} + \sqrt{(7 - 1)^2 + (8 - 1)^2(3)} \\
+ \sqrt{(6 - 1)^2 + (9 - 1)^2(1)} + \sqrt{(8 - 1)^2 + (9 - 1)^2(3)} \\
+ \sqrt{(9 - 1)^2 + (9 - 1)^2(1)} = 327.6648. \] (38)
4. Conclusion

In this paper, we studied the topological properties of some chemical compounds utilized to prevent COVID-19 outbreaks and transmission using degree-based indices. Drugs and other chemical substances are frequently shown as polygonal shapes, trees, graphs, and other geometrical shapes. We discussed the newly introduced atom-bond connectivity (ABC) index, Geometrically Arithmetic (GA) index, and Sombor invariants for the molecular graph of remdesivir (GS-5734), chloroquine, hydroxychloroquine, theaflavin, ritonavir, and arbidol. Figures 13–14 depict the graphical comparison of computed results for the aforementioned chemical structures. Topological indices can determine a variety of properties and functions including boiling point, entropy, enthalpy, acentric factor, and critical pressure. Our findings can be helpful in designing new drugs and vaccines for the treatment of COVID-19.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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