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Some degree-based topological indices of the molecular structure of drugs in the treatment RNA-viruses

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Abstract

The topological index is a molecular descriptor used to study the Quantitative Structure-Property Relationship (QSPR) study of drugs to examine their molecular characteristics by graph theory modeling. Predicting a drug's mechanism of action through theoretical evaluation of its molecular structure speeds up the process of finding and developing new medications.

In this study, we analyse the structure of several drugs, namely Oseltamivir, Favipiravir, and Chloroquine in the treatment of RNA viruses by computing some new topological indices. Through graph theory, we derive precise formulas for these topological indices of both the molecular graph and its corresponding line graph. The accuracy and validity of the obtained results are rigorously evaluated using computational tools like Matlab and Mathematica.

Subject Classification: *05C92, 05C09, 05C90, 92E10.*

Keywords: *RNA viruses, Sombor index, Line graph, Degree-based topological index.*

1. Introduction

RNA viruses are a type of virus that utilizes RNA for its genetic information. These viruses are responsible for a wide spectrum of human diseases, encompassing respiratory illnesses like the common cold and influenza, viral hemorrhagic fevers like Ebola and SARS, and other

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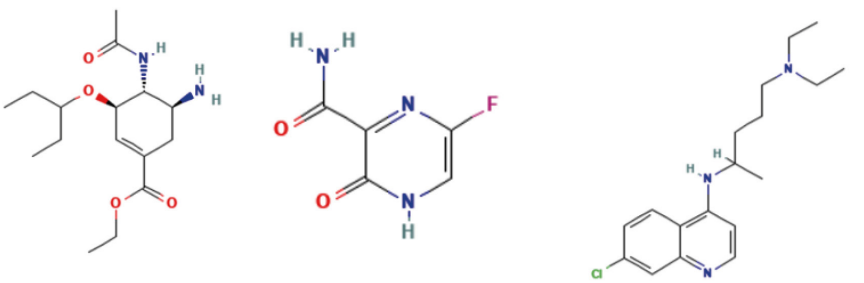
conditions like Hepatitis C, Dengue fever, and childhood diseases such as polio, mumps, and measles [1].

Oseltamivir, a medicine that fights viruses, is effective in treating and preventing influenza A and B, the viruses that cause the common flu. This medication belongs to a group of drugs called neuraminidase inhibitors. Oseltamivir is a medication that fights influenza by interfering with an enzyme (neuraminidase) that helps new viruses escape infected cells. This enzyme cuts a sugar molecule (sialic acid) on the cell surface, which viruses need to break free. By blocking this enzyme, Oseltamivir prevents the spread of new influenza particles [2]. This drug has the molecular formula $C_{16}H_{28}N_2O_4$. The chemical structure of Oseltamivir is presented in Figure 1(a).

Originally developed for its antiviral properties against RNA viruses, Favipiravir (a pyrazinecarboxamide derivative) works by being transformed within the host cell. This transformed version selectively disrupts the RNA polymerase enzyme of influenza viruses, hindering their replication. Due to this mechanism, Favipiravir is being investigated as a potential treatment for life-threatening RNA viral diseases like Ebola, Lassa, and most recently, COVID-19 [3]. The Molecular formula of Favipiravir is $C_5H_4FN_3O_2$ and its chemical structure is presented in Figure 1(b).

Chloroquine (CQ), traditionally employed for treating malaria, exhibits positive effects in reducing viral replication. Additionally, CQ seems to be effective against other viral infections like SARS and COVID-19 [4]. CQ inhibits endosomal viral RNA release and leads to a decrease in antigen processing and presentation [5]. The molecular formula of Chloroquine is $C_{18}H_{26}ClN_3$ (see Figure 1(c)).



a) ***b***) ***c***)

Figure 1

The chemical structure of a) Oseltamivir, b) Favipiravir, and c) Chloroquine.

Mathematical modeling is an essential tool in medical studies [6, 7]. As the development of medicines continues to grow, there is a need for research on how these structures interact with the body (pharmacological properties) of medications. Mathematical chemistry is an interdisciplinary field that analyses molecular structures using mathematical methods without requiring chemical testing. Chemical graph theory is a branch of mathematical chemistry that deals with the relationship between mathematics, chemistry, and graph theory [8, 9]. Using a graph theory approach called the topological index, the researchers established a strong correlation between the chemical, pharmacodynamic, and molecular structures of drugs. The structure of a chemical compound is depicted using a graph theory concept called a molecular graph. In this representation, vertices are the individual atoms and edges signify the bonds between them. Topological indices assign a numerical value to a molecule's structure. This value helps researchers understand the molecule's physical and chemical properties, as well as its potential biological effects [10].

Consider a molecular graph denoted by G_M with a vertex set $V(G_M) = \{v_1, \ldots, v_n\}$ and an edge set $E(G_M) = \{e_1, \ldots, e_m\}$. The set $N_{G_M}(u_i) = \{u_j \in V(G_M) \mid u_i u_j \in E(G_M)\}$ represents the neighborhood of vertex $u_i \in V(G_M)$ within the graph G_M and $|N_{G_M}(u_i)|$ is called the degree of u_i and is denoted by $\eta(u)$. The line graph $L(G_M)$ of a graph G_M is constructed which each edge in G_M becomes a vertex in $L(G_M)$. In $L(G_M)$, two vertices are connected if the corresponding edges in G_M are adjacent [11].

In [12], Gutman defined a novel family of topological indices as follows.

- The Sombor index

$$SO(G_M) = \sum_{uv \in E(G_M)} \sqrt{\eta(u)^2 + \eta(v)^2}.$$

- The reduced Sombor index

$$SO_{red}(G_M) = \sum_{uv \in E(G_M)} \sqrt{(\eta(u)-1)^2 + (\eta(v)-1)^2}.$$

- The average Sombor index

$$SO_{avg}(G_M) = \sum_{uv \in E(G_M)} \sqrt{\left(\eta(u)-\Omega\right)^2 + \left(\eta(v)-\Omega\right)^2}.$$

where $\Omega = \frac{2|E(G_M)|}{|V(G_M)|}$ and $\eta(x)$ denotes the degree of vertex x. For further reading on Sombor indices, interested readers may refer to [13-16].

