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Irregularity Invariants for Chemical Structures used in the Treatment of COVID-19

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Abstract

The world is going through the pandemic of COVID-19. Remdesivir, chloroquine, hydroxychloroquine and theaflavin are some drugs currently in use for the treatment of the COVID-19 patients. This manuscript aims to compute the irregularity measures for these chemical structures. We believe that our results can be utilized to improve the capacity of these chemical structures.

Keywords: COVID-19, chloroquine, hydroxychloroquine, irregularity indices, remdesivir, theaflavin

Introduction

Historically, the epidemics of influenza and cholera were regarded as the most devastating. Recently, the COVID-19 pandemic which originated from China has affected the health of people all around the world [1]. By September 2020, there were over 32.7 million confirmed cases of COVID-19 including 991,000 deaths. According to WHO, no particular medication for this disease is available. So, it's very important to choose suitable medicine for its treatment. Researchers have tested some chemical compounds [2, 3, 4, 5, 6] and obtained favorable results. These compounds include chloroquine, hydroxylchloroquine, remdesivir (GS5734), and theaflavin.

Molecular graph is a [7, 8] simple graph in which the vertices and edges are considered as the atoms and bonds of the compound, respectively.

Let $G = (V,E)$ be a simple connected graph, where V is the set of vertices and E represents the number of edges present in the graph. The degree of vertex depicts the number of edges attached with that vertex and it is denoted by d_v, where $v \in V(G)$ and e represents an edge $e = uv \in E(G)$. Topological indices (TIs) help us to describe the structure of the graph [9, 10, 11, 12, 13, 14, 15, 16, 17, 18]. The first ever TI was presented by Wiener in 1947 [19], when he was trying to find out the boiling point of alkanes.

$$W(G) = \sum_{(uv)\subseteq V(G)} d_G(u,v)$$

Gutman, in 1975, presented the definition [20] of Zagreb indices. the oldest degree-based descriptors are two indices known as the first and second Zagreb indices, respectively. The properties of these indices were investigated extensively [21, 22]. These properties can be represented by the mathematical formulae given below.

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

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

TI is recognized as an irregularity index [23] if certain conditions are met. Firstly, if the TI of a graph is greater than zero or equal to zero. Secondly, if the TI of a graph is equal to zero, given the graph is regular. Table 1 shows the irregularity indices.

Table 1. Irregularity Indices and their Mathematical Formulae

Irregularity Index	**Mathematical Formula**
VAR	$\sum_{u\grave{o}V}(d_u - \frac{2m}{n})^2 = \frac{M_1(G)}{n} - (\frac{2m}{n})^2$
AL	$\sum_{uv\in E(G)} \lvert d_u - d_v \rvert$
IR1	$\sum_{u\in V}(d_u)^3 - \frac{2m}{n}\sum_{u\in V}(d_u)^2 = F(G) - \frac{2m}{n}M_1(G)$
IR2	$\sqrt{\frac{\sum_{uv\in E(G)} d_u d_v}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(G)}{m}} - \frac{2m}{n}$
IRF	$\sum_{uv\in E(G)} (d_u - d_v)^2 = F(G) - 2M_2(G)$
IRFW	$\frac{IRF(G)}{M_2(G)}$

Irregularity Index	Mathematical Formula
IRA	$\sum_{uv\in E(G)} (d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(G)$
IRB	$\sum_{uv\in E(G)} (d_u^{1/2} - d_v^{1/2})^2 = M_1(G) - 2RR(G)$
IRC	$\frac{\sum_{uv\in E(G)} \sqrt{d_u d_v}}{m} - \frac{2m}{n} = \frac{RR(G)}{m} - \frac{2m}{n}$
IRDIF	$\sum_{uv\in E(G)} \lvert \frac{d_u}{d_v} - \frac{d_v}{d_u} \rvert = \sum_{i<j} m_{i,j} (\frac{j}{i} - \frac{i}{j})$
IRL	$\sum_{uv\in E(G)} \lvert lnd_u - lnd_v \rvert = \sum_{i<j} m_{i,j} ln(\frac{j}{i})$
IRLU	$\sum_{uv\in E(G)} \frac{\lvert d_u - d_v \rvert}{min(d_u, d_v)} = \sum_{i<j} m_{i,j} ln(\frac{j-i}{i})$
IRLF	$\sum_{uv\in E(G)} \frac{\lvert d_u - d_v \rvert}{\sqrt{(d_u d_v)}} = \sum_{i<j} m_{i,j} (\frac{j-i}{\sqrt{ij}})$
IRLA	$2\sum_{uv\in E(G)} \frac{\lvert d_u - d_v \rvert}{(d_u + d_v)} = 2\sum_{i<j} m_{i,j} (\frac{j-i}{i+j})$
IRDI	$\sum_{uv\in E(G)} ln1 + \lvert d_u - d_v \rvert = \sum_{i<j} m_{i,j} ln(i+j-1)$
IRGA	$\sum_{uv\in E(G)} ln(\frac{d_u + d_v}{2\sqrt{d_u d_v}}) \sum_{i<j} m_{i,j} (\frac{i+j}{2\sqrt{ij}})$

2. Irregularities of the Chemical Structures used for the Treatment of the Patients of COVID-19

In this section, we discuss some chemical structures used for the treatment and management of the patients of COVID-19 by means of the chemical graph theory. We associate these structures with a molecular graph. We can observe from these two-dimensional molecular structures that all of them belong to the family of the irregular graph, so the best way to express these irregularities are irregularity indices. Here, we discuss sixteen irregularity indices for chloroquine, hydroxychloroquine, remdesivir, and theaflavin in four subsections.

