

**Original Research Article****Investigation of Closed Formula and Topological Properties of Remdesivir ($C_{27}H_{35}N_6O_8P$)**

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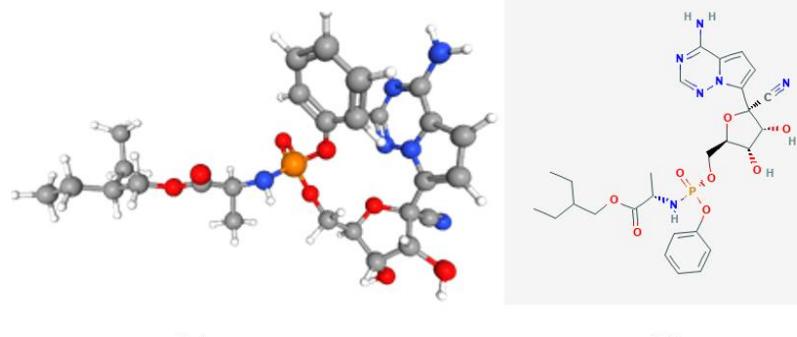
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ABSTRACT

Coronavirus is able to cause illnesses ranging from the common flu to severe respiratory disease. Today there is great competition among researchers and physicians to cure COVID-19. Remdesivir is being studied for the COVID-19 treatment. In this article, we presented the topological analysis of remdesivir with the help of M-polynomial. Proofs of the closed form of some topological indices via M-polynomial are also included in this article.

GRAPHICAL ABSTRACT

Molecular structure of remdesivir (a) 3D structure (b) 2D structure.

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Introduction

In December 2019, a new epidemic started in the city of China (Wuhan) and rapidly spread all over the world, causing a serious health problem. This virus is named severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) [1]. Personal protective equipment and physical distance are the best means to reduce the spread of this epidemic. A great deal of time is required to find the cure of COVID-19.

Remdesivir is a monophosphoramidate prodrug of an adenosine analogue. It is a broad-spectrum antiviral substance that act against coronaviruses, flaviviruses and paramyxoviruses. Several clinical trials reflect its *vitro* activity on human airway epithelial cells against SARS-CoV-2 that shows encouraging results [2, 3]. The chemical formula of remdesivir is $C_{27}H_{35}N_6O_8P$ with molecular weight of 602.6 g/mol. 3D and 2D structure of remdesivir is shown in Figure 1.

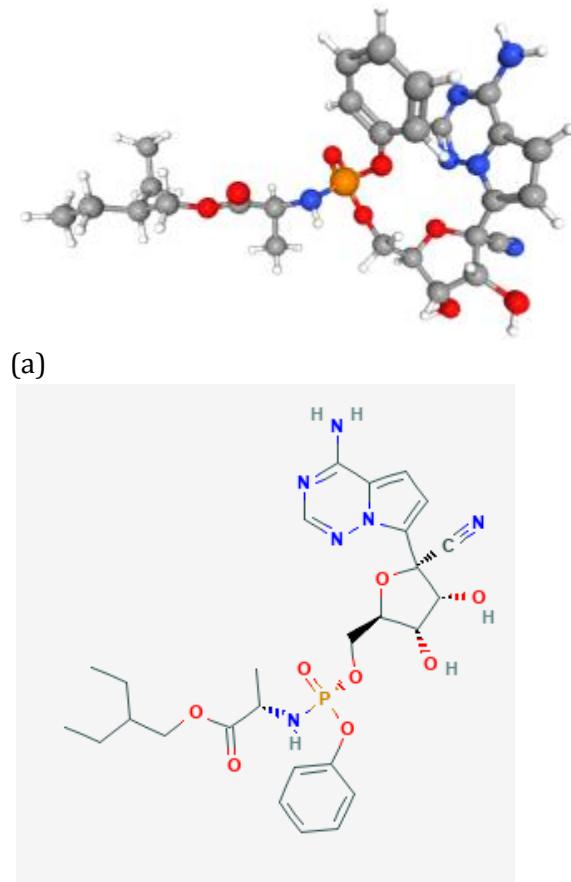


Figure 1: Molecular structure of remdesivir (a) 3D structure (b) 2D structure

A graph $G(V_G, E_G)$ is a relation between vertex set V_G and edge set E_G . The degree of a vertex d_x is the count of edges meet at vertex X . The molecular structure of the substance can be converted in graph in which atoms act as vertex and bonds behave as edges of the graph. By using the computational technique, the graph can be converted into a real number. This real number is known as topological index. This number is capable of displaying the physical, chemical and biological characteristics of the substance [4- 6]. C-H bond does not have a serious effect on the characteristics of the chemical species. So, during the computational analysis, we ignore it.

For a graph G , a degree dependent topological index is defined as equation 1:

$$I(G) = \sum_{e=xy \in E_G} f(d_x, d_y). \quad 1$$

By counting edges which have same end-degrees in the chemical graph, then we can rewrite equation 1 as:

$$I(G) = \sum_{j \leq k} m_{jk} f(j, k). \quad (2)$$

where the relation $\{d_x, d_y\} = \{j, k\}$ shows the satisfaction and m_{jk} is the total count of edges xy of the graph G .

Estrada et al. (1998) set out an important degree dependent topological indices named as atom-bond connectivity invariant [7]. This index is denoted by ABC calculated as:

$$ABC[G] = \sum_{xy \in E(G)} \sqrt{\frac{d_x + d_y - 2}{d_x \cdot d_y}}$$

In 2009, Damir Vukčević and Boris Furtula [23] proposed an important index named as geometric arithmetic index and defined as:

$$GA[G] = \sum_{xy \in E(G)} \frac{2\sqrt{d_x \cdot d_y}}{d_x + d_y}$$

V.R. Kulli [18- 20] introduced new indices in 2016 and 2017,

first K Banhatti index

$$B_1[G] = \sum_{xy \in E(G)} (d_x + d_{xy}),$$

second K Bahtti index

$$B_2[G] = \sum_{xy \in E(G)} (d_x \cdot d_{xy}),$$

first K hyper Bahatti index

$$HB_1[G] = \sum_{xy \in E(G)} (d_x + d_{xy})^2,$$

Second K hyper Bahatti index

$$HB_2[G] = \sum_{xy \in E(G)} (d_x \cdot d_{xy})^2,$$

modified first K Banhatti index

$$^mB_1[G] = \sum_{xy \in E(G)} \frac{1}{d_x + d_{xy}},$$

modified second K Banhatti index

$$^mB_2[G] = \sum_{xy \in E(G)} \frac{1}{d_x \cdot d_{xy}},$$

Harmonic K Banhatti index

$$H_b[G] = \sum_{xy \in E(G)} \frac{2}{d_x + d_{xy}}.$$

These topological indices are either calculated directly by their formula or by using the graph polynomials such as M-polynomial. E. Deutsch and S. Klavzar define the M-polynomial in 2015 as [9]: $M_G(u, v) = \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k$.