A study by Radžeporić [17] demonstrates the effectiveness of the Sombor index, the reduced Sombor index, and the average Sombor index in modeling the thermodynamic properties of chemical structures. Liu et al. [18] reported that there is a high correlation between boiling points and these indices of some aromatic hydrocarbons.

Deng et al. [19] investigated the Sombor index in terms of application. Their study suggests that this index is a more accurate predictor of certain chemical properties compared to existing methods.

In a study by Liu et al. [20] the reduced Sombor index was compared to several established topological indices such that all tested on octane isomers. The study revealed that the reduced Sombor index can outperform these existing methods in some cases. In the following, we state some definitions of other types of Sombor indices that we need in this study.

- The modified Sombor index [21]

$$^{m}SO(G_M) = \sum_{uv \in E(G_M)} \frac{1}{\sqrt{\eta(u)^2 + \eta(v)^2}}.$$

- The multiplicative Sombor index [22]

$$SOII(G_M) = \prod_{uv \in E(G_M)} \sqrt{\eta(u)^2 + \eta(v)^2}.$$

- The multiplicative modified Sombor index [23]

$$MSOII(G_M) = \prod_{uv \in E(G_M)} \frac{1}{\sqrt{\eta(u)^2 + \eta(v)^2}}.$$

- The multiplicative reduced Sombor index [23]

$$RSOII(G_M) = \prod_{uv \in E(G_M)} \sqrt{(\eta(u)-1)^2 + (\eta(v)-1)^2}.$$

Sarkar et al. [24] examined a group of special indices, called multiplicative topological indices, to see if they could predict certain physical and chemical properties of octane isomers. These properties included AcentFac, molar volume, HVAP, density, entropy, and DHAVP.

Recently, analysing molecular structures by using the Sombor-type topological indices has received much attention. The Sombor indices are investigated for the molecular structures such as dendrimers in [25], the

hyaluronic acid-methotrexate conjugate in [26], some alkanes in [27], the polycyclic aromatic hydrocarbons in [28] and the antiviral drugs in [29].

This study focuses on calculating precise formulas of some Sombor indices for drugs used to treat RNA viruses. We also explore line graphs of these drug structures and perform the same calculations. Finally, we investigate the numerical data and give the results visually using graphs.

2. Methodology and Main Results

The structure of drug molecules such as Oseltamivir, Favipiravir, Ritonavir, Chloroquine, and Lopinavir in the treatment of RNA-viruses are studied in this section. We compute some Sombor indices for the graph and line graph of these drugs. We consider the edge partitions of the molecular graph G_M as $W_{ij} = \{xy \in E(G_M) \mid \eta(x) = i,\ \eta(y) = j\}$.

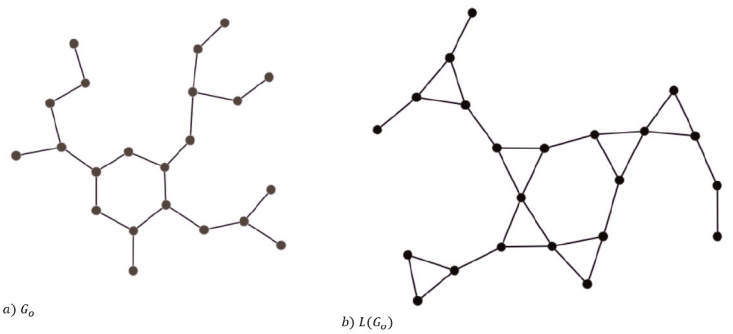


Figure 2

a) The molecular graph, and b) the line graph of Oseltamivir.

First, we consider the graph G_O corresponding to Oseltamivir, which consists of 22 vertices and 22 edges (see Figure 2(a)).

Table 1 displays the edge partitions of the molecular graph G_O (associated with Oseltamivir) along with their respective cardinalities. Thus, $|E(G_O)| = \sum_{i \le j} |W_{ij}| = |W_{12}| + |W_{13}| + |W_{22}| + |W_{23}| + |W_{33}| = 22$.

Table 1

The cardinality of edge partitions of G_o.

Edge partitions	W_{12}	W_{13}	W_{22}	W_{23}	W_{33}
Number of edges	3	4	1	11	3

Theorem 2.1: *Assume that G_O is the molecular graph of Oseltamivir. Then*

(i) $SO(G_O) = 11\sqrt{2} + 3\sqrt{5} + 4\sqrt{10} + 11\sqrt{13}$,

(ii) $SO_{red}(G_O) = 11 + 7\sqrt{2} + 11\sqrt{5}$,

(iii) ${}^{m}SO(G_O) = 2\sqrt{\frac{2}{5}} + \frac{3}{2\sqrt{2}} + \frac{3}{\sqrt{5}} + \frac{11}{\sqrt{13}}$,

(iv) $SO_{avg}(G_O) = 14 + 7\sqrt{2}$.

Proof: Using Table 1, we get

(i)

$$\begin{aligned} SO(G_O) &= |W_{12}|\sqrt{1^2+2^2} + |W_{13}|\sqrt{1^2+3^2} + |W_{22}|\sqrt{2^2+2^2} \\ &\quad + |W_{23}|\sqrt{2^2+3^2} + |W_{33}|\sqrt{3^2+3^2} \\ &= 3\sqrt{5} + 4\sqrt{10} + \sqrt{8} + 11\sqrt{13} + 3\sqrt{18} \\ &= 11\sqrt{2} + 3\sqrt{5} + 4\sqrt{10} + 11\sqrt{13}. \end{aligned}$$

(ii)

$$\begin{aligned} SO_{red}(G_O) &= |W_{12}|\sqrt{(1-1)^2+(2-1)^2} + |W_{13}|\sqrt{(1-1)^2+(3-1)^2} \\ &\quad + |W_{22}|\sqrt{(2-1)^2+(2-1)^2} + |W_{23}|\sqrt{(2-1)^2+(3-1)^2} \\ &\quad + |W_{33}|\sqrt{(3-1)^2+(3-1)^2} \\ &= 3 + 4\sqrt{4} + \sqrt{2} + 11\sqrt{5} + 3\sqrt{8} \\ &= 11 + 7\sqrt{2} + 11\sqrt{5}. \end{aligned}$$