2.1. Irregularity Indices for Remdesivir

This section covers the irregularity indices of remdesivir.

Figure 1 shows the two dimensional molecular graph of remdesivir.

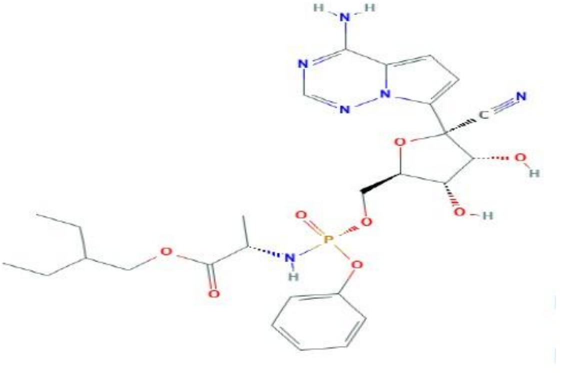

Figure 1. Molecular structure of Remdesivir [24]

The degree-based edge partition of remdesivir is given in Table 2

Table 2. Partition of *E* (*Remdesivir)*

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

Theorem 2.1. Let's suppose G is the graph of remdesivir. The irregularity indices are as follows:

(1) $VAR(G) = 13.60$.
(2) $AL(G) = 42$.

(3) $IR1(G) = 133.42$.
(4) $IR2(G) = 0.315$.
(5) $IRF(G) = 72$.
(6) $IRFW(G) = 0.280$.
(7) $IRA(G) = 3.04$.
(8) $IRB(G) = 7.93$.
(9) $IRC(G) = -1.67$.
(10) $IRDIF(G) = 34.76$.
(11) $IRL(G) = 18.53$.
(12) $IRLU(G) = 29.66$. (13) $IRLF(G) = 19.28$. (14) $IRLA(G) = 17.56$.
(15) $IRD1(G) = 42$.
(16) $IRGA(G) = 0.518$.

***Proof**:* Using the edge partition (Table 1), the irregularities of remdesivir are computed as follows:

$$
\begin{aligned}
VAR(G) &= \sum_{u\epsilon V}\left(d_u - \frac{2m}{n}\right)^2 = \frac{M_1(G)}{n} - \left(\frac{2m}{n}\right)^2 \\
&= \frac{216}{42} - \left(\frac{44}{42}\right)^2 \\
&= 13.60.
\end{aligned}
$$

$$
\begin{aligned}
AL(G) &= \sum_{uv\epsilon E(G)} |d_u - d_v| \\
&= |1-2|(2) + |1-3|(5) + |1-4|(2) + |2-2|(9) \\
&\quad + |2-3|(14) + |2-4|(4) + |3-3|(6) + |3-4|(2) \\
&= 42.
\end{aligned}
$$

$$
\begin{aligned}
IR1(G) &= \sum_{u\epsilon V} d_u^3 - \frac{2m}{n}\sum_{u\epsilon V} d_u^2 = F(G) - \left(\frac{2m}{n}\right) M_1(G) \\
&= 586 - \left(\frac{88}{42}\right) 216 \\
&= 133.42.
\end{aligned}
$$

$$
\begin{aligned}
IR2(G) &= \sqrt{\frac{\sum_{uv\epsilon E(G)} d_u d_v}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(G)}{m}} - \frac{2m}{n} \\
&= \sqrt{\frac{257}{44}} - \frac{2(44)}{42} \\
&= 0.315.
\end{aligned}
$$

$$\begin{aligned} IRF(G) &= \sum_{uv\epsilon E(G)} (d_u - d_v)^2 \\ &= (1-2)^2(2) + (1-3)^2(5) + (1-4)^2(2) + (2-2)^2(9) \\ &\quad +(2-3)^2(14) + (2-4)^2(4) + (3-3)^2(6) + (3-4)^2(2) \\ &= 72. \end{aligned}$$

$$\begin{aligned} IRFW(G) &= \frac{IRF(G)}{M_2(G)} \\ &= 0.280. \end{aligned}$$

$$\begin{aligned} IRA(G) &= \sum_{uv\epsilon E(G)} (d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(G) \\ &= (42) - 2(19.48) \\ &= 3.04. \end{aligned}$$

$$\begin{aligned} IRB(G) &= \sum_{uv\epsilon E(G)} (d_u^{1/2} - d_v^{1/2})^2 = M_1(G) - 2RR(G) \\ &= (\sqrt{1}-\sqrt{2})^2 \times 2 + (\sqrt{1}-\sqrt{3})^2 \times 5 + (\sqrt{1}-\sqrt{4})^2 \times 2 + (\sqrt{2}-\sqrt{2})^2 \times 9 \\ &\quad +(\sqrt{2}-\sqrt{3})^2 \times 14 + (\sqrt{2}-\sqrt{4})^4 \times 9 + (\sqrt{3}-\sqrt{3})^2 \times 6(\sqrt{3}-\sqrt{4})^2 \times 9 \\ &= 7.93. \end{aligned}$$