Here $\psi = \min\{d_x | x \in V_G\}$, $\Psi = \max\{d_x | x \in V_G\}$. Numerous graphs have been studied in the past through M-Polynomial and topological indices [1-3, 6-8, 14-17, 22, 25-28]. Some operators which are used further, are defined as:

$$D_u M_G(u, v) = u \frac{\partial}{\partial u} M_G(u, v),$$

$$D_u^{\frac{1}{2}} M_G(u, v) = \sqrt{u \frac{\partial}{\partial u} M_G(u, v) \times \sqrt{M_G(u, v)}},$$

$$D_v M_G(u, v) = v \frac{\partial}{\partial v} M_G(u, v),$$

$$D_v^{\frac{1}{2}} M_G(u, v) = \sqrt{v \frac{\partial}{\partial v} M_G(u, v) \times \sqrt{M_G(u, v)}},$$

$$S_u M_G(u, v) = \int_0^u \frac{M_G(t, v)}{t} dt,$$

$$S_u^{\frac{1}{2}} M_G(u, v) = \sqrt{\int_0^u \left(\frac{M_G(t, v)}{t} \right) dt \times \sqrt{M_G(u, v)}},$$

$$S_v M_G(u, v) = \int_0^v \frac{M_G(u, t)}{t} dt,$$

$$S_v^{\frac{1}{2}} M_G(u, v) = \sqrt{\int_0^v \left(\frac{M_G(u, t)}{t} \right) dt \times \sqrt{M_G(u, v)}},$$

$$Q_\alpha M_G(u, v) = u^\alpha M_G(u, v),$$

$$JM_G(u, v) = M_G(u, u),$$

$$L_u M_G(u, v) = M_G(u^2, v),$$

$$L_v M_G(u, v) = M_G(u, v^2).$$

Results and Discussion

In the present section, proofs of some closed formulas of topological indices depend on vertex degree are calculated with the help of M-polynomial. These indices are taken from [4].

Theorem 2.1 Let $M_G(u, v)$ be the M-polynomial for the graph G , then the atom bond index is also calculated as

$$ABC(G) = D_u^{\frac{1}{2}} Q_{-2} J S_u^{\frac{1}{2}} S_v^{\frac{1}{2}} M_G(u, v) |_{u=1}.$$

Proof. By taking

$$= D_u^{\frac{1}{2}} Q_{-2} J S_u^{\frac{1}{2}} S_v^{\frac{1}{2}} M_G(u, v)$$

$$= D_u^{\frac{1}{2}} Q_{-2} J S_u^{\frac{1}{2}} S_v^{\frac{1}{2}} \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k$$

$$= D_u^{\frac{1}{2}} Q_{-2} J \sum_{\psi \leq j \leq k \leq \Psi} \frac{1}{\sqrt{jk}} m_{jk} u^j v^k$$

$$= D_u^{\frac{1}{2}} Q_{-2} J \sum_{\psi \leq j \leq k \leq \Psi} \frac{1}{\sqrt{jk}} m_{jk} u^{j+k}$$

$$= D_u^{\frac{1}{2}} \sum_{\psi \leq j \leq k \leq \Psi} \frac{1}{\sqrt{jk}} m_{jk} u^{j+k-2}$$

$$= \sum_{\psi \leq j \leq k \leq \Psi} \sqrt{\frac{j+k-2}{jk}} m_{jk} u^{j+k-2}.$$

$$D_u^{\frac{1}{2}} Q_{-2} J S_u^{\frac{1}{2}} S_v^{\frac{1}{2}} M_G(u, v) |_{u=1}$$

$$= \sum_{\psi \leq j \leq k \leq \Psi} \sqrt{\frac{j+k-2}{jk}} m_{jk} = \sum_{xy \in E_G} \sqrt{\frac{d_x + d_y - 2}{d_x d_y}}$$

Now Hence $ABC(G) = D_u^{\frac{1}{2}} Q_{-2} J S_u^{\frac{1}{2}} S_v^{\frac{1}{2}} M_G(u, v) |_{u=1}$.

Theorem 2.2 If $M_G(u, v)$ be the M-polynomial of the graph G , then the geometric arithmetic index is given by

$$GA(G) = 2 S_u J D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} M_G(u, v) |_{u=1}.$$

Proof. By taking

$$\begin{aligned}
& 2S_u JD_u^{\frac{1}{2}} D_v^{\frac{1}{2}} M_G(u, v) \\
&= 2S_u JD_u^{\frac{1}{2}} D_v^{\frac{1}{2}} \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k \\
&= 2S_u JD_u^{\frac{1}{2}} \sum_{\psi \leq j \leq k \leq \Psi} \sqrt{jk} m_{jk} u^j v^k \\
&= 2S_u J \sum_{\psi \leq j \leq k \leq \Psi} \sqrt{jk} m_{jk} u^j v^k \\
&= 2S_u \sum_{\psi \leq j \leq k \leq \Psi} \sqrt{jk} m_{jk} u^{j+k} \\
&= 2 \sum_{\psi \leq j \leq k \leq \Psi} \frac{\sqrt{jk}}{j+k} m_{jk} u^{j+k} \\
&= \sum_{\psi \leq j \leq k \leq \Psi} \frac{2\sqrt{jk}}{j+k} m_{jk} u^{j+k} \\
&= D_x \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k + D_y \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k + 2D_x Q_{-2} J \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k, \\
&= \sum_{\psi \leq j \leq k \leq \Psi} jm_{jk} u^j v^k + \sum_{\psi \leq j \leq k \leq \Psi} km_{jk} u^j v^k + 2D_x Q_{-2} \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^{j+k}, \\
&= \sum_{\psi \leq j \leq k \leq \Psi} (j+k)m_{jk} u^j v^k + 2D_x \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^{j+k-2}, \\
&= \sum_{\psi \leq j \leq k \leq \Psi} (j+k)m_{jk} u^j v^k + 2 \sum_{\psi \leq j \leq k \leq \Psi} (j+k-2)m_{jk} u^{j+k-2}, \\
&= \sum_{\psi \leq j \leq k \leq \Psi} (j+k)m_{jk} u^j v^k + \sum_{\psi \leq j \leq k \leq \Psi} 2(j+k-2)m_{jk} u^{j+k-2}, \\
&= \sum_{\psi \leq j \leq k \leq \Psi} \{j+k+2(j+k-2)\}m_{jk} u^{j+k-2}. \blacksquare
\end{aligned}$$

Now

$$\begin{aligned}
& (D_x + D_y + 2D_x Q_{-2} J) M_G(u, v) |_{u=v=1} \\
&= \sum_{\psi \leq j \leq k \leq \Psi} \{j+k+ (j+k-2)\}m_{jk} \\
&= \sum_{xy \in E_G} [d_x + d_y + (d_x + d_y - 2)] \\
&= \sum_{xy \in E_G} \{d_x + d_y\}.
\end{aligned}$$

Hence

$$B_1(G) = D_x + D_y + 2D_x Q_{-2} J M_G(u, v) |_{u=v=1}.$$

Theorem 2.4 If $M_G(u, v)$ is the M-polynomial of the graph G , then second K Banhatti index is computed as $B_2(G) = D_u Q_{-2} J (D_u + D_v) M_G(u, v) |_{u=1}$.