(iii)

$$\begin{aligned} {}^{m}SO(G_O) &= |W_{12}|\left(\frac{1}{\sqrt{1^2+2^2}}\right) + |W_{13}|\left(\frac{1}{\sqrt{1^2+3^2}}\right) + |W_{22}|\left(\frac{1}{\sqrt{2^2+2^2}}\right) \\ &\quad + |W_{23}|\left(\frac{1}{\sqrt{2^2+3^2}}\right) + |W_{33}|\left(\frac{1}{\sqrt{3^2+3^2}}\right) \\ &= \frac{3}{\sqrt{5}} + \frac{4}{\sqrt{10}} + \frac{1}{\sqrt{8}} + \frac{11}{\sqrt{13}} + \frac{3}{\sqrt{18}} \\ &= 2\sqrt{\frac{2}{5}} + \frac{3}{2\sqrt{2}} + \frac{3}{\sqrt{5}} + \frac{11}{\sqrt{13}}. \end{aligned}$$

(iv) Since $|V(G_O)| = |E(G_O)| = 22$, we have $\frac{2|E(G_O)|}{|V(G_O)|} = 2$. Thus,

$$\begin{aligned} SO_{avg}(G_O) &= |W_{12}|\sqrt{(1-2)^2+(2-2)^2} + |W_{13}|\sqrt{(1-2)^2+(3-2)^2} \\ &\quad + |W_{22}|\sqrt{(2-2)^2+(2-2)^2} + |W_{23}|\sqrt{(2-2)^2+(3-2)^2} \\ &\quad + |W_{33}|\sqrt{(3-2)^2+(3-2)^2} \\ &= 3+4\sqrt{2}+11+3\sqrt{2} \\ &= 14+7\sqrt{2}. \end{aligned}$$

Theorem 2.2: *Assume that* G_O *is the molecular graph of Oseltamivir. Then*

(i) $SOII(G_O) = 4.00996\times(10)^{10}\times\sqrt{65}$,

(ii) $MSOII(G_O) = 3.8366\times(10)^{-13}\times\sqrt{65}$,

(iii) $RSOII(G_O) = 16\times(10)^{5}\times\sqrt{5}$.

Proof:

(i)

$$\begin{aligned} SOII(G_O) &= (\sqrt{1^2+2^2})^{|W_{12}|}\times(\sqrt{1^2+3^2})^{|W_{13}|}\times(\sqrt{2^2+2^2})^{|W_{22}|} \\ &\quad \times(\sqrt{2^2+3^2})^{|W_{23}|}\times(\sqrt{3^2+3^2})^{|W_{33}|} \\ &= (\sqrt{5})^3\times(\sqrt{10})^4\times\sqrt{8}\times(\sqrt{13})^{11}\times(\sqrt{18})^3 \\ &= 40099644\times(10)^3\times\sqrt{65}. \end{aligned}$$

(ii)

$$\begin{aligned} MSOII(G_O) &= \left(\frac{1}{\sqrt{1^2+2^2}}\right)^{|W_{12}|}\times\left(\frac{1}{\sqrt{1^2+3^2}}\right)^{|W_{13}|}\times\left(\frac{1}{\sqrt{2^2+2^2}}\right)^{|W_{22}|} \\ &\quad \times\left(\frac{1}{\sqrt{2^2+3^2}}\right)^{|W_{23}|}\times\left(\frac{1}{\sqrt{3^2+3^2}}\right)^{|W_{33}|} \\ &= \left(\frac{1}{\sqrt{5}}\right)^3\times\left(\frac{1}{\sqrt{10}}\right)^4\times\frac{1}{\sqrt{8}}\times\left(\frac{1}{\sqrt{13}}\right)^{11}\times\left(\frac{1}{\sqrt{18}}\right)^3 \\ &= \frac{1}{40099644\times(10)^3\times\sqrt{65}}. \end{aligned}$$

(iii)

$$\begin{aligned} RSOII(G_O) &= (\sqrt{(1-1)^2+(2-1)^2})^{|W_{12}|}\times(\sqrt{(1-1)^2+(3-1)^2})^{|W_{13}|} \\ &\quad \times(\sqrt{(2-1)^2+(2-1)^2})^{|W_{22}|}\times(\sqrt{(2-1)^2+(3-1)^2})^{|W_{23}|} \end{aligned}$$

$$\times(\sqrt{(3-1)^2+(3-1)^2})^{|W_{33}|}$$
$$=(\sqrt{4})^4\times\sqrt{2}\times(\sqrt{5})^{11}\times(\sqrt{8})^3$$
$$=16\times(10)^5\times\sqrt{5}.$$

We have the line graph $L(G_O)$ corresponding to Oseltamivir, which consists of 22 vertices and 29 edges (see Figure 2(b)). Table 2 displays the edge partitions of the molecular graph G_O (associated with Oseltamivir) along with their respective cardinalities. Thus, $|E(L(G_O))| = \sum_{i\le j}|W_{ij}| = 29$.

Table 2

The cardinality of edge partitions of $L(G_O)$.

Edge partitions	W_{12}	W_{13}	W_{22}	W_{23}	W_{24}	W_{33}	W_{34}	W_{44}
Number of edges	1	2	1	5	2	9	8	1

Similar to Theorems 2.1 and 2.2, the following results are given for the graph $L(G_O)$.

Theorem 2.3: *Assume that $L(G_O)$ is the line graph of Oseltamivir. Then*

(i) $SO(L(G_O)) = 40+33\sqrt{2}+5\sqrt{5}+2\sqrt{10}$,

(ii) $SO_{red}(L(G_O)) = 5+22\sqrt{2}+5\sqrt{5}+2\sqrt{10}+8\sqrt{13}$,

(iii) $^{m}SO(L(G_O)) = \frac{8}{5}+\sqrt{\frac{2}{5}}+\frac{15}{4\sqrt{2}}+\frac{2}{\sqrt{5}}+\frac{5}{\sqrt{13}}$,

(iv) $SO_{avg}(L(G_O)) = \frac{1}{29}(473\sqrt{2}+\sqrt{421}+4\sqrt{1345}+5\sqrt{2045}+2\sqrt{2074}+8\sqrt{7033})$.