$$\begin{aligned} IRC(G) &= \frac{\sum_{uv\epsilon E(G)} \sqrt{d_u d_v}}{m} - \frac{2m}{n} = \frac{RR(G)}{m} - \frac{2m}{n} \\ &= \frac{18.88}{44} - \left(\frac{88}{42}\right) \\ &= -1.67. \end{aligned}$$

$$\begin{aligned} IRDIF(G) &= \sum_{uv\epsilon E(G)} |\frac{d_u}{d_v} - \frac{d_v}{d_u}| \\ &= |\frac{1}{2} - \frac{2}{1}|(2) + |\frac{1}{3} - \frac{3}{1}|(5) + |\frac{1}{4} - \frac{4}{1}|(2) + |\frac{2}{2} - \frac{2}{2}|(9) \\ &\quad +|\frac{2}{3} - \frac{3}{2}|(14) + |\frac{2}{4} - \frac{4}{2}|(4) + |\frac{3}{3} - \frac{3}{3}|(6) + |\frac{3}{4} - \frac{4}{3}|(2) \\ &= 34.76. \end{aligned}$$

$$\begin{aligned} IRL(G) &= \sum_{uv\epsilon E(G)} |ln d_u - ln d_v| \\ &= |ln1 - ln2|(2) + |ln1 - ln3|(5) + |ln1 - ln4|(2) + |ln2 - ln2|(9) \\ &\quad +|ln2 - ln3|(14) + |ln2 - ln4|(4) + |ln3 - ln3|(6) + |ln3 - ln4|(2) \\ &= 18.53. \end{aligned}$$

$$
\begin{aligned}
IRLU(G) &= \sum_{uv\epsilon E(G)} \frac{|d_u - d_v|}{min(d_u, d_v)} \\
&= \left(\frac{|1-2|}{1}\right)(2) + \left(\frac{|1-3|}{1}\right)(5) + \left(\frac{|1-4|}{1}\right)(2) + \left(\frac{|2-2|}{2}\right)(9) \\
&= \left(\frac{|2-3|}{2}\right)(14) + \left(\frac{|2-4|}{2}\right)(4) + \left(\frac{|3-3|}{3}\right)(6) + \left(\frac{|3-4|}{3}\right)(2) \\
&= 29.66.
\end{aligned}
$$

$$
\begin{aligned}
IRLF(G) &= \sum_{uv\epsilon E(G)} \frac{|d_u - d_v|}{\sqrt{d_u.d_v}} \\
&= \left(\frac{|1-2|}{\sqrt{2}}\right)(2) + \left(\frac{|1-3|}{\sqrt{3}}\right)(5) + \left(\frac{|1-4|}{\sqrt{4}}\right)(2) + \left(\frac{|2-2|}{\sqrt{4}}\right)(9) \\
&= \left(\frac{|2-3|}{\sqrt{6}}\right)(14) + \left(\frac{|2-4|}{\sqrt{8}}\right)(4) + \left(\frac{|3-3|}{\sqrt{9}}\right)(6) + \left(\frac{|3-4|}{\sqrt{12}}\right)(2) \\
&= 19.28.
\end{aligned}
$$

$$
\begin{aligned}
IRLA(G) &= \sum_{uv\epsilon E(G)} 2\frac{|d_u - d_v|}{(d_u + d_v)} \\
&= 2\left(\frac{|1-2|}{1+2}\right)(2) + 2\left(\frac{|1-3|}{1+3}\right)(5) + 2\left(\frac{|1-4|}{1+4}\right)(2) + 2\left(\frac{|2-2|}{2+2}\right)(9) \\
&\quad +2\left(\frac{|2-3|}{2+3}\right)(14) + 2\left(\frac{|2-4|}{2+4}\right)(4) + 2\left(\frac{|3-3|}{3+3}\right)(6) + 2\left(\frac{|3-4|}{3+4}\right)(2) \\
&= 17.56.
\end{aligned}
$$

$$
\begin{aligned}
IRD1(G) &= \sum_{uv\epsilon E(G)} ln\{1 + |d_u - d_v|\} \\
&= ln\{1+|1-2|\}(2) + ln\{1+|1-3|\}(5) + ln\{1+|1-4|\}(2) + ln\{1+|2-2|\}(9) \\
&\quad +ln\{1+|2-3|\}(14) + ln\{1+|2-4|\}(4) + ln\{1+|3-3|\}(6) + ln\{1+|3-4|\}(2) \\
&= 42.
\end{aligned}
$$

$$
\begin{aligned}
IRGA(G) &= \sum_{uv\epsilon E(G)} ln(\frac{d_u + d_v}{2\sqrt{d_u d_v}}) \\
&= ln\left(\frac{1+2}{2\sqrt{1\times 2}}\right)(2) + ln\left(\frac{1+3}{2\sqrt{1\times 3}}\right)(5) + ln\left(\frac{1+4}{2\sqrt{1\times 4}}\right)(2) + ln\left(\frac{2+2}{2\sqrt{2\times 2}}\right)(9) \\
&\quad +ln\left(\frac{2+3}{2\sqrt{2\times 3}}\right)(14) + ln\left(\frac{2+4}{2\sqrt{2\times 4}}\right)(4) + ln\left(\frac{3+3}{2\sqrt{3\times 3}}\right)(6) + ln\left(\frac{3+4}{2\sqrt{3\times 4}}\right)(2) \\
&= 0.518.
\end{aligned}
$$

2.2. Irregularity Indices for Chloroquine

This section focuses on the irregularity indices for chloroquine. The two-dimensional molecular graph of chloroquine (Figure 2) has three types of vertices.