Proof. By taking

$$\begin{aligned}
& 2S_u JD_u^{\frac{1}{2}} D_v^{\frac{1}{2}} M_G(u, v) |_{u=1} \\
&= \sum_{\psi \leq j \leq k \leq \Psi} \frac{2\sqrt{jk}}{j+k} m_{jk} = \sum_{xy \in E_G} \frac{2\sqrt{d_x d_y}}{d_x + d_y} \\
&\text{Hence } GA(G) = 2S_u JD_u^{\frac{1}{2}} D_v^{\frac{1}{2}} M_G(u, v) |_{u=1}. \\
&\text{Theorem 2.3 If } M_G(u, v) \text{ is represented the M-polynomial of the graph } G, \text{ then first K Banhatti index is computed by } B_1(G) = (D_x + D_y + 2D_x Q_{-2} J) M_G(u, v) |_{u=v=1}. \\
&\text{Proof. By taking} \\
& (D_x + D_y + 2D_x Q_{-2} J) M_G(u, v) \\
&= (D_x + D_y + 2D_x Q_{-2} J) \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k, \\
&= D_u Q_{-2} J (D_u + D_v) M_G(u, v) \\
&= D_u Q_{-2} J (D_u + D_v) \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k \\
&= D_u Q_{-2} J (D_u \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k + D_v \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k), \\
&= D_u Q_{-2} J (\sum_{\psi \leq j \leq k \leq \Psi} jm_{jk} u^j v^k + \sum_{\psi \leq j \leq k \leq \Psi} km_{jk} u^j v^k), \\
&= D_u Q_{-2} J \sum_{\psi \leq j \leq k \leq \Psi} (j+k)m_{jk} u^j v^k, \\
&= D_u Q_{-2} \sum_{\psi \leq j \leq k \leq \Psi} (j+k)m_{jk} u^{j+k}, \\
&= D_u \sum_{\psi \leq j \leq k \leq \Psi} (j+k)m_{jk} u^{j+k-2}, \\
&= \sum_{\psi \leq j \leq k \leq \Psi} (j+k)(j+k-2)m_{jk} u^{j+k-2}. \\
&\text{Now } D_u Q_{-2} J (D_u + D_v) M_G(u, v) |_{u=1}
\end{aligned}$$

$$\begin{aligned}
&= \sum_{\psi \leq j \leq k \leq \Psi} (j+k)(j+k-2)m_{jk}, \\
&= \sum_{xy \in E_G} (d_x + d_y)(d_x + d_y - 2) = \sum_{xy \in E_G} \{d_x d_{xy} . \\
\text{Hence } &B_2(G) = D_u Q_{-2} J(D_u + D_v) M_G(u, v) \Big|_{u=1} .
\end{aligned}$$

Theorem 2.5 Let $M_G(u, v)$ be the M -polynomial for the graph G , then first K hyper Banhatti index is given by

$$\begin{aligned}
HB_1(G) &= \{D_u^2 + D_v^2 + 2D_u^2 Q_{-2} J + 2D_u Q_{-2} J(D_u + D_v)\} M_G(u, v) \Big|_{u=v=1} .
\end{aligned}$$

Proof. By taking

$$\begin{aligned}
&\{D_u^2 + D_v^2 + 2D_u^2 Q_{-2} J + 2D_u Q_{-2} J(D_u + D_v)\} M_G(u, v) \\
&= \{D_u^2 + D_v^2 + 2D_u^2 Q_{-2} J + 2D_u Q_{-2} J(D_u + D_v)\} \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k, \\
&= D_u^2 \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k + D_v^2 \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k \\
&\quad + 2D_u^2 Q_{-2} J \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k + 2D_u Q_{-2} J(D_u + D_v) \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k, \\
&= \sum_{\psi \leq j \leq k \leq \Psi} j^2 m_{jk} u^j v^k + \sum_{\psi \leq j \leq k \leq \Psi} k^2 m_{jk} u^j v^k + 2D_u^2 Q_{-2} \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^{j+k} \\
&\quad + 2D_u Q_{-2} J(D_u \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k + D_v \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k), \\
&= \sum_{\psi \leq j \leq k \leq \Psi} (j^2 + k^2) m_{jk} u^j v^k + 2D_u^2 \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^{j+k-2} \\
&\quad + 2D_u Q_{-2} J \left(\sum_{\psi \leq j \leq k \leq \Psi} j m_{jk} u^j v^k + \sum_{\psi \leq j \leq k \leq \Psi} k m_{jk} u^j v^k \right), \\
&= \sum_{\psi \leq j \leq k \leq \Psi} (j^2 + k^2) m_{jk} u^j v^k + 2 \sum_{\psi \leq j \leq k \leq \Psi} (j+k-2)^2 m_{jk} u^{j+k-2} \\
&\quad + 2D_u Q_{-2} J \sum_{\psi \leq j \leq k \leq \Psi} (j+k) m_{jk} u^j v^k, \\
&= \sum_{\psi \leq j \leq k \leq \Psi} (j^2 + k^2) m_{jk} u^j v^k + \sum_{\psi \leq j \leq k \leq \Psi} 2(j+k-2)^2 m_{jk} u^{j+k-2} \\
&\quad + 2D_u Q_{-2} \sum_{\psi \leq j \leq k \leq \Psi} (j+k) m_{jk} u^{j+k}, \\
&= \sum_{\psi \leq j \leq k \leq \Psi} (j^2 + k^2) m_{jk} u^j v^k + \sum_{\psi \leq j \leq k \leq \Psi} 2(j+k-2)^2 m_{jk} u^{j+k-2} \\
&\quad + 2D_u \sum_{\psi \leq j \leq k \leq \Psi} (j+k) m_{jk} u^{j+k-2}, \\
&= \sum_{\psi \leq j \leq k \leq \Psi} (j^2 + k^2) m_{jk} u^j v^k + \sum_{\psi \leq j \leq k \leq \Psi} 2(j+k-2)^2 m_{jk} u^{j+k-2} \\
&\quad + 2 \sum_{\psi \leq j \leq k \leq \Psi} (j+k)(j+k-2) m_{jk} u^{j+k-2}, \\
&= \sum_{\psi \leq j \leq k \leq \Psi} (j^2 + k^2) m_{jk} u^j v^k + \sum_{\psi \leq j \leq k \leq \Psi} 2(j+k-2)^2 m_{jk} u^{j+k-2} \\
&\quad + \sum_{\psi \leq j \leq k \leq \Psi} 2(j+k)(j+k-2) m_{jk} u^{j+k-2}.
\end{aligned}$$

