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Measuring the Energy for the molecular graphs of antiviral agents: Hydroxychloroquine, Chloroquine and Remdesivir

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Abstract: We consider the energy for the molecular graphs of antiviral agents like Hydroxychloroquine, Remdesivir and Chloroquine. These drugs play a vital role in the treatment of COVID-19. Let $\acute{\Gamma}_1, \acute{\Gamma}_2$ and $\acute{\Gamma}_3$ be the n-dimensional graphs of the molecular structures of antiviral agents Hydroxychloroquine, Chloroquine and Remdesivir, respectively. We define their energies as $E'(\acute{\Gamma}_1) = \sum|\lambda'_i|$, $E'(\acute{\Gamma}_2) = \sum|\lambda'_j|$ and $E'(\acute{\Gamma}_3) = \sum|\lambda'_k|$, respectively. Where the sets $\{\lambda'_1(\acute{\Gamma}_1), \lambda'_2(\acute{\Gamma}_1), \lambda'_3(\acute{\Gamma}_1), \ldots, \lambda'_n(\acute{\Gamma}_1)\}$, $\{\lambda'_1(\acute{\Gamma}_2), \lambda'_2(\acute{\Gamma}_2), \lambda'_3(\acute{\Gamma}_2), \ldots, \lambda'_n(\acute{\Gamma}_2)\}$ and

$\{\lambda'_1(\acute{\Gamma}_3),\ \lambda'_2(\acute{\Gamma}_3),\ \lambda'_3(\acute{\Gamma}_3),\ \ldots,\lambda'_n(\acute{\Gamma}_3)\}$ depict the eigenvalues for the adjacency matrices of $\acute{\Gamma}_1, \acute{\Gamma}_2$ and $\acute{\Gamma}_3$, respectively. We have developed some basic ideas and properties in order to measure the energies for the antiviral agents Hydroxychloroquine, Chloroquine and Remdesivir.

Keywords: Eigenvalues, Energy, Hydroxychloroquine, Chloroquine, Remdesivir, Molecule, Adjacency matrix.

1 Introduction

The chemical graph theory (CGT) is the study of formulation and formation of graphs used in chemical study. CGT is associated with the computation, generalization and development in the construction and conversion of chemical structures into mathematical graphs with the help of several math tools to understand the basic ideas of their topologies. We explore the mathematical firmness of the problems, questions, queries, disputes and issues outstretched in the molecular chemistry. The study of energy of the graphs is very famous these days especially in the field of mathematical chemistry [1, 2]. The study of energy of the graph is purely chemically originated and interoperated [3]. Abundant of researches have been made on the energy of simple as well as molecular graphs using various topological invariants [4, 5]. The disease of Covid-19 started in Dec, 2019 in Wuhan, China [6]. The Chinese invented three antidotes named Hydroxychloroquine, Chloroquine and Remdesivir for the medications of Covid-19 [7-9]. The drug Chloroquine has primarily been used in the treatment of Malaria.

After that, a new medication named Hydroxychloroquine [10] has been utilized for the cure of different diseases such as Systemic lupus erythematosus, HIV and rheumatoid arthritis.
In this study, we have determined the energies as $E'(\acute{\Gamma}_1) = \sum|\lambda'_i|$, $E'(\acute{\Gamma}_2) = \sum|\lambda'_j|$ and $E'(\acute{\Gamma}_3) = \sum|\lambda'_k|$, respectively for the antidotes Hydroxychloroquine, Chloroquine and Remdesivir, whereas the sets $\{\lambda'_1(\acute{\Gamma}_{1,2,3}),\ \lambda'_2(\acute{\Gamma}_{1,2,3}),\ \lambda'_3(\acute{\Gamma}_{1,2,3}),\ \ldots,\lambda'_n(\acute{\Gamma}_{1,2,3})\}$ describe the eigenvalues for the adjacency matrices of $\acute{\Gamma}_1, \acute{\Gamma}_2$ and $\acute{\Gamma}_3$. Basic concepts and features have been developed for measuring the energies of these antiviral agents Hydroxychloroquine, Chloroquine and Remdesivir. The eigenvalues of any network are in fact the eigenvalues of the given matrix known as adjacency matrix. The maximum absolute eigenvalue of a graph is called as its spectral radius. Eigenvalues has its extreme importance in the field of frequency analysis, differential equations, physics, and computer graphics and in many more subjects [11-13]. For more details see [18-24].