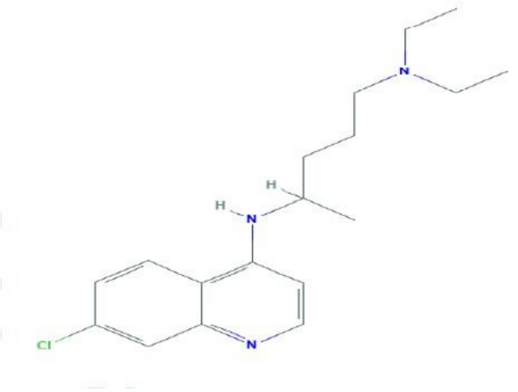

Figure 2. Molecular structure of Chloroquine [25]

Table 3 shows the degree-based edge partition of chloroquine

Table 3. Partition of *E* (*Chloroquine*)

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

Theorem 2.2. Let's suppose G is the graph of chloroquine. The irregularity indices are as follows:

(1) $VAR(G) = 0.44$.
(2) $AL(G) = 18$.
(3) $IR1(G) = 40.36$.
(4) $IR2(G) = 0.19$.
(5) $IRF(G) = 22$.
(6) $IRFW(G) = 0.183$.
(7) $IRA(G) = 1$.
(8) $IRB(G) = 2.623$.
(9) $IRC(G) = -1.63$.
(10) $IRDIF(G) = 18.42$.
(11) $IRL(G) = 8.37$.
(12) $IRLU(G) = 12$.
(13) $IRLF(G) = 7.84$.
(14) $IRLA(G) = 7.13$.

(15) $IRD1(G) = 11.88$.
(16) $IRGA(G) = 16.66$.

Proof. Using the edge partition of chloroquine given in Table 3, the irregularities of chloroquine are computed as follows:

$$VAR(G) = \sum_{u \epsilon V}\left(d_u - \frac{2m}{n}\right)^2 = \frac{M_1(G)}{n} - \left(\frac{2m}{n}\right)^2$$
$$= \frac{106}{22} - \left(\frac{2(23)}{22}\right)^2$$
$$= 0.44.$$

$$AL(G) = \sum_{uv \epsilon E(G)} |d_u - d_v|$$
$$= |1-2|(2) + |1-3|(2) + |2-2|(5) + |2-3|(12) + |3-3|(2)$$
$$= 18.$$

$$IR1(G) = \sum_{u\epsilon V)} d_u^3 - \left(\frac{2m}{n}\right)\sum_{u\epsilon V)} d_u^2 = F(G) - \frac{2m}{n}M_1(G)$$
$$= (262) - \left(\frac{2(23)}{22}\right)(106)$$
$$= 40.36.$$

$$IR2(G) \quad \sqrt{\frac{\sum_{uv\epsilon E(G)} d_u d_v}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(G)}{m}} - \frac{2m}{n}$$
$$= \sqrt{\frac{120}{23}} - \frac{2(23)}{22}$$
$$= 0.19.$$

$$IRF(G) = \sum_{uv\epsilon E(G)} (d_u - d_v)^2$$
$$= (1-2)^2(2) + (1-3)^2(2) + (2-2)^2(5) + (2-3)^2(12) + (3-3)^2(2)$$
$$= 22.$$

$$IRFW(G) = \frac{IRF(G)}{M_2(G)}$$
$$= 0.183.$$

$$IRA(G) = \sum_{uv\epsilon E(G)} (d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(G)$$
$$= (22) - 2(10.5)$$
$$= 1.$$

$$\begin{aligned}
IRB(G) &= \sum_{uv\epsilon E(G)} (d_u^{1/2} - d_v^{1/2})^2 = M_1(G) - 2RR(G) \\
&= (1\sqrt{1} - \sqrt{2})^2(2) + (1\sqrt{1} - \sqrt{3})^2(2)(1\sqrt{2} - \sqrt{2})^2(12) + (1\sqrt{2} - \sqrt{3})^2(12) \\
&= (1\sqrt{3} - \sqrt{3})^2(2) \\
&= 2.623.
\end{aligned}$$

$$\begin{aligned}
IRC(G) &= \frac{\sum_{uv\epsilon E(G)} \sqrt{d_u d_v}}{m} - \frac{2m}{n} = \frac{RR(G)}{m} - \frac{2m}{n} \\
&= \frac{10.58}{23} - \frac{46}{22} \\
&= -1.63.
\end{aligned}$$

$$\begin{aligned}
IRDIF(G) &= \sum_{uv\epsilon E(G)} |\frac{d_u}{d_v} - \frac{d_v}{d_u}| \\
&= |\frac{1}{2} - \frac{2}{1}|(2) + |\frac{1}{3} - \frac{3}{1}|(2) + |\frac{2}{2} - \frac{2}{2}|(5) \\
&\quad + |\frac{2}{3} - \frac{3}{2}|(12) + |\frac{3}{3} - \frac{3}{3}|(2) \\
&= 18.42.
\end{aligned}$$