$$\begin{aligned}
& \text{Now } \{D_u^2 + D_v^2 + 2D_u^2 Q_{-2} J + 2D_u Q_{-2} J(D_u + D_v)\} M_G(u, v)|_{u=v=1} \\
& = \sum_{\psi \leq j \leq k \leq \Psi} \{j^2 + k^2 + 2(j+k-2)^2 + 2(j+k)(j+k-2)\} m_{jk}, \\
& = \sum_{xy \in E_G} \{d_x^2 + d_y^2 + 2(d_x + d_y - 2) + 2(d_x + d_y)(d_x + d_y - 2)\}, \\
& = \sum_{xy \in E_G} (d_x + d_{xy})^2.
\end{aligned}$$

$$\text{Hence } HB_1(G) = \{D_u^2 + D_v^2 + 2D_u^2 Q_{-2} J + 2D_u Q_{-2} J(D_u + D_v)\} M_G(u, v)|_{u=v=1}.$$

Theorem 2.6 IF $M_G(u, v)$ is the M-polynomial of the graph G, then second K hyper Banhatti index is given by $HB_2(G) = D_u^2 Q_{-2} J(D_u^2 + D_v^2) M_G(u, v)|_{u=1}$.

Proof. By taking

$$\begin{aligned}
& D_u^2 Q_{-2} J(D_u^2 + D_v^2) M_G(u, v) \\
& = D_u^2 Q_{-2} J(D_u^2 + D_v^2) \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k, \\
& = D_u^2 Q_{-2} J(D_u^2) \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k + D_v^2 \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k S_x Q_{-2} \\
& = D_u^2 Q_{-2} J \left(\sum_{\psi \leq j \leq k \leq \Psi} j^2 m_{jk} u^j v^k + \sum_{\psi \leq j \leq k \leq \Psi} k^2 m_{jk} u^j v^k \right) S_x \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} (u^{2j+k} + u^{j+2k}), \\
& = D_u^2 Q_{-2} J \sum_{\psi \leq j \leq k \leq \Psi} (j^2 + k^2) m_{jk} u^j v^k, \\
& = D_u^2 Q_{-2} \sum_{\psi \leq j \leq k \leq \Psi} (j^2 + k^2) m_{jk} u^{j+k}, \\
& = D_u^2 \sum_{\psi \leq j \leq k \leq \Psi} (j^2 + k^2) m_{jk} u^{j+k-2}, \\
& = \sum_{\psi \leq j \leq k \leq \Psi} (j^2 + k^2) (j+k-2)^2 m_{jk} u^{j+k-2}.
\end{aligned}$$

$$\text{Now } D_u^2 Q_{-2} J(D_u^2 + D_v^2) M_G(u, v)|_{u=1}$$

$$\begin{aligned}
& = \sum_{\psi \leq j \leq k \leq \Psi} (j^2 + k^2) (j+k-2)^2 m_{jk}, \\
& = \sum_{xy \in E_G} (d_x^2 + d_y^2) (d_x + d_y - 2)^2 = \sum_{xy \in E_G} (d_x d_{xy})^2.
\end{aligned}$$

$$\text{Hence } HB_2(G) = D_u^2 Q_{-2} J(D_u^2 + D_v^2) M_G(u, v)|_{u=1}.$$

Theorem 2.7 If $M_G(u, v)$ is the M-polynomial of the graph G, then modified first K Banhatti index is computed as ${}^m B_1(G) = S_x Q_{-2} J(L_u + L_v) M_G(u, v)|_{u=1}$.

Proof. By taking

$$S_x Q_{-2} J(L_x + L_y) M_G(u, v)$$

$$\begin{aligned}
& = S_x Q_{-2} J(L_x + L_y) \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k, \\
& = S_x Q_{-2} J(L_x \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k + L_y \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k), \\
& = S_x Q_{-2} J \left(\sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^{2j} v^k + \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^{2k} \right), \\
& = S_x Q_{-2} J \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} (u^{2j} v^k + u^j v^{2k}), \\
& = S_x Q_{-2} J \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} (u^{2j+k} + u^{j+2k}), \\
& = \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} \left(\frac{1}{2j+k-2} u^{2j+k-2} + \frac{1}{j+2k-2} u^{j+2k-2} \right).
\end{aligned}$$

$$\begin{aligned}
& \text{Now } S_x Q_{-2} J(L_x + L_y) M_G(u, v)|_{u=1} \\
& = \sum_{\psi \leq j \leq k \leq \Psi} \left(\frac{1}{2j+k-2} + \frac{1}{j+2k-2} \right) m_{jk}, \\
& = \sum_{xy \in E_G} \left(\frac{1}{2d_x + d_y - 2} + \frac{1}{d_x + 2d_y - 2} \right), \\
& = \sum_{xy \in E_G} \left(\frac{1}{d_x + d_y - 2} + \frac{1}{d_y + d_x - 2} \right), \\
& = \sum_{xy \in E_G} \frac{1}{d_x + d_{xy}}.
\end{aligned}$$

$$\text{Hence } {}^m B_1(G) = S_x Q_{-2} J(L_x + L_y) M_G(u, v)|_{u=1}.$$

Theorem 2.8 Let $M_G(u, v)$ be the M-polynomial for the graph G, then modified second K Banhatti index is computed as ${}^m B_2(G) = S_u Q_{-2} J(S_u + S_v) M_G(u, v)|_{u=1}$.