Theorem 2.4: *Assume that $L(G_O)$ is the line graph of Oseltamivir. Then*

(i) $SOII(L(G_O)) = 6.65285\times(10)^{16}\times\sqrt{130}$,

(ii) $MSOII(L(G_O)) = 1.15624\times(10)^{-19}\times\sqrt{130}$,

(iii) $RSOII(L(G_O)) = 1.40383\times(10)^{12}\times\sqrt{10}$.

We have the molecular graph G_F corresponding to Favipiravir, which consists of 32 vertices and 33 edges (see Figure 3(a)). Table 3 displays the edge partitions of the molecular graph G_O (associated with Favipiravir) along with their respective cardinalities. Thus, $|E(G_F)| = \sum_{i\le j}|W_{ij}| = 33$.

$a)\ G_F$ $b)\ L(G_F)$

Figure 3

a) The molecular graph and b) the line graph of Favipiravir.

Table 3

The cardinality of edge partitions of G_F.

Edge partitions	W_{13}	W_{14}	W_{22}	W_{23}	W_{24}	W_{33}
Number of edges	6	7	1	7	5	7

Theorem 2.5: *Assume that G_F is the molecular graph of Favipiravir. Then*

(i) $SO(G_F) = 23\sqrt{2} + 10\sqrt{5} + 6\sqrt{10} + 7\sqrt{13} + 7\sqrt{17}$,

(ii) $SO_{red}(G_F) = 33 + 15\sqrt{2} + 7\sqrt{5} + 5\sqrt{10}$,

(iii) ${}^{m}SO(G_F) = 3\sqrt{\frac{2}{5}} + \frac{17}{6\sqrt{2}} + \frac{\sqrt{5}}{2} + \frac{7}{\sqrt{13}} + \frac{7}{\sqrt{17}}$,

(iv) $SO_{avg}(G_F) = \frac{1}{33}(247\sqrt{2} + 10\sqrt{1157} + 7\sqrt{1229} + 6\sqrt{2186} + 7\sqrt{5585})$.

Proof: Using Table 3, we get

(i)

$$\begin{aligned} SO(G_F) &= |W_{13}|\sqrt{1^2+3^2} + |W_{14}|\sqrt{1^2+4^2} \\ &\quad + |W_{22}|\sqrt{2^2+2^2} + |W_{23}|\sqrt{2^2+3^2} \\ &\quad + |W_{24}|\sqrt{2^2+4^2} + |W_{33}|\sqrt{3^2+3^2} \\ &= 6\sqrt{10} + 7\sqrt{17} + \sqrt{8} + 7\sqrt{13} + 5\sqrt{20} + 7\sqrt{18} \\ &= 23\sqrt{2} + 10\sqrt{5} + 6\sqrt{10} + 7\sqrt{13} + 7\sqrt{17}. \end{aligned}$$

(ii)

$$\begin{aligned}SO_{red}(G_F) &= |W_{13}|\sqrt{(1-1)^2+(3-1)^2}+|W_{14}|\sqrt{(1-1)^2+(4-1)^2}\\ &\quad+|W_{22}|\sqrt{(2-1)^2+(2-1)^2}+|W_{23}|\sqrt{(2-1)^2+(3-1)^2}\\ &\quad+|W_{24}|\sqrt{(2-1)^2+(4-1)^2}+|W_{33}|\sqrt{(3-1)^2+(3-1)^2}\\ &= 6\sqrt{4}+7\sqrt{9}+\sqrt{2}+7\sqrt{5}+5\sqrt{10}+7\sqrt{8}\\ &= 33+15\sqrt{2}+7\sqrt{5}+5\sqrt{10}.\end{aligned}$$

(iii)

$$\begin{aligned}{}^{m}SO(G_F) &= |W_{13}|\left(\frac{1}{\sqrt{1^2+3^2}}\right)+|W_{14}|\left(\frac{1}{\sqrt{1^2+4^2}}\right)+|W_{22}|\left(\frac{1}{\sqrt{2^2+2^2}}\right)\\ &\quad+|W_{23}|\left(\frac{1}{\sqrt{2^2+3^2}}\right)+|W_{24}|\left(\frac{1}{\sqrt{2^2+4^2}}\right)+|W_{33}|\left(\frac{1}{\sqrt{3^2+3^2}}\right)\\ &= \frac{6}{\sqrt{10}}+\frac{7}{\sqrt{17}}+\frac{1}{\sqrt{8}}+\frac{7}{\sqrt{13}}+\frac{5}{\sqrt{20}}+\frac{7}{\sqrt{18}}\\ &= 3\sqrt{\frac{2}{5}}+\frac{17}{6\sqrt{2}}+\frac{\sqrt{5}}{2}+\frac{7}{\sqrt{13}}+\frac{7}{\sqrt{17}}.\end{aligned}$$

(iv) Since $|V(G_F)|=32$ and $|E(G_F)|=33$, we have $\frac{2|E(G_F)|}{|V(G_F)|}=\frac{33}{16}$. Thus,

$$\begin{aligned}SO_{avg}(G_F) &= |W_{13}|\sqrt{\left(1-\tfrac{33}{16}\right)^2+\left(3-\tfrac{33}{16}\right)^2}+|W_{14}|\sqrt{\left(1-\tfrac{33}{16}\right)^2+\left(4-\tfrac{33}{16}\right)^2}\\ &\quad+|W_{22}|\sqrt{\left(2-\tfrac{33}{16}\right)^2+\left(2-\tfrac{33}{16}\right)^2}+|W_{23}|\sqrt{\left(2-\tfrac{33}{16}\right)^2+\left(3-\tfrac{33}{16}\right)^2}\\ &\quad+|W_{24}|\sqrt{\left(2-\tfrac{33}{16}\right)^2+\left(4-\tfrac{33}{16}\right)^2}+|W_{33}|\sqrt{\left(3-\tfrac{33}{16}\right)^2+\left(3-\tfrac{33}{16}\right)^2}\\ &= \frac{1}{33}(247\sqrt{2}+10\sqrt{1157}+7\sqrt{1229}+6\sqrt{2186}+7\sqrt{5585}).\end{aligned}$$

Theorem 2.6: *Assume that G_F is the molecular graph of Favipiravir. Then*

(i) $SOII(G_F)=6.04318\times(10)^{17}\times\sqrt{1105}$,

(ii) $MSOII(G_F)=1.49752\times(10)^{-21}\times\sqrt{1105}$,

(iii) $RSOII(G_F)=1.79159\times(10)^{13}\times\sqrt{2}$.