$$\begin{aligned}
IRL(G) &= \sum_{uv\epsilon E(G)} |lnd_u - lnd_v| \\
&= |ln1 - ln2|(2) + |ln1 - ln3|(2) + |ln2 - ln2|(5) \\
&\quad + |ln2 - ln3|(12) + |ln3 - ln3|(2)
\end{aligned}$$

$$= 8.37.$$

$$\begin{aligned}
IRLU(G) &= \sum_{uv\epsilon E(G)} \frac{|d_u - d_v|}{min(d_u, d_v)} \\
&= \left(\frac{|1-2|}{1}\right)(2) + \left(\frac{|1-3|}{1}\right)(2) + \left(\frac{|2-2|}{2}\right)(5) \\
&\quad + \left(\frac{|2-3|}{2}\right)(12) + \left(\frac{|3-3|}{3}\right)(2) \\
&= 12.
\end{aligned}$$

$$\begin{aligned}
IRLF(G) &= \sum_{uv\epsilon E(G)} \frac{|d_u - d_v|}{\sqrt{d_u.d_v}} \\
&= \left(\frac{|1-2|}{\sqrt{2}}\right)(2) + \left(\frac{|1-3|}{\sqrt{3}}\right)(2) + \left(\frac{|2-2|}{\sqrt{4}}\right)(5)) \\
&\quad + \left(\frac{|2-3|}{\sqrt{6}}\right)(12) + \left(\frac{|3-3|}{\sqrt{9}}\right)(2) \\
&= 7.84.
\end{aligned}$$

$$
\begin{aligned}
IRLA(G) &= \sum_{uv\epsilon E(G)} 2\frac{|d_u - d_v|}{(d_u + d_v)} \\
&= 2\frac{|1-2|}{1+2}(2) + 2\frac{|1-3|}{1+3}(2) + 2\frac{|2-2|}{2+2}(5) \\
&\quad +2\frac{|2-3|}{2+3}(12) + 2\frac{|3-3|}{3+3}(2) \\
&= 7.13. \\
IRD1(G) &= \sum_{uv\epsilon E(G)} ln\{1 + |d_u - d_v|\} \\
&= ln\{1+|1-2|\}(2) + ln\{1+|1-3|\}(2) + ln\{1+|2-2|\}(5) \\
&\quad +ln\{1+|2-3|\}(12) + ln\{1+|3-3|\}(2) \\
&= 11.88. \\
IRGA(G) &= \sum_{uv\epsilon E(G)} ln(\frac{d_u + d_v}{2\sqrt{d_u d_v}}) \\
&= ln\left(\frac{1+2}{2\sqrt{1\times 2}}\right)(2) + ln\left(\frac{1+3}{2\sqrt{1\times 3}}\right)(2) + ln\left(\frac{2+2}{2\sqrt{2\times 2}}\right)(5) \\
&\quad +ln\left(\frac{2+3}{2\sqrt{2\times 3}}\right)(12)) + ln\left(\frac{3+3}{2\sqrt{3\times 3}}\right)(2) \\
&= 16.66.
\end{aligned}
$$

2.3. Irregularities of Hydroxychloroquine

In this section, irregularity indices for hydroxychloroquine are discussed. The two-dimensional molecular graph of hydroxychloroquine is given in Figure 3. There are three types of vertices present in the graph.

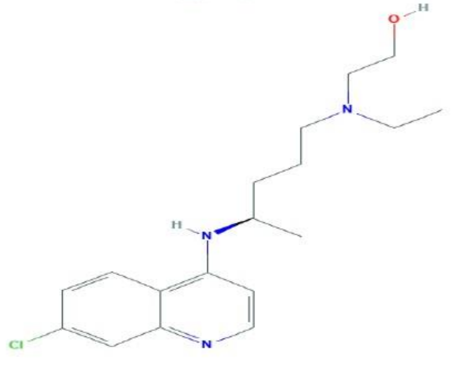

Figure 3. Molecular graph of Hydroxychloroquine [26]

The degree-based edge partition of hydroxychloroquine is given below in Table 4.

Table 4. Partition of E (*Chloroquine*)

(du,dv)	**Frequency**
(1,2)	2
(1,3)	2
(2,2)	6
(2, 3)	12
(3,3)	2

Theorem 2.3. Let's suppose G is the graph of hydroxychloroquine. The irregularity indices are as follows:

(1) $VAR(G) = 0.43.$

(2) $AL(G) = 18.$

(3) $IR1(G) = 40.43.$

(4) $IR2(G) = 0.19.$

(5) $IRF(G) = 22.$

(6) $IRFW(G) = 0.177.$

(7) $IRA(G) = 5.78.$

(8) $IRB(G) = 2.62.$

(9) $IRC(G) = -1.64.$

(10) $IRDIF(G) = 18.40.$

(11) $IRL(G) = 13.29.$

(12) $IRLU(G) = 12.$

(13) $IRLF(G) = 8.6.$

(14) $IRLA(G) = 8.13.$

(15) $IRD1(G) = 11.88.13.$

(16) $IRGA(G) = 0.63.$

Proof. Using the edge partition of hydroxychloroquine given in Table 4, the irregularities of hydroxychloroquine are computed as follows:

$$\begin{aligned} VAR(G) &= \sum_{u\epsilon V}\left(d_u - \frac{2m}{n}\right)^2 = \frac{M_1(G)}{n} - \left(\frac{2m}{n}\right)^2 \\ &= \frac{110}{23} - \left(\frac{2(24)}{23}\right)^2 \\ &= 0.43. \end{aligned}$$

$$\begin{aligned} AL(G) &= \sum_{uv\epsilon E(G)} |d_u - d_v| \\ &= |1-2|(2) + |1-3|(2) + |2-2|(6) + |2-3|(12) + |3-3|(2) \\ &= 18. \end{aligned}$$

$$\begin{aligned} IR1(G) &= \sum_{u\epsilon V)} d_u^3 - \left(\frac{2m}{n}\right)\sum_{u\epsilon V)} d_u^2 = F(G) - \frac{2m}{n}M_1(G) \\ &= (270) - \left(\frac{2(24)}{23}\right)(110) \\ &= 40.43. \end{aligned}$$

$$\begin{aligned} IR2(G) &= \sqrt{\frac{\sum_{uv\epsilon E(G)} d_u d_v}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(G)}{m}} - \frac{2m}{n} \\ &= \sqrt{\frac{124}{24}} - \frac{2(24)}{23} \\ &= 0.19. \end{aligned}$$

$$\begin{aligned} IRF(G) &= \sum_{uv\epsilon E(G)} (d_u - d_v)^2 \\ &= (1-2)^2(2) + (1-3)^2(2) + (2-2)^2(6) + (2-3)^2(12) + (3-3)^2(2) \\ &= 22. \end{aligned}$$

$$\begin{aligned} IRFW(G) &= \frac{IRF(G)}{M_2(G)} \\ &= 0.177. \end{aligned}$$

$$\begin{aligned} IRA(G) &= \sum_{uv\epsilon E(G)} (d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(G) \\ &= (23) - 2(8.61) \\ &= 5.78. \end{aligned}$$

$$\begin{aligned} IRB(G) &= \sum_{uv\epsilon E(G)} (d_u^{1/2} - d_v^{1/2})^2 = M_1(G) - 2RR(G) \\ &= (1\sqrt{1} - \sqrt{2})^2(2) + (1\sqrt{1} - \sqrt{3})^2(2) + (1\sqrt{2} - \sqrt{2})^2(6) \\ &\quad + (1\sqrt{2} - \sqrt{3})^2(12) + (1\sqrt{3} - \sqrt{3})^2(2) \\ &= 2.62. \end{aligned}$$

$$\begin{aligned} IRC(G) &= \frac{\sum_{uv\epsilon E(G)}\sqrt{d_u d_v}}{m} - \frac{2m}{n} = \frac{RR(G)}{m} - \frac{2m}{n} \\ &= \frac{10.59}{24} - \frac{48}{23} \\ &= -1.64. \end{aligned}$$

$$\begin{aligned} IRDIF(G) &= \sum_{uv\epsilon E(G)} |\frac{d_u}{d_v} - \frac{d_v}{d_u}| \\ &= |\frac{1}{2} - \frac{2}{1}|(2) + |\frac{1}{3} - \frac{3}{1}|(2) + |\frac{2}{2} - \frac{2}{2}|(6) \\ &\quad +|\frac{2}{3} - \frac{3}{2}|(12) + |\frac{3}{3} - \frac{3}{3}|(2) \\ &= 18.42. \end{aligned}$$

$$IRL(G) = \sum_{uv\in E(G)} \left|\ln d_u - \ln d_v\right|$$

$$= \left|\ln 1 - \ln 2\right|(2) + \left|\ln 1 - \ln 3\right|(2) + \left|\ln 2 - \ln 2\right|(6)$$

$$+ \left|\ln 2 - \ln 3\right|(12) + \left|\ln 3 - \ln 3\right|(2)$$

$$= 13.29$$

$$\begin{aligned} IRLU(G) &= \sum_{uv\epsilon E(G)} \frac{|d_u - d_v|}{min(d_u, d_v)} \\ &\left(\frac{|1-2|}{1}\right)(2) + \left(\frac{|1-3|}{1}\right)(2) + \left(\frac{|2-2|}{2}\right)(6) \\ &+ \left(\frac{|2-3|}{2}\right)(12) + \left(\frac{|3-3|}{3}\right)(2) \end{aligned}$$

.

