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Some Temperature Indices of the Chemical Structure of Favipiravir

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Abstract. Favipiravir is an antiviral medication that has shown potential in treating COVID-19. Topological indices, on the other hand are mathematical descriptors used to quantify the molecular structure of compounds. These indices provide insights into the physical, chemical and biological properties of molecules. In this manuscript when applied to favipiravir, topological indices can help analyse its molecular structure and predict various features related to its bioactivity and pharmacological properties. These indices may include parameters such as. First and second temperature indices, hyper first and second temperature indices, reciprocal product connectivity temperature, first and second general temperature indexes, and general temperature index of a molecular graph. Consequently, the results and findings were compute and investigated with the help of MATLAB. The correlation between the indices that define the Physico-chemical properties and biological activities. These findings and results may help design new medicine to treat COVID-19.

Keywords: topological indices, favipiravir, chemical graph

Introduction

Covid-19, also known as the novel corona virus is a highly contagious respiratory illness caused by the severe acute respiratory syndrome corona virus 2 (SARS-CoV-2). It was first identified in Wuhan, China, in late 2019 and quickly spread globally, leading to a pandemic. The virus primarily spreads through respiratory droplets when an infected person coughs, sneezes or talks, and it can also spread by touching contaminated surfaces. Symptoms can vary from mild to severe, including fever, cough and fatigue, loss of taste or smell and difficulty breathing. Certain individuals, such as the elderly and those with pre-existing medical conditions are at a higher risk of experiencing severe illness or complications. O contains the spread, countries have implemented measures like social distancing, mask-wearing, frequent hand washing and lockdowns. Vaccination efforts have been initiated worldwide to protect people from the virus. However, the emergence of new variants poses ongoing challenges. Coronavirus was first reported in Wuhan, PR China. Favipiravir are taken from Pub Chem which are depicted in Fig. 1.

Consequently, discovering a proper and safe drug or vaccine to treat this disease is critical. Several antiviral agents have been researched by (Lung *et al*., 2020; Morse *et al*., 2020). Favipiravir is an example of an antiviral compound (agent). Favipiravir has revealed encouraging and beneficial results in clinical research studies in countries like Russia, China and Japan. In contrast, several trials were carried out in different countries showing the UK, India, USA etc. Graph theory is a mathematical field that studies relationships between objects called vertices, connected by edges. It has numerous applications in computer science, operations research and social network analysis. Chemical graph theory is a branch of mathematical chemistry that focuses on the study of chemical compounds using graph theory science by (Zaman *et al*., 2023; Hakeem *et al*., 2023; Liu *et al*., 2023; Assadullah *et al*., 2022; Qasim *et al*., 2022; Havare, 2019). It uses graphs to represent molecules, where atoms are represented as vertices and chemical bonds as edges and chemical graph theory plays a vital role in drug discovery by providing valuable insights into molecular similarity, structure activity relationships, pharma-cokinetics, reaction mechanisms and target interactions. These applications aid in the rational design and optimization of drugs, leading to faster and more efficient development processes. Topological indices have been widely use in QSPR analysis to predict the properties of different

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chemical structures. For instance, Achieved diverse topological properties for cerium oxide by (Assadllah *et al*., 2022; Qasim *et al*., 2022). In 2023, conducted a study on the 3D structures of ant anxiety disorder drugs using QSAR (Quantitative Structure-Activity Relationship) analysis. They used linear regres-sion model and degree-based topological indices to analyse the relationship between the chemical structures of the drugs and their effectiveness in treating anxiety disorders by (Azeem *et al*., 2023). Authors conducted extensive computational analysis to generate various innovative versions of molecular descriptors within local communities. Additionally, they formulated equations specifically tailored for two carbon Nano sheets (Khabyah *et al*., 2022). Topological indices provide valuable information for drug discovery, they are just one of many tools used by researchers in the field. The integration of various computational and experimental techniques is necessary for comprehensive drug development. Quantitative Structure-Activity Relationship (QSAR). (Hakeem *et al*., 2023; Kosar *et al*., 2023; Shahid *et al*., 2023; Zaman *et al*., 2023). Topological indices are essential in developing QSAR models, which establish a relationship between the chemical structure of molecules and their biological activities.