Proof:

(i)

$$SOII(G_F)=(\sqrt{1^2+3^2})^{|W_{13}|}\times(\sqrt{1^2+4^2})^{|W_{14}|}\times(\sqrt{2^2+2^2})^{|W_{22}|}$$

$$\times(\sqrt{2^2+3^2})^{|W_{23}|}\times(\sqrt{2^2+4^2})^{|W_{24}|}\times(\sqrt{3^2+3^2})^{|W_{33}|}$$
$$=(\sqrt{10})^6\times(\sqrt{17})^7\times\sqrt{8}\times(\sqrt{13})^7\times(\sqrt{20})^5\times(\sqrt{18})^7$$
$$=6.04318\times(10)^{17}\times\sqrt{1105}.$$

(ii)

$$MSOII(G_F)=\left(\frac{1}{\sqrt{1^2+3^2}}\right)^{|W_{13}|}\times\left(\frac{1}{\sqrt{1^2+4^2}}\right)^{|W_{14}|}\times\left(\frac{1}{\sqrt{2^2+2^2}}\right)^{|W_{22}|}$$
$$\times\left(\frac{1}{\sqrt{2^2+3^2}}\right)^{|W_{23}|}\times\left(\frac{1}{\sqrt{2^2+4^2}}\right)^{|W_{24}|}\times\left(\frac{1}{\sqrt{3^2+3^2}}\right)^{|W_{33}|}$$
$$=\left(\frac{1}{\sqrt{10}}\right)^6\times\left(\frac{1}{\sqrt{17}}\right)^7\times\frac{1}{\sqrt{8}}\times\left(\frac{1}{\sqrt{13}}\right)^7\times\left(\frac{1}{\sqrt{20}}\right)^5\times\left(\frac{1}{\sqrt{180}}\right)^7$$
$$=1.49752\times(10)^{-21}\times\sqrt{1105}.$$

(iii)

$$RSOII(G_F)=(\sqrt{(1-1)^2+(3-1)^2})^{|W_{13}|}\times(\sqrt{(1-1)^2+(4-1)^2})^{|W_{14}|}$$
$$\times(\sqrt{(2-1)^2+(2-1)^2})^{|W_{22}|}\times(\sqrt{(2-1)^2+(3-1)^2})^{|W_{23}|}$$
$$\times(\sqrt{(2-1)^2+(4-1)^2})^{|W_{24}|}\times(\sqrt{(3-1)^2+(3-1)^2})^{|W_{33}|}$$
$$=(\sqrt{4})^6\times(\sqrt{9})^7\times\sqrt{2}\times(\sqrt{10})^7\times(\sqrt{8})^5\times(\sqrt{8})^7$$
$$=1.79159\times(10)^{13}\times\sqrt{2}.$$

We have the line graph $L(G_F)$ corresponding to Favipiravir, which consists of 33 vertices and 52 edges (see Figure 3(b)). Table 4 displays the edge partitions of the line graph $L(G_F)$ along with their respective cardinalities. Thus, $|E(L(G_F))| = \sum_{i\le j}|W_{ij}| = 52$.

Table 4

The cardinality of edge partitions of $L(G_F)$.

Edge partitions	W_{22}	W_{23}	W_{24}	W_{33}	W_{34}	W_{44}
Number of edges	1	3	9	10	19	10

Similar to Theorems 2.5 and 2.6, the following results are obtained for $L(G_F)$.

Theorem 2.7: *Assume that $L(G_F)$ is the line graph of Favipiravir. Then*

(i) $SO(L(G_F)) = 95 + 72\sqrt{2} + 18\sqrt{5} + 3\sqrt{13}$,

(ii) $SO_{red}(L(G_F)) = 51\sqrt{2} + 3\sqrt{5} + 9\sqrt{10} + 19\sqrt{13}$,

(iii) ${}^{m}SO(L(G_F)) = \frac{19}{5} + \frac{19}{3\sqrt{2}} + \frac{9}{2\sqrt{5}} + \frac{3}{\sqrt{13}}$,

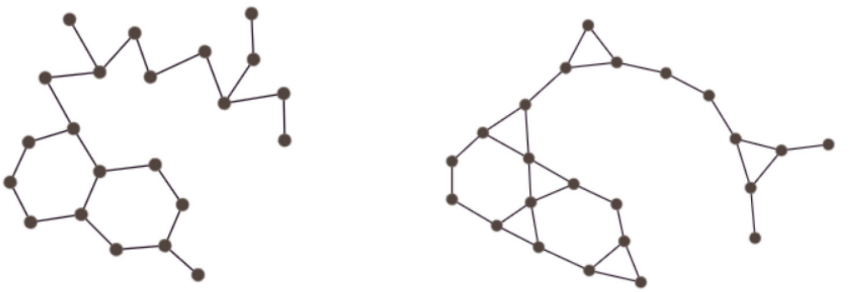
(iv) $SO_{avg}(L(G_F)) = \frac{1}{26}(1179\sqrt{2} + 3\sqrt{2386} + 9\sqrt{5402} + 19\sqrt{7066})$.

Theorem 2.8: *Suppose that* $L(G_F)$ *bis the line graph of Favipiravir. Then*

(i) $SOII(L(G_F)) = 1.00616 \times (10)^{34} \times \sqrt{130}$,

(ii) $MSOII(L(G_F)) = 7.64523 \times (10)^{-37} \times \sqrt{130}$,

(iii) $RSOII(L(G_F)) = 3.28301 \times (10)^{26} \times \sqrt{13}$.



$a)\ G_C$ $b)\ L(G_C)$

Figure 4

a) The molecular graph and b) the line graph of Chloroquine.