2 Potential Applications

Applications of graph energy in the field of physical chemistry of unsaturated conjugated molecules are obvious, rather numerous such as in crystallography [14, 15], theory of macromolecules [16], analysis and comparison of protein sequences [17]. They also include the problems raised in computer science, image analysis and processing, engineering, complex system design and analysis, air transportation, biology, medicine, construction of spacecrafts, face recognition systems, and satellite communication. Less mysterious applications for this are the usage in epidemics and neuronal networks. As considered graph energy [18-22] are able to guess various properties and activities including entropy, boiling point, enthalpy, critical pressure, and acentric factor and many more. Our conclusions can be supportive in conniving new drugs and vaccine for the treatment of COVID-19 with the help of QSARs and QSPRs models that are frequently used in mathematical chemistry.

3 Material and Methods

To get better understanding of eigenvalues of any molecular structure, first of all, we build a mathematical graph of the molecular structure by transforming it into a planar graph. And then we label its nodes in two different methods, by coloring and numbering. But here we have selected the method in which we assign numbers to all nodes. After that we construct its adjacency matrix to get the eigenvalues. We consider three chemical structures known as Hydroxychloroquine, Chloroquine and Remdesivir. Moreover, let $\acute{\Gamma}_1$ be a schlicht, finite, undirected and connected graph with node set $V(\acute{\Gamma}_1) = \{v_1^1, v_1^2, v_1^3, \dots, v_1^n\}$ and edge set $E(\acute{\Gamma}_1) = \{e_1^1, e_1^2, e_1^3, \dots, e_1^n\}$. Similarly, by supposing $\acute{\Gamma}_2$ and $\acute{\Gamma}_3$ are the schlicht, finite, undirected and connected graphs with node sets $V(\acute{\Gamma}_2) = \{v_2^1, v_2^2, v_2^3, \dots, v_2^n\}$, $V(\acute{\Gamma}_3) = \{v_3^1, v_3^2, v_3^3, \dots, v_3^n\}$ and edge sets $E(\acute{\Gamma}_2) = \{e_2^1, e_2^2, e_2^3, \dots, e_2^n\}$, $E(\acute{\Gamma}_3) = \{e_3^1, e_3^2, e_3^3, \dots, e_3^n\}$, respectively. Whereas $|V(\acute{\Gamma}_1)|$ and $|\mathrm{E}(\acute{\Gamma}_1)|$ describe the cardinality of the graph $\acute{\Gamma}_1$ for all $v_1^i \in V(\acute{\Gamma}_1)$ and $v_1^1 v_1^2 \in E(\acute{\Gamma}_1)$. Similarly, $|V(\acute{\Gamma}_2)|$ and $|\mathrm{E}(\acute{\Gamma}_2)|$ explain the cardinality of the graph $\acute{\Gamma}_2$ for all $v_2^i \in V(\acute{\Gamma}_2)$ and $v_2^1 v_2^2 \in E(\acute{\Gamma}_2)$ and $|V(\acute{\Gamma}_3)|$ and $|\mathrm{E}(\acute{\Gamma}_3)|$ show the cardinality of the graph $\acute{\Gamma}_3$ for all $v_3^i \in V(\acute{\Gamma}_3)$ and $v_3^1 v_3^2 \in E(\acute{\Gamma}_3)$. We define n^{th} order adjacency matrix $A(\acute{\Gamma}_{h=1,\ 2,\ 3})$ whose (i, j)-number is formulated as:

$$A(\acute{\Gamma}_{h=1,\ 2,\ 3})_{i,j} = \begin{cases} 1 & \text{for the nodes } v_{h=1,\ 2,\ 3}^i \text{ and } v_{h=1,\ 2,\ 3}^j \text{ to be adjacent,} \\ 0 & \text{for the nodes } v_{h=1,\ 2,\ 3}^i \text{ and } v_{h=1,\ 2,\ 3}^j \text{ not to be adjacent,} \\ 0 & \quad i = j. \end{cases}$$

Where $A(\acute{\Gamma}_{h=1,\ 2,\ 3})$ is a square symmetric matrix. To compute the eigenvalues and analyze the data from adjacency matrices, we have used the software MATLAB.