$$=12$$

$$IRLF(G) = \sum_{uv\in E(G)} \frac{\left|d_u - d_v\right|}{\sqrt{d_u . d_v}}$$

$$= (\frac{\left|1-2\right|}{\sqrt{2}})(2) + (\frac{\left|1-3\right|}{\sqrt{3}})(2) + (\frac{\left|2-2\right|}{\sqrt{4}})(6) + (\frac{\left|2-3\right|}{\sqrt{6}})(12) + (\frac{\left|3-3\right|}{\sqrt{9}})(2)$$

$$= 8.6$$

$$
\begin{aligned}
IRLA(G) &= \sum_{uv\epsilon E(G)} 2\frac{|d_u - d_v|}{(d_u + d_v)} \\
&= 2\frac{|1-2|}{1+2}(2) + 2\frac{|1-3|}{1+3}(2) + 2\frac{|2-2|}{2+2}(6) \\
&\quad +2\frac{|2-3|}{2+3}(12) + 2\frac{|3-3|}{3+3}(2) \\
&= 8.13. \\
IRD1(G) &= \sum_{uv\epsilon E(G)} ln\{1 + |d_u - d_v|\} \\
&= ln\{1+|1-2|\}(2) + ln\{1+|1-3|\}(2) + ln\{1+|2-2|\}(6) \\
&\quad +ln\{1+|2-3|\}(12) + ln\{1+|3-3|\}(2) \\
&= 11.88.
\end{aligned}
$$

$$
\begin{aligned}
IRGA(G) &= \sum_{uv\epsilon E(G)} ln(\frac{d_u + d_v}{2\sqrt{d_u d_v}}) \\
&= ln\left(\frac{1+2}{2\sqrt{1\times 2}}\right)(2) + ln\left(\frac{1+3}{2\sqrt{1\times 3}}\right)(2) + ln\left(\frac{2+2}{2\sqrt{2\times 2}}\right)(6) \\
&\quad +ln\left(\frac{2+3}{2\sqrt{2\times 3}}\right)(12)) + ln\left(\frac{3+3}{2\sqrt{3\times 3}}\right)(2) \\
&= 16.66.
\end{aligned}
$$

2.4. Irregularities of Theaflavin

In this section, irregularity indices for theaflavin are computed. The two-dimensional molecular graph of theaflavin (Figure 4) depicts that three types of vertices are present in the graph.

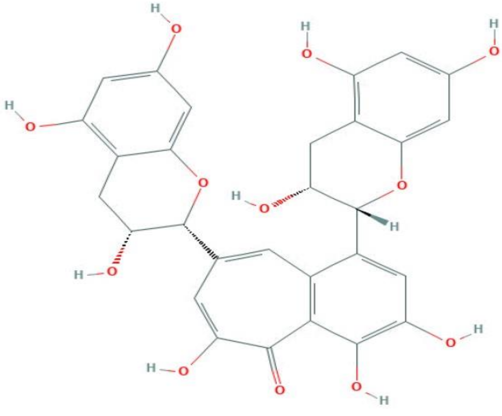

Figure 4. Molecular structure of Theaflavin [27]

Table 5 shows the degree-based edge partition of theaflavin.

Table 5. Partition of E (*Theaflavin*)

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

Theorem 2.4. Let's suppose G is the graph of theaflavin. The irregularity indices are as follows:

(1) $VAR(G) = 0.67$.
(2) $AL(G) = 44$.
(3) $IR1(G) = 112.92$.
(4) $IR2(G) = 0.25$.
(5) $IRF(G) = 62$.
(6) $IRFW(G) = 0.21$.
(7) $IRA(G) = 2.18$.
(8) $IRB(G) = 3.13$.
(9) $IRC(G) = -2.07$.
(10) $IRDIF(G) = 45.18$.
(11) $IRL(G) = 19.78$.
(12) $IRLU(G) = 31$.
(13) $IRLF(G) = 20.52$.
(14) $IRLA(G) = 18.8$.
(15) $IRD1(G) = 26.22$.
(16) $IRGA(G) = 1.87$.

Proof. Using the edge partition of theaflavin given in Table 5, the irregularity indices of theaflavin are computed as follows:

$$
\begin{aligned}
VAR(G) &= \sum_{u\epsilon V}\left(d_u - \frac{2m}{n}\right)^2 = \frac{M_1(G)}{n} - \left(\frac{2m}{n}\right)^2 \\
&= \frac{234}{41} - \left(\frac{2(46)}{41}\right)^2 \\
&= 0.67.
\end{aligned}
$$

$$\begin{aligned} AL(G) &= \sum_{uv\epsilon E(G)} |d_u - d_v| \\ &= |1-3|(10) + |2-3|(22) + |3-3|(14) \\ &= 44. \end{aligned}$$

$$\begin{aligned} IR1(G) &= \sum_{u\epsilon V)} d_u^3 - \left(\frac{2m}{n}\right) \sum_{u\epsilon V)} d_u^2 = F(G) - \frac{2m}{n} M_1(G) \\ &= (638) - \left(\frac{2(46)}{41}\right)(234) \\ &= 112.92. \end{aligned}$$

$$\begin{aligned} IR2(G) &= \sqrt{\frac{\sum_{uv\epsilon E(G)} d_u d_v}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(G)}{m}} - \frac{2m}{n} \\ &= \sqrt{\frac{288}{46}} - \frac{2(46)}{41} \\ &= 0.25. \end{aligned}$$

$$\begin{aligned} VAR(G) &= \sum_{u\epsilon V} \left(d_u - \frac{2m}{n}\right)^2 = \frac{M_1(G)}{n} - \left(\frac{2m}{n}\right)^2 \\ &= \frac{234}{41} - \left(\frac{2(46)}{41}\right)^2 \\ &= 0.67. \end{aligned}$$

$$\begin{aligned} AL(G) &= \sum_{uv\epsilon E(G)} |d_u - d_v| \\ &= |1-3|(10) + |2-3|(22) + |3-3|(14) \\ &= 44. \end{aligned}$$