Proof. By taking

$$S_u Q_{-2} J(S_u + S_v) M_G(u, v)$$

$$\begin{aligned}
&= S_u Q_{-2} J(S_v + S_v) \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k, \\
&= S_u Q_{-2} J(S_u) \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k + S_v \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k, \\
&= S_u Q_{-2} J \left(\sum_{\psi \leq j \leq k \leq \Psi} \frac{1}{j} m_{jk} u^j v^k + \sum_{\psi \leq j \leq k \leq \Psi} \frac{1}{k} m_{jk} u^j v^k \right), \\
&= S_u Q_{-2} J \sum_{\psi \leq j \leq k \leq \Psi} \left(\frac{1}{j} + \frac{1}{k} \right) m_{jk} u^j v^k, \\
&= S_u Q_{-2} \sum_{\psi \leq j \leq k \leq \Psi} \left(\frac{1}{j} + \frac{1}{k} \right) m_{jk} u^{j+k}, \\
&= S_u \sum_{\psi \leq j \leq k \leq \Psi} \left(\frac{1}{j} + \frac{1}{k} \right) m_{jk} u^{j+k-2}, \\
&= \sum_{\psi \leq j \leq k \leq \Psi} \left(\frac{1}{j} + \frac{1}{k} \right) \frac{1}{j+k-2} m_{jk} u^{j+k-2}.
\end{aligned}$$

$$\begin{aligned}
&= 2S_x Q_{-2} J \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} (u^{2j} v^k + u^j v^{2k}), \\
&= 2S_x Q_{-2} J \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} (u^{2j+k} + u^{j+2k}), \\
&= 2S_x \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} (u^{2j+k-2} + u^{j+2k-2}), \\
&= 2 \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} \left(\frac{1}{2j+k-2} u^{2j+k-2} \right. \\
&\quad \left. + \frac{1}{j+2k-2} u^{j+2k-2} \right), \\
&= \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} \left(\frac{2}{2j+k-2} u^{2j+k-2} \right. \\
&\quad \left. + \frac{2}{j+2k-2} u^{j+2k-2} \right),
\end{aligned}$$

Now $S_x Q_{-2} J(S_x + S_y) M_G(u, v)|_{u=1}$

$$\begin{aligned}
&= \sum_{\psi \leq j \leq k \leq \Psi} \left(\frac{1}{j} + \frac{1}{k} \right) \frac{1}{j+k-2} m_{jk}, \\
&= \sum_{xy \in E_G} \left(\frac{1}{d_x} + \frac{1}{d_y} \right) \frac{1}{d_x + d_y - 2}, \\
&= \sum_{xy \in E_G} \frac{1}{d_x d_{xy}}.
\end{aligned}$$

Hence $mB_2(G) = S_x Q_{-2} J(S_x + S_y) M_G(u, v)|_{u=1}$.

Theorem 2.9 If $M_G(u, v)$ is the M-polynomial of the graph G, then harmonic K Banhatti index is computed as $HB(G) = 2S_x Q_{-2} J(L_x + L_y) M_G(u, v)|_{u=1}$.

Proof. By taking

$$\begin{aligned}
&2S_x Q_{-2} J(L_x + L_y) M_G(u, v) \\
&= 2S_x Q_{-2} J(L_x + L_y) \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k, \\
&= 2S_x Q_{-2} J(L_x) \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k + L_y \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^k, \\
&= 2S_x Q_{-2} J \left(\sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^{2j} v^k + \sum_{\psi \leq j \leq k \leq \Psi} m_{jk} u^j v^{2k} \right)
\end{aligned}$$

Table 1: Vertex partition of Rd

d_x	1	2	3	4
Number of vertices	9	8	7	4

Table 2: Edge partition of Rd.

(d_x, d_y)	(1,2)	(1,3)	(1,4)	(2,2)	(2,3)	(2,4)	(3,3)	(3,4)
Number of edges	3	5	1	9	14	5	6	2

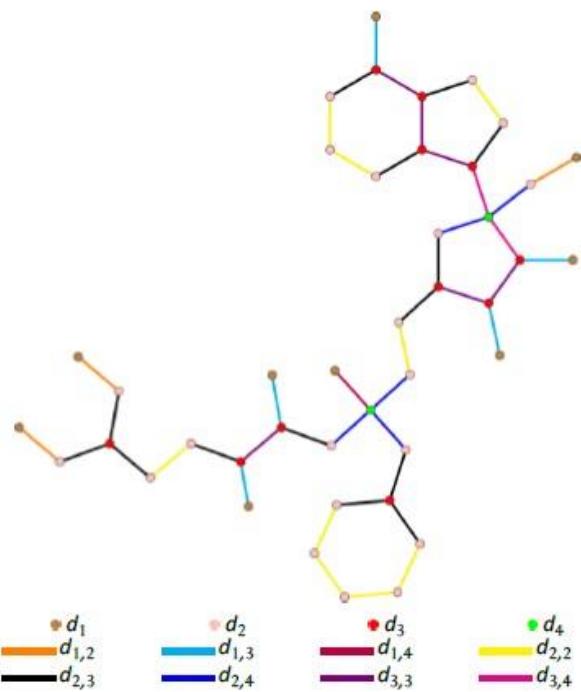
Now $2S_x Q_{-2} J(L_x + L_y) M_G(u, v)|_{u=1}$

$$\begin{aligned}
&= \sum_{\psi \leq j \leq k \leq \Psi} \left(\frac{2}{2j+k-2} + \frac{2}{j+2k-2} \right) m_{jk}, \\
&= \sum_{xy \in E_G} \left(\frac{2}{2d_x + d_y - 2} + \frac{2}{d_x + 2d_y - 2} \right), \\
&= \sum_{xy \in E_G} \left(\frac{2}{d_x + d_y - 2} + \frac{2}{d_y + d_x - 2} \right), \\
&= \sum_{xy \in E_G} \frac{2}{d_x + d_{xy}},
\end{aligned}$$

Hence $HB(G) = 2S_x Q_{-2} J(L_x + L_y) M_G(u, v)|_{u=1}$.

Chemical Graph of Remdesivir

The chemical graph of remdesivir (Rd) is shown in Figure 2, in which brown, pink, red and green dot represent the vertices of degree 1, 2, 3 and 4 respectively, orange, cyan, purple, yellow, black, blue, violet and magenta edges represent the edges having degree of end vertices (1,2), (1,3), (1,4), (2,2), (2,3), (2,4), (3,3) and (3,4) respectively. In this present work, we extract some topological indices via M-polynomial of (Rd).

**Figure 2:** Chemical graph of remdesivir (*Rd*)

M-Polynomial and Topological Indices of Remdesivir

Theorem 4.1 Let Rd be a remdesivir then M -polynomial of Rd is $M_{Rd}(u, v) = 3uv^2 + 5uv^3 + uv^4 + 9u^2v^2 + 14u^2v^3 + 5u^2v^4 + 6u^3v^3 + 2v^3v^4$.

Proof. Let Rd represented the remdesivir then by using Figures 1, 2 and Table 1, we have there are four partition of the vertex set with respect of the vertex degree defined as $V_n = \{x \in V_{Rd}, d_x = n\}$ where $n = 1, 2, 3, 4$.