3.1 Antidote Hydroxychloroquine

Suppose $\acute{\Gamma}_1$ is the graph of chemical structure of Hydroxychloroquine shown below in Fig. 1. And $\lambda_1'(\acute{\Gamma}_1),\ \lambda_2'(\acute{\Gamma}_1),\ \lambda_3'(\acute{\Gamma}_1),\ \dots, \lambda_n'(\acute{\Gamma}_1)$ are the eigenvalues of $A(\acute{\Gamma}_1)$.

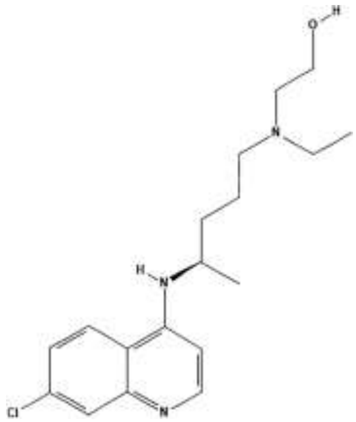

Fig. 1: Hydroxychloroquine ($\acute{\Gamma}_1$)

The energy of the graph $\acute{\Gamma}_1$ is defined as:

$$E'(\acute{\Gamma}_1) = \sum_{z=1}^{n} |\lambda'_z(\acute{\Gamma}_1)| \tag{1}$$

Adjacency matrix of the graph $\acute{\Gamma}_1$ is given by:

$$A(\acute{\Gamma}_1) = \begin{pmatrix}
0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1\\
0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0\\
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0&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&0&0&0&0\\
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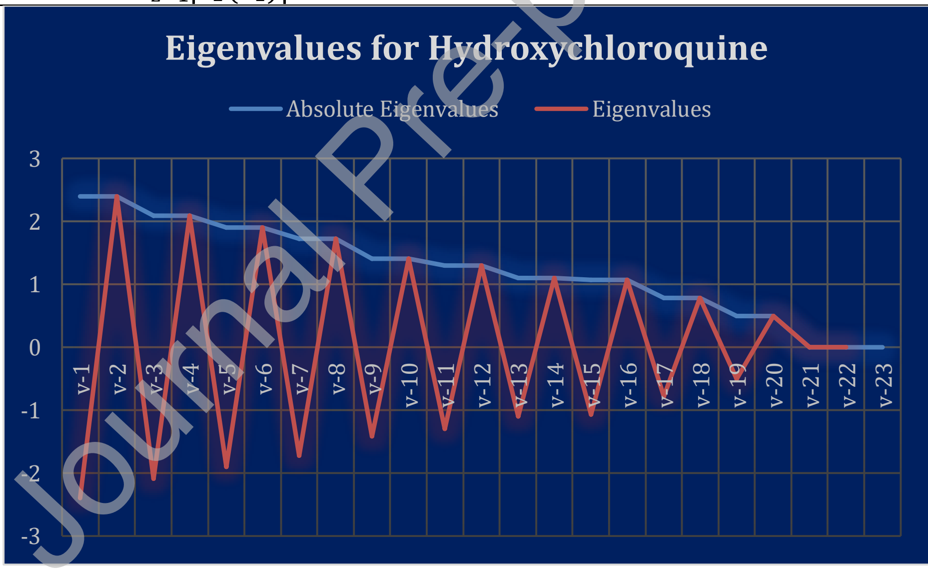
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0\\
0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0\\
0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1\\
0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0
\end{pmatrix}$$

Definition: The energy of a graph $\acute{\Gamma}_r$ is defined as the sum of the absolute eigenvalues of $\acute{\Gamma}_r$. The eigenvalues that are computed from the above-mentioned adjacency matrix of the graph $\acute{\Gamma}_1$ are given in Tab. 1:

Table 1: Shows eigenvalues of $\acute{\Gamma}_1$.