Here, we consider the graph G_C as the molecular graph of Chloroquine with $|V(G_C)| = 22$ vertices and $|E(G_C)| = 23$ edges (see Figure 4(a)). Table 5 displays the edge partitions of the molecular graph G_C along with their respective cardinalities. Thus, $|E(G_C)| = \sum_{i \le j} |W_{ij}| = 23$.

Table 5

The cardinality of edge partitions of G_C.

Edge partitions	W_{12}	W_{13}	W_{22}	W_{23}	W_{33}
Number of edges	2	2	5	12	2

Theorem 2.9: *Assume that G_C is the molecular graph of Chloroquine. Then*

(i) $SO(G_C) = 16\sqrt{2} + 2\sqrt{5} + 2\sqrt{10} + 12\sqrt{13}$,

(ii) $SO_{red}(G_C) = 6 + 9\sqrt{2} + 12\sqrt{5}$,

(iii) ${}^{m}SO(G_C) = \sqrt{\frac{2}{5}} + \frac{19}{6\sqrt{2}} + \frac{2}{\sqrt{5}} + \frac{12}{\sqrt{13}}$,

(iv) $SO_{avg}(G_C) = \frac{1}{23}(60\sqrt{2} + 2\sqrt{445} + 12\sqrt{629} + 2\sqrt{1066})$.

Proof: Using Table 5, we get

(i)

$$\begin{aligned} SO(G_C) &= |W_{12}|\sqrt{1^2+2^2} + |W_{13}|\sqrt{1^2+3^2} + |W_{22}|\sqrt{2^2+2^2} \\ &\quad + |W_{23}|\sqrt{2^2+3^2} + |W_{33}|\sqrt{3^2+3^2} \\ &= 2\sqrt{5} + 2\sqrt{10} + 5\sqrt{8} + 12\sqrt{13} + 2\sqrt{18} \\ &= 16\sqrt{2} + 2\sqrt{5} + 2\sqrt{10} + 12\sqrt{13}. \end{aligned}$$

(ii)

$$\begin{aligned} SO_{red}(G_C) &= |W_{12}|\sqrt{(1-1)^2+(2-1)^2} + |W_{13}|\sqrt{(1-1)^2+(3-1)^2} \\ &\quad + |W_{22}|\sqrt{(2-1)^2+(2-1)^2} + |W_{23}|\sqrt{(2-1)^2+(3-1)^2} \\ &\quad + |\ \ _{33}|\sqrt{(3-1)^2+(3-1)^2} \\ &= 2 + 2\sqrt{4} + 5\sqrt{2} + 12\sqrt{5} + 2\sqrt{8} \\ &= 6 + 9\sqrt{2} + 12\sqrt{5}. \end{aligned}$$

(iii)

$$\begin{aligned} {}^{m}SO(G_C) &= |W_{12}|\left(\frac{1}{\sqrt{1^2+2^2}}\right) + |W_{13}|\left(\frac{1}{\sqrt{1^2+3^2}}\right) + |W_{22}|\left(\frac{1}{\sqrt{2^2+2^2}}\right) \\ &\quad + |W_{23}|\left(\frac{1}{\sqrt{2^2+3^2}}\right) + |W_{33}|\left(\frac{1}{\sqrt{3^2+3^2}}\right) \\ &= \frac{2}{\sqrt{5}} + \frac{2}{\sqrt{10}} + \frac{5}{\sqrt{8}} + \frac{12}{\sqrt{13}} + \frac{2}{\sqrt{18}} \\ &= \sqrt{\frac{2}{5}} + \frac{19}{6\sqrt{2}} + \frac{2}{\sqrt{5}} + \frac{12}{\sqrt{13}}. \end{aligned}$$

(iv) Since $|V(G_C)| = 22$ and $|E(G_C)| = 23$, we have $\frac{2|E(G_C)|}{|V(G_C)|} = \frac{23}{11}$. Thus,

$$SO_{avg}(G_C) = |W_{12}|\sqrt{\left(1-\frac{23}{11}\right)^2+\left(2-\frac{23}{11}\right)^2} + |W_{13}|\sqrt{\left(1-\frac{23}{11}\right)^2+\left(3-\frac{23}{11}\right)^2}$$
$$+ |W_{22}|\sqrt{\left(2-\frac{23}{11}\right)^2+\left(2-\frac{23}{11}\right)^2} + |W_{23}|\sqrt{\left(2-\frac{23}{11}\right)^2+\left(3-\frac{23}{11}\right)^2}$$
$$+ |W_{33}|\sqrt{\left(3-\frac{23}{11}\right)^2+\left(3-\frac{23}{11}\right)^2}$$
$$= \frac{1}{23}(60\sqrt{2} + 2\sqrt{445} + 12\sqrt{629} + 2\sqrt{1066}).$$

Theorem 2.10: *Assume that G_C is the molecular graph of Chloroquine. Then*

(i) $SOII(G_C) = 5.56048 \times (10)^{11} \times \sqrt{2}$,

(ii) $MSOII(G_C) = 8.99202 \times (10)^{-13} \times \sqrt{2}$,

(iii) $RSOII(G_C) = 2 \times (10)^6 \times \sqrt{2}$.

Proof:

(i)

$$SOII(G_C) = (\sqrt{1^2+2^2})^{|W_{12}|} \times (\sqrt{1^2+3^2})^{|W_{13}|} \times (\sqrt{2^2+2^2})^{|W_{22}|}$$
$$\times (\sqrt{2^2+3^2})^{|W_{23}|} \times (\sqrt{3^2+3^2})^{|W_{33}|}$$
$$= (\sqrt{5})^2 \times (\sqrt{10})^2 \times (\sqrt{8})^5 \times (\sqrt{13})^{12} \times (\sqrt{18})^2$$
$$= 5560483968 \times (10)^2 \times \sqrt{2}.$$