$$\begin{aligned} IR1(G) &= \sum_{u\epsilon V)} d_u^3 - \left(\frac{2m}{n}\right) \sum_{u\epsilon V)} d_u^2 = F(G) - \frac{2m}{n} M_1(G) \\ &= (638) - \left(\frac{2(46)}{41}\right)(234) \\ &= 112.92. \end{aligned}$$

$$\begin{aligned} IR2(G) &= \sqrt{\frac{\sum_{uv\epsilon E(G)} d_u d_v}{m} - \frac{2m}{n}} = \sqrt{\frac{M_2(G)}{m} - \frac{2m}{n}} \\ &= \sqrt{\frac{288}{46} - \frac{2(46)}{41}} \\ &= 0.25. \end{aligned}$$

$$\begin{aligned} IRF(G) &= \sum_{uv\epsilon E(G)} (d_u - d_v)^2 \\ &= (1-2)^2(2) + (1-3)^2(2) + (2-2)^2(6) + (2-3)^2(12) + (3-3)^2(2) \\ &= 62. \end{aligned}$$

$$\begin{aligned} IRFW(G) &= \frac{IRF(G)}{M_2(G)} \\ &= 0.21. \end{aligned}$$

$$\begin{aligned} IRA(G) &= \sum_{uv\epsilon E(G)} (d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(G) \\ &= (41) - 2(19.41) \\ &= 2.18. \end{aligned}$$

$$\begin{aligned} IRB(G) &= \sum_{uv\epsilon E(G)} (d_u^{1/2} - d_v^{1/2})^2 = M_1(G) - 2RR(G) \\ &= (1\sqrt{1} - \sqrt{3})^2(10) + (1\sqrt{2} - \sqrt{3})^2(22) + (1\sqrt{3} - \sqrt{3})^2(14) \\ &= 3.13. \end{aligned}$$

$$\begin{aligned} IRC(G) &= \frac{\sum_{uv\epsilon E(G)} \sqrt{d_u d_v}}{m} - \frac{2m}{n} = \frac{RR(G)}{m} - \frac{2m}{n} \\ &= \frac{7.18}{41} - \frac{92}{41} \\ &= -2.07. \end{aligned}$$

$$\begin{aligned} IRDIF(G) &= \sum_{uv\epsilon E(G)} |\frac{d_u}{d_v} - \frac{d_v}{d_u}| \\ &= |\frac{1}{3} - \frac{3}{1}|(10) + |\frac{2}{3} - \frac{3}{2}|(22) + |\frac{3}{3} - \frac{3}{3}|(14) \\ &= 45.18. \end{aligned}$$

$$\begin{aligned} IRL(G) &= \sum_{uv\epsilon E(G)} |lnd_u - lnd_v| \\ &= |ln1 - ln3|(10) + |ln2 - ln3|(22) + |ln3 - ln3|(14) \\ &= 19.78. \end{aligned}$$

$$
\begin{aligned}
IRLU(G) &= \sum_{uv\epsilon E(G)} \frac{|d_u - d_v|}{min(d_u, d_v)} \\
&= \left(\frac{|1-3|}{1}\right)(10) + \left(\frac{|2-3|}{2}\right)(22) + \left(\frac{|3-3|}{3}\right)(14) \\
&= 31 \\
IRLF(G) &= \sum_{uv\epsilon E(G)} \frac{|d_u - d_v|}{\sqrt{d_u.d_v}} \\
&= \left(\frac{|1-3|}{\sqrt{3}}\right)(10) + \left(\frac{|2-3|}{\sqrt{6}}\right)(22) + \left(\frac{|3-3|}{\sqrt{9}}\right)(14) \\
&= 20.52.
\end{aligned}
$$

$$
\begin{aligned}
IRLA(G) &= \sum_{uv\epsilon E(G)} 2\frac{|d_u - d_v|}{(d_u + d_v)} \\
&= 2\frac{|1-3|}{1+3}(10) + 2\frac{|2-3|}{2+3}(22) + 2\frac{|3-3|}{3+3}(14) \\
&= 18.8.
\end{aligned}
$$

$$
\begin{aligned}
IRD1(G) &= \sum_{uv\epsilon E(G)} ln\{1 + |d_u - d_v|\} \\
&= ln\{1+|1-3|\}(10) + ln\{1+|2-3|\}(22) + ln\{1+|3-3|\}(14) \\
&= 26.22.
\end{aligned}
$$

$$
\begin{aligned}
IRGA(G) &= \sum_{uv\epsilon E(G)} ln(\frac{d_u + d_v}{2\sqrt{d_u d_v}}) \\
&= ln\left(\frac{1+3}{2\sqrt{1\times 3}}\right)(10) + ln\left(\frac{2+3}{2\sqrt{2\times 3}}\right)(22)) + ln\left(\frac{3+3}{2\sqrt{3\times 3}}\right)(14) \\
&= 1.87.
\end{aligned}
$$

3. Conclusion

TIs are very helpful in predicting the physicochemical properties of chemical structures without involving laboratory work. This paper discusses the irregularity indices for chemical structures used in the treatment of COVID-19 namely chloroquine, hydroxychloroquine, remdesivir, and theaflavin. All these chemical structures have an irregular structure, so the best way of predicting their properties is through irregularity indices.

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