Figures 1, 2 and Table 2 show that there are nine partition of the edge set with respect of degree of end-vertices of the edge. These partitions is represented with E_n , where $E_n = \{e = xy \in E_{Rd}, d_x = a, d_y = b\}$ where $n = 1, 2, 3, \dots, 8$ and $a, b = 1, 2, 3, 4$ with $a < b$ and $a = b$ only for $a = 2, 3$. We have the following results by using the definition of M -polynomial.

$$\begin{aligned} M_{Rd}(u, v) &= \sum_{\psi \leq j \leq k \leq \Psi} m_{jk}(Rd)u^jv^k = \sum_{1 \leq j \leq k \leq 4} m_{jk}(Rd)u^jv^k, \\ M_{Rd}(u, v) &= \sum_{1 \leq 2} m_{12}(Rd)u^1v^2 + \sum_{1 \leq 3} m_{13}(Rd)u^1v^3 + \sum_{1 \leq 4} m_{14}(Rd)u^1v^4 + \sum_{2 \leq 2} m_{22}(Rd)u^2v^2 \\ &\quad + \sum_{2 \leq 3} m_{23}(Rd)u^2v^3 + \sum_{2 \leq 4} m_{24}(Rd)u^2v^4 + \sum_{3 \leq 3} m_{33}(Rd)u^3v^3 \\ &\quad + \sum_{3 \leq 4} m_{34}(Rd)u^3v^4, \\ M_{Rd}(u, v) &= |E_1(Rd)|u^1v^2 + |E_2(Rd)|u^1v^3 + |E_3(Rd)|u^1v^4 + |E_4(Rd)|u^2v^2 + |E_5(Rd)|u^2v^3 \\ &\quad + |E_6(Rd)|u^2v^4 + |E_7(Rd)|u^3v^3 + |E_8(Rd)|u^3v^4, \\ M_{Rd}(u, v) &= 3uv^2 + 5uv^3 + uv^4 + 9u^2v^2 + 14u^2v^3 + 5u^2v^4 + 6u^3v^3 + 2v^3v^4. \end{aligned}$$

The plot of M -polynomial Rd is shown in Figures 3 and 4.

Theorem 4.2 Let Rd represent the remdesivir and $M_{Rd}(u, v) = 3uv^2 + 5uv^3 + uv^4 + 9u^2v^2 + 14u^2v^3 + 5u^2v^4 + 6u^3v^3 + 2u^3v^4$.

Then

$$\begin{aligned} 1. ABC[Rd] &= \frac{1}{6}(24 + 51\sqrt{2} + 3\sqrt{3} \\ &\quad + 10\sqrt{6} + 2\sqrt{15} + 14\sqrt{18}). \end{aligned}$$

$$\begin{aligned} 2. GA[Rd] &= \frac{1}{210}[3318 + 1120\sqrt{2} \\ &\quad + 765\sqrt{3} + 1176\sqrt{6}]. \end{aligned}$$

$$3. B_1[Rd] = 480.$$

$$4. B_2[Rd] = 680.$$

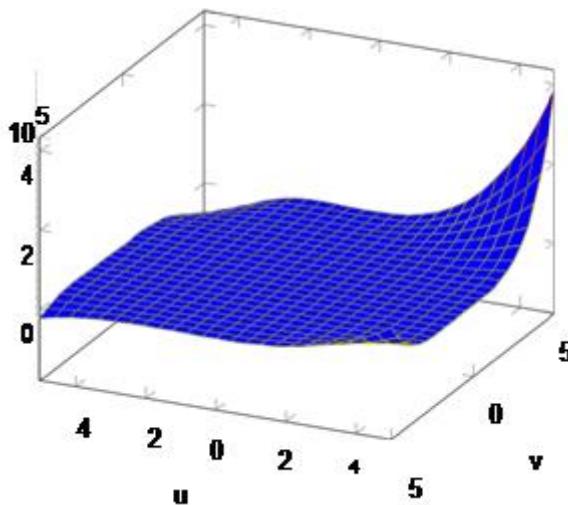
$$5. HB_1[Rd] = 2794.$$

$$6. HB_2[Rd] = 6872.$$

$$7. {}^mB_1[Rd] = \frac{5947}{315}.$$

$$8. {}^mB_2[Rd] = \frac{13543}{720}.$$

$$9. H_b[Rd] = \frac{11894}{315}.$$

**Figure 3:** 3D plot of M-polynomial of remdesivir (*Rd*) for $p = q = 4$.

Proof.

1. The atom-bond connectivity index

$$\begin{aligned}
 S_v^{\frac{1}{2}}M_{Rd}(u, v) &= \frac{3\sqrt{2}}{2}uv^2 + \frac{5\sqrt{3}}{3}uv^3 + \frac{1}{2}uv^4 + \frac{9\sqrt{2}}{2}u^2v^2 + \frac{14\sqrt{3}}{3}u^2v^3 + \frac{5}{2}u^2v^4 + 2\sqrt{3}u^3v^3 \\
 &\quad + u^3v^4, \\
 S_u^{\frac{1}{2}}S_v^{\frac{1}{2}}M_{Rd}(u, v) &= \frac{3\sqrt{2}}{2}uv^2 + \frac{5\sqrt{3}}{3}uv^3 + \frac{1}{2}uv^4 + \frac{9}{2}u^2v^2 + \frac{7\sqrt{6}}{3}u^2v^3 + \frac{5\sqrt{2}}{4}u^2v^4 + 2u^3v^3 \\
 &\quad + \frac{\sqrt{3}}{3}u^3v^4, \\
 JS_u^{\frac{1}{2}}S_v^{\frac{1}{2}}M_{Rd}(u, v) &= \frac{3\sqrt{2}}{2}u^3 + \frac{1}{6}(27 + 10\sqrt{3})u^4 + \frac{1}{6}(3 + 14\sqrt{6})u^5 + \frac{1}{4}(8 + 5\sqrt{2})u^6 + \frac{\sqrt{3}}{3}u^7, \\
 Q_{-2}JS_u^{\frac{1}{2}}S_v^{\frac{1}{2}}M_{Rd}(u, v) &= \frac{3\sqrt{2}}{2}u + \frac{1}{6}(27 + 10\sqrt{3})u^2 + \frac{1}{6}(3 + 14\sqrt{6})u^3 + \frac{1}{4}(8 + 5\sqrt{2})u^4 + \frac{\sqrt{3}}{3}u^5, \\
 D_u^{\frac{1}{2}}Q_{-2}JS_u^{\frac{1}{2}}S_v^{\frac{1}{2}}M_{Rd}(u, v) &= \frac{3\sqrt{2}}{2}u + \frac{\sqrt{2}}{6}(27 + 10\sqrt{3})u^2 + \frac{\sqrt{3}}{6}(3 + 14\sqrt{6})u^3 + \frac{1}{2}(8 + 5\sqrt{2})u^4 + \frac{\sqrt{15}}{3}u^5, \\
 ABC[Rd] &= D_u^{\frac{1}{2}}Q_{-2}JS_u^{\frac{1}{2}}S_v^{\frac{1}{2}}M_{Rd}(u, v)|_{u=1} = \frac{1}{6}[24 + 51\sqrt{2} + 3\sqrt{3} + 10\sqrt{6} + 2\sqrt{15} + 14\sqrt{18}].
 \end{aligned}$$