Eigenvalues	$\acute{\Gamma}_1$	Absolute eigenvalues $\lvert\lambda'_z(\acute{\Gamma}_1)\rvert$ for $z = 1, 2, \ldots, 23$
λ'_1	-2.39761	2.39761
λ'_2	2.39761	2.39761
λ'_3	-2.09285	2.09285

λ'_4	2.09285	2.09285
λ'_5	−1.94465	1.94465
λ'_6	1.94465	1.94465
λ'_7	−1.72823	1.72823
λ'_8	1.72823	1.72823
λ'_9	−1.41421	1.41421
λ'_{10}	1.41421	1.41421
λ'_{11}	−1.30518	1.30518
λ'_{12}	1.30518	1.30518
λ'_{13}	−1.168	1.168
λ'_{14}	1.168	1.168
λ'_{15}	−1.07499	1.07499
λ'_{16}	1.07499	1.07499
λ'_{17}	−0.784918	0.784918
λ'_{18}	0.784918	0.784918
λ'_{19}	−0.513339	0.513339
λ'_{20}	0.513339	0.513339
λ'_{21}	0	0
λ'_{22}	0	0
λ'_{23}	0	0
Sum of eigenvalues = $\sum_{z=1}^{23} \lvert \lambda'_z(\acute{\Gamma}_1) \rvert$	0	28.84795



It can be seen from this graph that the maximum energy obtained is 2.39761 Joules. While the minimum energy obtained is 0 Joule. The total energy for the molecular structure $\acute{\Gamma}_1$ is 28.84795 Joules.

3.2 Antidote Chloroquine

Suppose $\acute{\Gamma}_2$ is the graph of chemical structure of Chloroquine shown below in Fig. 2. And $\lambda'_1(\acute{\Gamma}_2),\ \lambda'_2(\acute{\Gamma}_2),\ \lambda'_3(\acute{\Gamma}_2),\ \ldots,\lambda'_n(\acute{\Gamma}_2)$ are the eigenvalues of $A(\acute{\Gamma}_2)$.

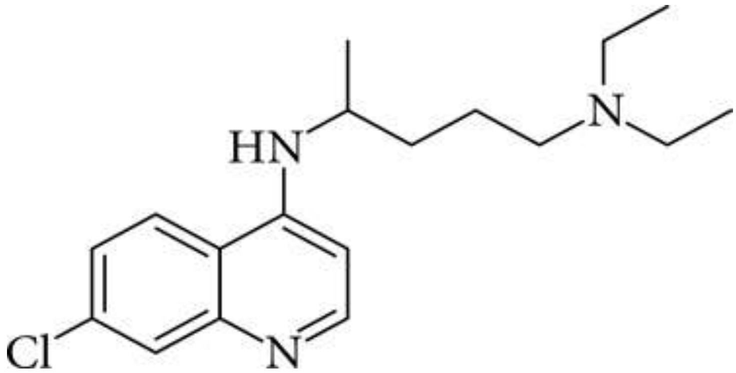


Fig. 2: Chloroquine $(\acute{\Gamma}_2)$

The energy of the graph $\acute{\Gamma}_2$ is defined as:

$$E'(\acute{\Gamma}_2) = \sum_{z=1}^{n} |\lambda'_z(\acute{\Gamma}_2)| \tag{2}$$

Adjacency matrix of the graph $\acute{\Gamma}_2$ is given by:

$$A(\acute{\Gamma}_2) = \begin{pmatrix}
0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1\\
0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
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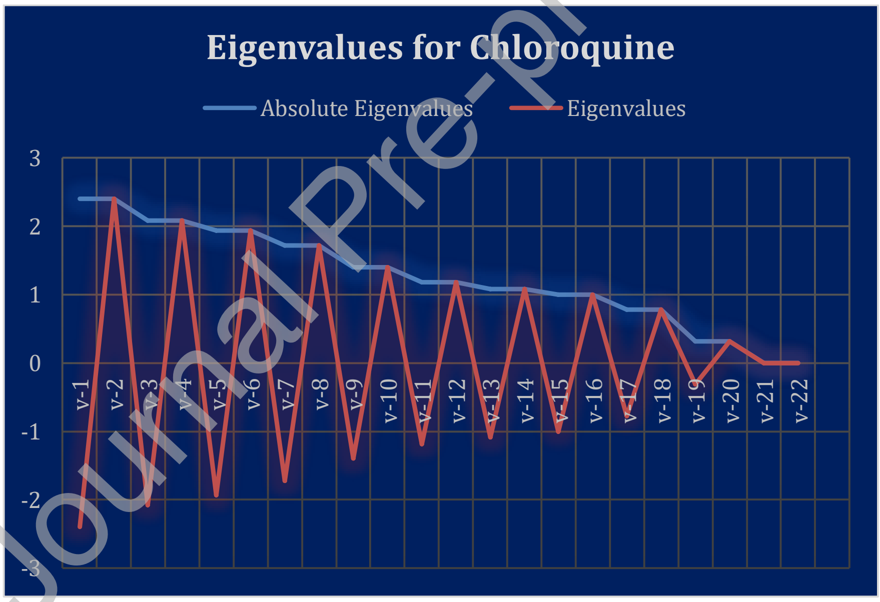
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0\\
0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1\\
0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0
\end{pmatrix}$$

The eigenvalues that are computed from the above-mentioned adjacency matrix of the graph $\acute{\Gamma}_2$ are given in Tab. 2:

Table 2: Shows eigenvalues of $\acute{\Gamma}_2$.

Eigenvalues	$\acute{\Gamma}_2$	Absolute eigenvalues $\lvert\lambda'_z(\acute{\Gamma}_2)\rvert$ for $z = 1, 2, \ldots, 22$
λ'_1	-2.3976	2.3976
λ'_2	2.3976	2.3976
λ'_3	-2.07953	2.07953
λ'_4	2.07953	2.07953
λ'_5	-1.93277	1.93277

λ'_6	1.93277	1.93277
λ'_7	−1.72193	1.72193
λ'_8	1.72193	1.72193
λ'_9	−1.39567	1.39567
λ'_{10}	1.39567	1.39567
λ'_{11}	−1.18244	1.18244
λ'_{12}	1.18244	1.18244
λ'_{13}	−1.08429	1.08429
λ'_{14}	1.08429	1.08429
λ'_{15}	−1	1
λ'_{16}	1	1
λ'_{17}	−0.778054	0.778054
λ'_{18}	0.778054	0.778054
λ'_{19}	−0.315125	0.315125
λ'_{20}	0.315125	0.315125
λ'_{21}	0	0
λ'_{22}	0	0
Sum of eigenvalues $= \sum_{z=1}^{22} \lvert \lambda'_z(\acute{\Gamma}_2) \rvert$	0	27.774818



It can be seen from this graph that the maximum energy obtained is 2.3976 Joules. While the minimum energy obtained is 0 Joule. The total energy for the molecular structure $\acute{\Gamma}_2$ is 27.774818 Joules.

3.3 Antidote Remdesivir

Suppose $\acute{\Gamma}_2$ is the graph of chemical structure of Remdesivir shown below in Fig. 3. And $\lambda'_1(\acute{\Gamma}_3)$, $\lambda'_2(\acute{\Gamma}_3)$, $\lambda'_3(\acute{\Gamma}_3)$, . . . , $\lambda'_n(\acute{\Gamma}_3)$ are the eigenvalues of $A(\acute{\Gamma}_3)$.