(ii)

$$MSOII(G_C) = \left(\frac{1}{\sqrt{1^2+2^2}}\right)^{|W_{12}|} \times \left(\frac{1}{\sqrt{1^2+3^2}}\right)^{|W_{13}|} \times \left(\frac{1}{\sqrt{2^2+2^2}}\right)^{|W_{22}|}$$
$$\times \left(\frac{1}{\sqrt{2^2+3^2}}\right)^{|W_{23}|} \times \left(\frac{1}{\sqrt{3^2+3^2}}\right)^{|W_{33}|}$$
$$= \left(\frac{1}{\sqrt{5}}\right)^2 \times \left(\frac{1}{\sqrt{10}}\right)^2 \times \left(\frac{1}{\sqrt{8}}\right)^5 \times \left(\frac{1}{\sqrt{13}}\right)^{12} \times \left(\frac{1}{\sqrt{18}}\right)^2$$
$$= \frac{1}{5560483968 \times (10)^2 \times \sqrt{2}}.$$

(iii)

$$RSOII(G_C) = (\sqrt{(1-1)^2+(2-1)^2})^{|W_{12}|} \times (\sqrt{(1-1)^2+(3-1)^2})^{|W_{13}|}$$
$$\times (\sqrt{(2-1)^2+(2-1)^2})^{|W_{22}|} \times (\sqrt{(2-1)^2+(3-1)^2})^{|W_{23}|}$$

$$\times(\sqrt{(3-1)^2+(3-1)^2})^{|W_{33}|}$$
$$=(\sqrt{4})^2\times(\sqrt{2})^5\times(\sqrt{5})^{12}\times(\sqrt{8})^2$$
$$=2\times(10)^6\times\sqrt{2}.$$

According to Figure 4(b), $L(G_C)$ (the line graph of Chloroquine) has 23 vertices and 30 edges. Table 6 displays the edge partitions of the molecular graph $L(G_C)$ along with their respective cardinalities. Thus, $|E(L(G_C))| = \sum_{i\le j}|W_{ij}| = 30$.

Table 6

The cardinality of edge partitions of $L(G_C)$.

Edge partitions	W_{13}	W_{22}	W_{23}	W_{33}	W_{34}	W_{44}
Number of edges	2	2	10	9	6	1

Similar to Theorems 2.9 and 2.10, the following results for line $L(G_C)$ are obtained.

Theorem 2.11: *Assume that $L(G_C)$ is the line graph of Chloroquine. Then*

(i) $SO(L(G_C)) = 30+35\sqrt{2}+2\sqrt{10}+10\sqrt{13}$,

(ii) $SO_{red}(L(G_C)) = 4+23\sqrt{2}+10\sqrt{5}+6\sqrt{13}$,

(iii) ${}^{m}SO(L(G_C)) = \frac{6}{5}+\frac{17}{4\sqrt{2}}+\frac{10}{\sqrt{13}}$,

(iv) $SO_{avg}(L(G_C)) = \frac{1}{15}(249\sqrt{2}+4\sqrt{137}+10\sqrt{533}+6\sqrt{1853})$.

Theorem 2.12: *Assume that $L(G_C)$ is the line graph of Chloroquine. Then*

(i) $SOII(L(G_C)) = 1.16931\times(10)^{18}$,

(ii) $MSOII(L(G_C)) = 8.55208\times(10)^{-19}$,

(iii) $RSOII(L(G_C)) = 2.69967\times(10)^{12}$.

3. Numerical comparison and discussion

The pharmaceutical model based on the QSAR analysis is effective for the design and development of drugs in the treatment of many diseases. Analysis of topological indices in QSAR models can play an important role in drug targets.

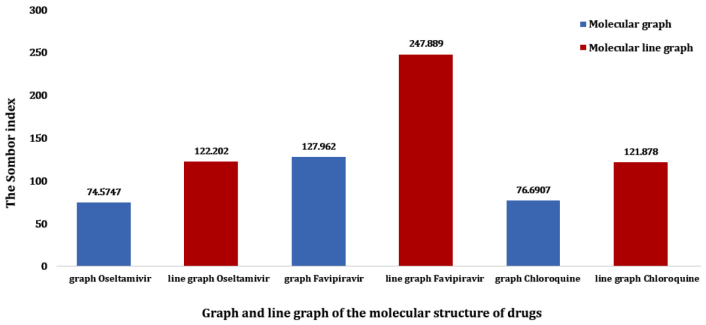


Figure 5

Comparison of *SO* of the graph and line graph Oseltamivir, Favipiravir, and Chloroquine.

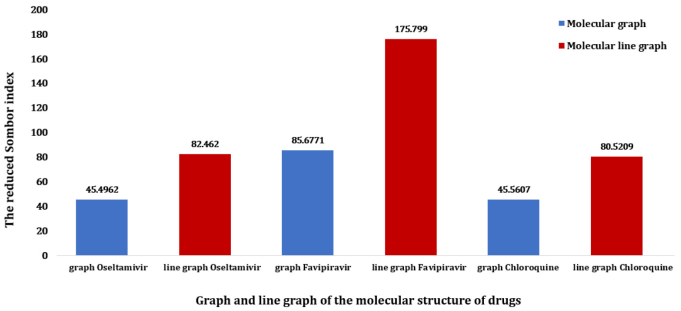


Figure 6

Comparison of SO_{red} of the graph and line graph Oseltamivir, Favipiravir, and Chloroquine.

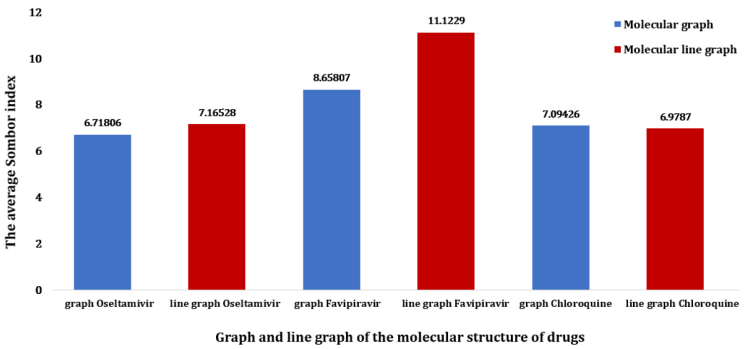


Figure 7

Comparison of SO_{avg} of the graph and line graph Oseltamivir, Favipiravir, and Chloroquine.