2. The geometric arithmetic index

$$\begin{aligned}
 D_v^{\frac{1}{2}}M_{Rd}(u, v) &= 3\sqrt{2}uv^2 + 5\sqrt{3}uv^3 + 2uv^4 + 9\sqrt{2}u^2v^2 + 14\sqrt{3}u^2v^3 \\
 &\quad + 10u^2v^4 + 6\sqrt{3}u^3v^3 + 4u^3v^4, \\
 D_u^{\frac{1}{2}}D_v^{\frac{1}{2}}M_{Rd}(u, v) &= 3\sqrt{2}uv^2 + 5\sqrt{3}uv^3 + 2uv^4 + 18u^2v^2 + 14\sqrt{6}u^2v^3 \\
 &\quad + 10\sqrt{2}u^2v^4 + 18u^3v^3 + 4\sqrt{3}u^3v^4, \\
 JD_u^{\frac{1}{2}}D_v^{\frac{1}{2}}M_{Rd}(u, v) &= 3\sqrt{2}u^3 + (18 + 5\sqrt{3})u^4 + 2(1 + 7\sqrt{6})u^5 \\
 &\quad + 2(9 + 5\sqrt{2})u^6 + 4\sqrt{3}u^7, \\
 S_uJD_u^{\frac{1}{2}}D_v^{\frac{1}{2}}M_{Rd}(u, v) &= \sqrt{2}u^3 + \frac{1}{4}(18 + 5\sqrt{3})u^4 + \frac{2}{5}(1 + 7\sqrt{6})u^5
 \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{3}(9 + 5\sqrt{2})u^6 + \frac{4\sqrt{3}}{7}u^7, \\
2S_u J D_u^{\frac{1}{2}} D_v^{\frac{1}{2}} M_{Rd}(u, v) = & 2\sqrt{2}u^3 + \frac{1}{2}(18 + 5\sqrt{3})u^4 + \frac{4}{5}(1 + 7\sqrt{6})u^5 \\
& + \frac{2}{3}(9 + 5\sqrt{2})u^6 + \frac{8\sqrt{3}}{7}u^7, \\
GA[Rd] = & 2S_x J D_x^{\frac{1}{2}} D_y^{\frac{1}{2}} M_{Rd}(u, v)|_{u=1}, \\
& \frac{1}{210}[3318 + 1120\sqrt{2} + 765\sqrt{3} + 1176\sqrt{6}].
\end{aligned}$$

3. The first K Banhatti index

$$\begin{aligned}
D_u M_{Rd}(u, v) = & 3uv^2 + 5uv^3 + uv^4 + 18u^2v^2 + 28u^2v^3 \\
& + 10u^2v^4 + 18u^3v^3 + 6u^3v^4, \\
D_v M_{Rd}(u, v) = & 6uv^2 + 15uv^3 + 4uv^4 + 18u^2v^2 + 42u^2v^3 \\
& + 20u^2v^4 + 18u^3v^3 + 8u^3v^4, \\
(D_u + D_v) M_{Rd}(u, v) = & 9uv^2 + 20uv^3 + 5uv^4 + 36u^2v^2 + 70u^2v^3 \\
& + 30u^2v^4 + 36u^3v^3 + 14u^3v^4, \\
(D_u + D_v) M_{Rd}(u, v)|_{u=v=1} = & 220. \\
JM_{Rd}(u, v) = & 3u^3 + 14u^4 + 15u^5 + 11u^6 + 2u^7, \\
Q_{-2}JM_{Rd}(u, v) = & 3u + 14u^2 + 15u^3 + 11u^4 + 2u^5, \\
D_u Q_{-2}JM_{Rd}(u, v) = & 3u + 28u^2 + 45u^3 + 44u^4 + 10u^5, \\
2D_u Q_{-2}JM_{Rd}(u, v) = & 6u + 56u^2 + 90u^3 + 88u^4 + 20u^5, \\
2D_u Q_{-2}JM_{Rd}(u, v)|_{u=1} = & 260. \\
B_1[Rd] = & (D_u + D_v + 2D_u Q_{-2}J) M_{Rd}(u, v)|_{u=v=1} = 480.
\end{aligned}$$

4. The second K Banhatti index

$$\begin{aligned}
J(D_u + D_v) M_{Rd}(u, v) = & 9u^3 + 56u^4 + 75u^5 + 66u^6 + 14u^7, \\
Q_{-2}J(D_u + D_v) M_{Rd}(u, v) = & 9u + 56u^2 + 75u^3 + 66u^4 + 14u^5, \\
D_u Q_{-2}J(D_u + D_v) M_{Rd}(u, v) = & 9u + 112u^2 + 225u^3 + 264u^4 + 70u^5, \\
B_2[Rd] = & D_u Q_{-2}J(D_u + D_v) M_{Rd}(u, v)|_{u=1} = 680.
\end{aligned}$$

5. The first K hyper Banhatti index

$$\begin{aligned}
D_u^2 M_{Rd}(u, v) = & 3uv^2 + 5uv^3 + uv^4 + 36u^2v^2 + 56u^2v^3 \\
& + 20u^2v^4 + 54u^3v^3 + 18u^3v^4, \\
D_v^2 M_{Rd}(u, v) = & 12uv^2 + 45uv^3 + 16uv^4 + 36u^2v^2 + 126u^2v^3 \\
& + 80u^2v^4 + 54u^3v^3 + 32u^3v^4, \\
(D_u^2 + D_v^2) M_{Rd}(u, v) = & 15uv^2 + 50uv^3 + 17uv^4 + 72u^2v^2 + 182u^2v^3 \\
& + 100u^2v^4 + 108u^3v^3 + 50u^3v^4, \\
(D_u^2 + D_v^2) M_{Rd}(u, v)|_{u=v=1} = & 594. \\
D_u^2 Q_{-2}JM_{Rd}(u, v) = & 3u + 56u^2 + 135u^3 + 176u^4 + 50u^5,
\end{aligned}$$

$$\begin{aligned}
2D_u^2 Q_{-2} J M_{Rd}(u, v) &= 6u + 112u^2 + 270u^3 + 352u^4 + 100u^5, \\
2D_u^2 Q_{-2} J M_{Rd}(u, v)|_{u=1} &= 840. \\
2D_u Q_{-2} J (D_u + D_v) M_{Rd}(u, v) &= 18u + 224u^2 + 450u^3 + 528u^4 + 140u^5, \\
2D_u Q_{-2} J (D_u + D_v) M_{Rd}(u, v)|_{u=1} &= 1360. \\
HB_1[Rd] &= (D_u^2 + D_v^2 + 2D_u^2 Q_{-2} J \\
&\quad + 2D_u Q_{-2} J (D_u + D_v)) M_{Rd}(u, v)|_{u=v=1} = 2794.
\end{aligned}$$