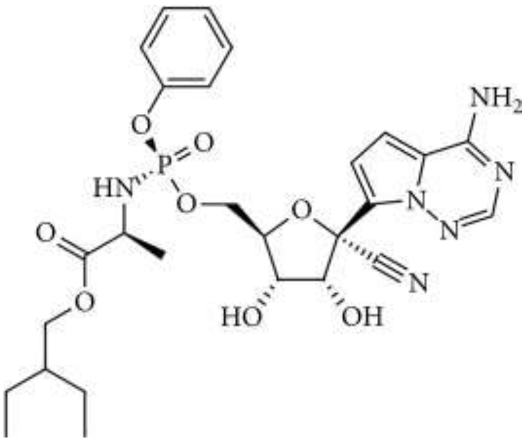


Fig. 3: Remdesivir ($\acute{\Gamma}_3$)

The energy of the graph $\acute{\Gamma}_3$ is defined as:

$$E'(\acute{\Gamma}_3) = \sum_{z=1}^{n} |\lambda'_z(\acute{\Gamma}_3)| \tag{3}$$

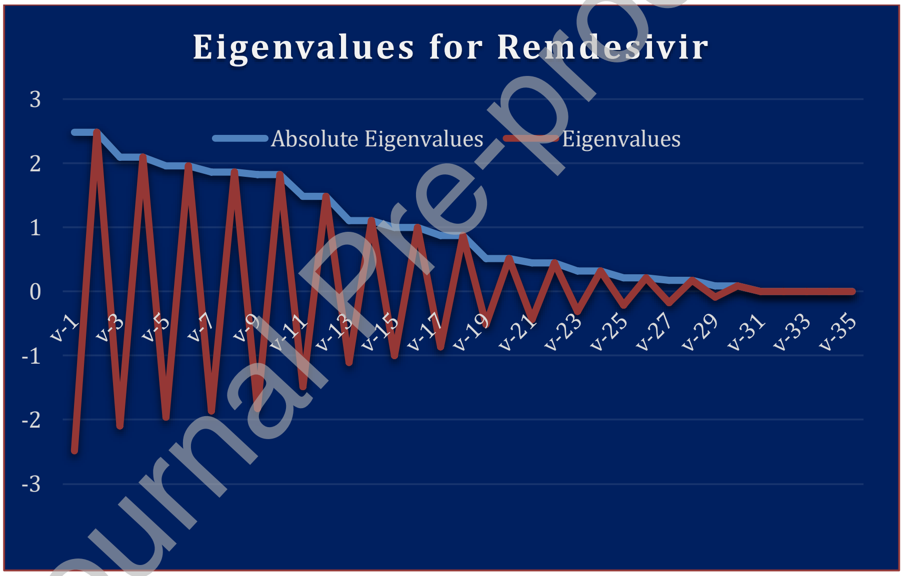
The eigenvalues that are computed for the graph $\acute{\Gamma}_3$ are given in Tab. 3:

Table 3: Shows eigenvalues of $\acute{\Gamma}_3$.

Eigenvalues	$\acute{\Gamma}_3$	Absolute eigenvalues $\lvert\lambda'_z(\acute{\Gamma}_3)\rvert$ for $z = 1, 2, \ldots, 35$
λ'_1	−2.4871	2.4871
λ'_2	2.4871	2.4871
λ'_3	−2.0993	2.0993
λ'_4	2.0993	2.0993
λ'_5	−1.9627	1.9627
λ'_6	1.9627	1.9627
λ'_7	−1.8619	1.8619
λ'_8	1.8619	1.8619
λ'_9	−1.8267	1.8267
λ'_{10}	1.8267	1.8267
λ'_{11}	−1.4831	1.4831
λ'_{12}	1.4831	1.4831
λ'_{13}	−1.1082	1.1082
λ'_{14}	1.1082	1.1082
λ'_{15}	−1.	1
λ'_{16}	1	1
λ'_{17}	−0.8680	0.8680
λ'_{18}	0.8680	0.8680
λ'_{19}	−0.5125	0.5125
λ'_{20}	0.5125	0.5125
λ'_{21}	−0.4418	0.4418
λ'_{22}	0.4418	0.4418
λ'_{23}	−0.3162	0.3162
λ'_{24}	0.3162	0.3162
λ'_{25}	−0.2129	0.2129
λ'_{26}	0.2129	0.2129