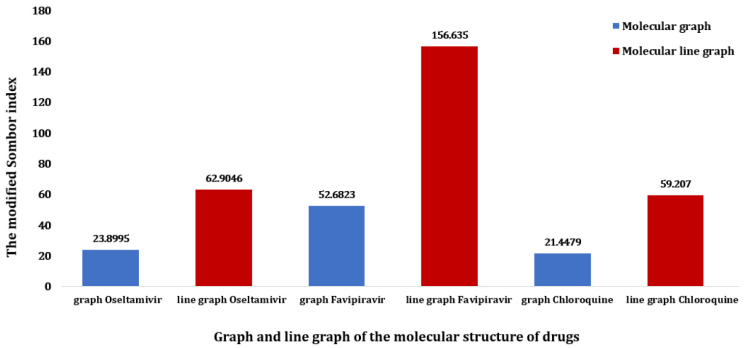


Figure 8

Comparison of ^{m}SO of the graph and line graph Oseltamivir, Favipiravir, and Chloroquine.

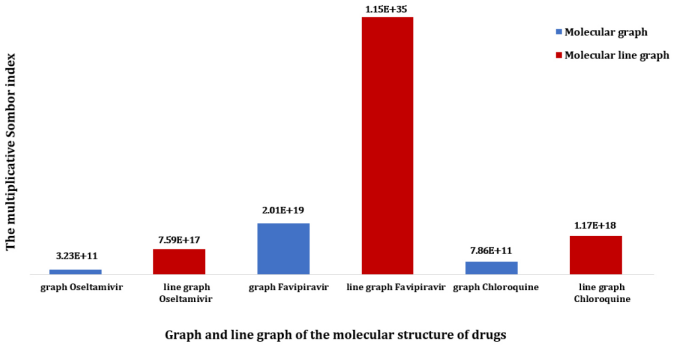


Figure 9

Comparison of *SOII* of the graph and line graph Oseltamivir, Favipiravir, and Chloroquine.

In this study, we analysed the molecular structures of Oseltamivir, Favipiravir, and Chloroquine in the treatment of RNA viruses. We computed some the Sombor indices and the multiplicative Sombor indices of drugs Oseltamivir, Favipiravir, and Chloroquine.

Since vertices in a line graph correspond to the edges in the graph, by studying the topological indices of the line graph, one can have a better analysis of the function of the bonds between atoms.

We have plotted Figures 5-11 for comparing the structure of the RNA-viruses drugs to study the behavior of the obtained Sombor-type topological indices to predict some physiochemical and medication properties of drugs.

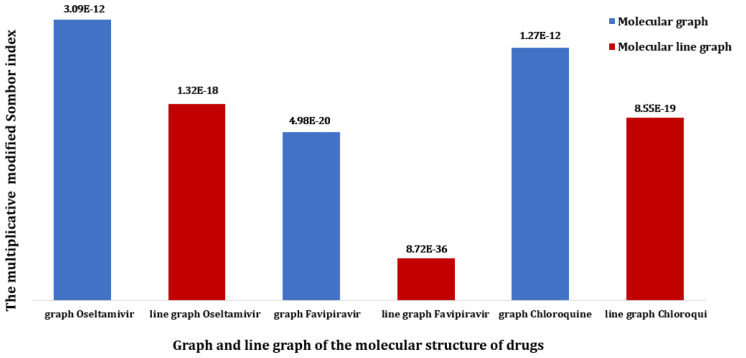


Figure 10

Comparison of *MSOII* of the graph and line graph Oseltamivir, Favipiravir, and Chloroquine.

The graphical comparison of obtained results for *SO* of drugs Oseltamivir, Favipiravir, and Chloroquine in the treatment of RNA viruses is shown in Figure 5.

It can be observed from Figure 5 that the value of *SO* of the graph and line graph of Favipiravir is more than others. Also, according to the molecular structure of Favipiravir, the topological indices studied of this drug have a higher value than other drugs except for *MSOII*.

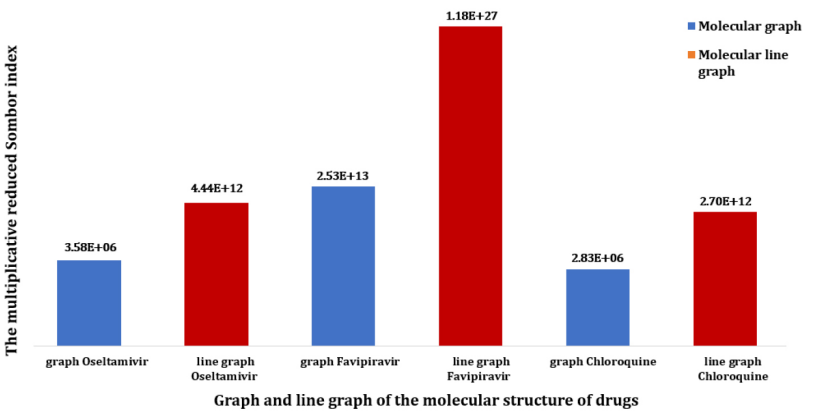


Figure 11

Comparison of *RSOII* of the graph and line graph Oseltamivir, Favipiravir, and Chloroquine.

On the contrary, according to Figure 10, the graph and the line graph of this drug have the lowest value for the multiplicative modified Sombor index among other drugs. Figures 5-7 show that SO, SO_{red}, and SO_{avg} of the molecular graph of Oseltamivir and the line graph of Chloroquine have the lowest values among the studied drugs. While the lowest value of the multiplicative Sombor index is obtained from the molecular graph and linear graph for the Oseltamivir drug (see Figure 9). According to Figures 8 and 11, ^{m}SO and $RSOII$ are obtained as the lower values for the graph and line graph of Chloroquine drug between others.

4. Conclusion

In this work, we investigated some new degree-based topological indices of Oseltamivir, Favipiravir, and Chloroquine in the treatment of RNA viruses. We obtained the Sombor indices and the multiplicative Sombor indices of their molecular graph and line graph using the graph theory.

The results obtained in this paper can help in the QSPR models for their applications in RNA virus drug research. The computation of other Sombor indices of the structure of drugs would be an interesting topic for further study.

Disclosure statement

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