6. The second K hyper Banhatti index

$$\begin{aligned}
J(D_u^2 + D_v^2) M_{Rd}(u, v) &= 15u^3 + 122u^4 + 199u^5 + 208u^6 + 50u^7, \\
Q_{-2} J (D_u^2 + D_v^2) M_{Rd}(u, v) &= 15u + 122u^2 + 199u^3 + 208u^4 + 50u^5, \\
D_u^2 Q_{-2} J (D_u^2 + D_v^2) M_{Rd}(u, v) &= 15u + 488u^2 + 1791u^3 + 3328u^4 + 1250u^5, \\
HB_2[Rd] &= D_u^2 Q_{-2} J (D_u^2 + D_v^2) M_{Rd}(u, v)|_{u=1} = 6872.
\end{aligned}$$

7. Modified first K Banhatti index

$$\begin{aligned}
L_u M_{Rd}(u, v) &= 3uv^4 + 5uv^6 + uv^8 + 9u^2v^4 + 14u^2v^6 \\
&\quad + 5u^2v^8 + 6u^3v^6 + 2u^3v^8, \\
L_v M_{Rd}(u, v) &= 3u^2v^2 + 5u^2v^3 + u^2v^4 + 9u^4v^2 + 14u^4v^3 \\
&\quad + 5u^4v^4 + 6u^6v^3 + 2u^6v^4, \\
J(L_u + L_v) M_{Rd}(u, v) &= 3u^4 + 10u^5 + 19u^6 + 19u^7 + 19u^8 + 13u^9 \\
&\quad + 2u^{10} + 2u^{11}, \\
Q_{-2} J (L_u + L_v) M_{Rd}(u, v) &= 3u^2 + 10u^3 + 19u^4 + 19u^5 + 19u^6 + 13u^7 \\
&\quad + 2u^8 + 2u^9, \\
S_u Q_{-2} J (L_u + L_v) M_{Rd}(u, v) &= \frac{3}{2}u^2 + \frac{10}{3}u^3 + \frac{19}{4}u^4 + \frac{19}{5}u^5 + \frac{19}{6}u^6 + \frac{13}{7}u^7 \\
&\quad + \frac{1}{4}u^8 + \frac{2}{9}u^9, \\
{}^m B_1[Rd] &= S_u Q_{-2} J (L_u + L_v) M_{Rd}(u, v)|_{u=1} = \frac{5947}{315}.
\end{aligned}$$

8. Modified second K Banhatti index

$$\begin{aligned}
S_u M_{Rd}(u, v) &= 3uv^2 + 5uv^3 + uv^4 + \frac{9}{2}u^2v^2 + 7u^2v^3 \\
&\quad + \frac{5}{2}u^2v^4 + 2u^3v^3 + \frac{2}{3}u^3v^4, \\
S_v M_{Rd}(u, v) &= \frac{3}{2}uv^2 + \frac{5}{3}uv^3 + \frac{1}{4}uv^4 + \frac{9}{2}u^2v^2 + \frac{14}{3}u^2v^3 \\
&\quad + \frac{5}{4}u^2v^4 + 2u^3v^3 + \frac{1}{2}u^3v^4, \\
(S_u + S_v) M_{Rd}(u, v) &= \frac{9}{2}uv^2 + \frac{20}{3}uv^3 + \frac{5}{4}uv^4 + 9u^2v^2 + \frac{35}{3}u^2v^3 \\
&\quad + \frac{15}{4}u^2v^4 + 4u^3v^3 + \frac{7}{6}u^3v^4, \\
J(S_u + S_v) M_{Rd}(u, v) &= \frac{9}{2}u^3 + \frac{47}{3}u^4 + \frac{155}{12}u^5 + \frac{31}{4}u^6 + \frac{7}{6}u^7,
\end{aligned}$$

$$Q_{-2}J(S_u + S_v)M_{Rd}(u, v) = \frac{9}{2}u + \frac{47}{3}u^2 + \frac{155}{12}u^3 + \frac{31}{4}u^4 + \frac{7}{6}u^5,$$

$$S_u Q_{-2}J(S_u + S_v)M_{Rd}(u, v) = \frac{9}{2}u + \frac{47}{6}u^2 + \frac{155}{36}u^3 + \frac{31}{16}u^4 + \frac{7}{30}u^5,$$

$${}^mB_2[Rd] = S_u Q_{-2}J(S_u + S_v)M_{Rd}(u, v)|_{u=1} = \frac{13543}{720}.$$

9. Harmonic K Banhatti index

$$2S_u Q_{-2}J(L_u + L_v)M_{Rd}(u, v) = 3u^2 + \frac{20}{3}u^3 + \frac{19}{2}u^4 + \frac{38}{5}u^5 + \frac{19}{3}u^6 + \frac{26}{7}u^7 + \frac{1}{2}u^8 + \frac{4}{9}u^9,$$

$$H_b[Rd] = 2S_u Q_{-2}J(L_u + L_v)M_{Rd}(u, v)|_{u=1} = \frac{11894}{315}.$$

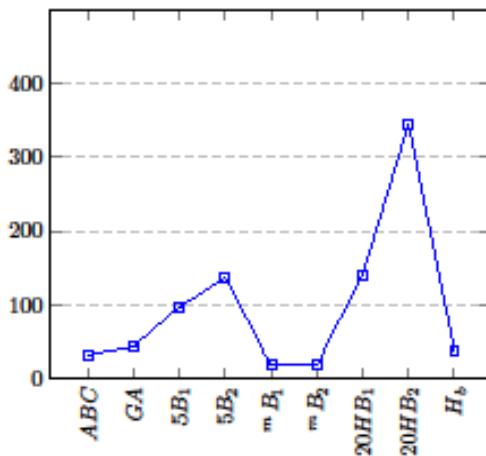


Figure 4: Plot of topological indices of remdesivir (Rd)

Conclusion

Computational techniques are the paramount ways to analyze the chemical compounds. Advanced study in this area can save a lot of resources and time. The results obtained in this article are helpful to improve the behavior of remdesivir and to study its properties. This work also provides proof of some already given topological indices that improve their credibility.

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Authors' contributions

All authors contributed toward data analysis, drafting and revising the paper and agreed to be responsible for all the aspects of this work.

Conflict of Interest

We have no conflicts of interest to disclose.

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