λ'_{27}	-0.1719	0.1719
λ'_{28}	0.1719	0.1719
λ'_{29}	-0.08923	0.08923
λ'_{30}	0.08923	0.08923
λ'_{31}	-0.00251	0.00251
λ'_{32}	0.00251	0.00251
λ'_{33}	0	0
λ'_{34}	0	0
λ'_{35}	0	0
Sum of eigenvalues $= \sum_{z=1}^{35} \lvert \lambda'_z(\acute{\Gamma}_3) \rvert$	0	32.88808

Similarly, an adjacency matrix of order $A_{35\times35}$ is derived and computed for thirty-five eigenvalues. It can be seen from this graph that the maximum energy obtained is 2.4871 Joules. While the minimum energy obtained is 0 Joule. The total energy for the molecular structure $\acute{\Gamma}_3$ is 32.88808 Joules. Graph shows different energy levels for the chemical compound *Remdesivir*.



4 Results and Discussion

We have discussed here three molecular structures of antiviral agents named Hydroxychloroquine, Chloroquine and Remdesivir. Furthermore, different graphs [23-26] have been constructed and observed for the above-mentioned antiviral agents to demonstrate some links between the structures of graphs and their energy levels mentioned in Equations (1-3). Moreover, the collective degree acquired from the characteristics polynomial which can be computed from eigenvalues, represents the cardinality of their vertex set. Different energy levels such as minimum, maximum and total energy are also determined.

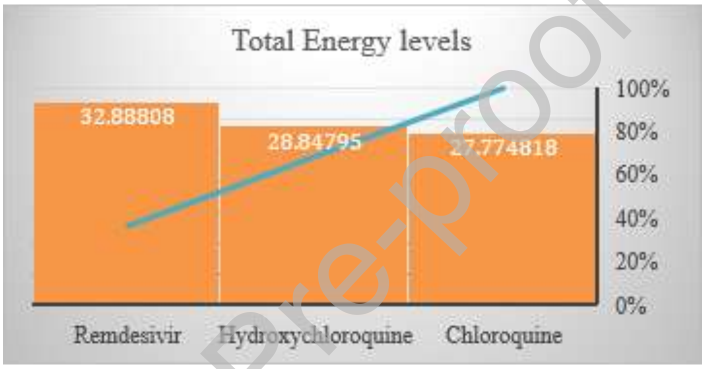
5 Conclusion

The following Table 4 shows the comparison among the total energy levels of Hydroxychloroquine, Remdesivir and Chloroquine.

Table 4: Comparison among the total energy levels of $\acute{\Gamma}_1$, $\acute{\Gamma}_2$, and $\acute{\Gamma}_3$.

Antiviral Agent	Total Energy level
Hydroxychloroquine	28.84795 Joules
Remdesivir	32.88808 Joules
Chloroquine	27.774818 Joules

Different values of total energy levels in joules and in percentages are depicted in graph shown below.



The principal component (*PC*) for the eigenvector is actually a parameter which is maximum among all the eigenvalues. If an eigenvalue $\lambda'_z < 1$, then the *PC* is said to have a unique original variable. This original variable obtained has a value which is better than the new value. The smallest eigenvalue is persistently interlinked with the classification of the given graphs. The obtained results can also be used in differential geometry [27-30]. The gap between the 1st & 2nd eigenvalues plays a vital role in the application of various fields in mathematics and subsequently, this gap is interlinked with a kind of "connectivity measure of the graph". It has been brought into notice that two antiviral agents Hydroxychloroquine and Chloroquine have a common maximum absolute eigenvalue which is 2.3976 and similarly, they have a common minimum absolute eigenvalue which is 0. Eigenvalues serve as energy and can be used in different physiochemical properties such as boiling point, entropy, enthalpy, acentric factor, and critical pressure. Our findings can aid in the development of new medications and vaccines for COVID-19 treatment.

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Conflict of Interest

The authors declare that they have no conflict of interest.