These indices help predict the activity, toxicity and other properties of drug molecules. (Colakoglu, 2022). Degree-based topological indices in chemical graph theory are numerical parameters calculated based on the degrees of vertices in a molecular graph. They provide insight into molecular structure and properties. These indices find applications in drug design, chemical synthesis and predicting physicochemical properties of chemical compounds. Topological indices aid in evaluating drug bioavailability, the rate and extent at which the active ingredient is absorbed by the body. By examining molecular descriptors, researchers can optimize drug structures to enhance absorption and overall efficacy. Described the temperature of a graph G vertex v (Fajtlowicz, 1988).

Material and Methods

$$T(U) = \frac{d(u)}{n - d(u)}$$

where:

$| V (G) |= n$ The topological indices discussed here were presented by Kulli (2019). The connectivity sum temperature index of graph G is how it is defined here.

$$ST(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{T(u) \times T(v)}}$$

The product connectivity temperature index

$$PT(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{T(u) \times T(v)}}$$

The reciprocal product connectivity temperature index

$$PT(G) = \sum_{uv \in E(G)} \sqrt{T(u) \times T(v)}$$

The first general temperature index

$$T_1^x = \sum_{uv \in E(G)} \left(T(u) + T(v)\right)^x$$

The second general temperature index

$$T_2^x = \sum_{uv \in E(G)} \left(T(u) + T(v)\right)^2$$

The first hyper-temperature index

$$HT_1 = \sum_{uv \in E(G)} \left(T(u) + T(v)\right)^2$$

The second hyper-temperature index

$$HT_2 = \sum_{uv \in E(G)} \left(T(u) \times T(v)\right)^2$$

The (x,y)-temperature index of graph G is described as follows:

$$T_{xy} = \sum_{uv \in E(G)} \left(T(u)^x \,(T(v)^y + T(u)^x \,(T(v)^y\,\right)^y$$

More recently, the biological activity of molecules and their structural characteristics have been modelled, leading to the complex modelling of compounds in QSAR/QSPR/QSTR research (Asadllah *et al*., 2023; Hakeem *et al*., 2023; Shahid *et al*., 2023; Zaman *et al*., 2023; Cancan *et al*., 2020; Ediz *et al*., 2020; Shanmukha *et al*., 2020; Kulli *et al*., 2019).

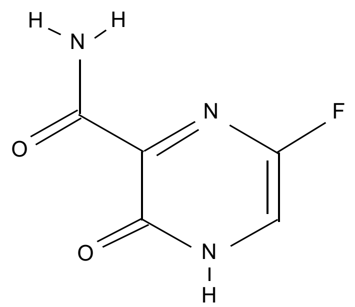

Fig. 1. Chemical Graph on behalf of the chemical compound of favipiravir.

Results and Discussion

Theorem 1. The chemical graph of favipiravir F has a general first temperature index of

Proof: Let G be the favipiravir chemical Graph. The Graph has 11 edges and 11 vertices, in Fig. 1, can see that the vertices of favipiravir are either 1 or 2 or 3 degrees. Therefore,there are four types of edges in favipiravir, in algebraic form, as follows:

$E_1 = uv \in E(G)|d_F(u) = 1, d_G(V) = 3, |E_1| = 4$
$E_2 = uv \in E(G)|d_F(u) = 2, d_G(V) = 2, |E_2| = 1$
$E_3 = uv \in E(G)|d_F(u) = 2, d_G(V) = 3, |E_3| = 4$
$E_4 = uv \in E(G)|d_F(u) = 3, d_G(V) = 3, |E_4| = 2$

As a result, the first general temperature index of F have the definition of

$$T_1^x = \sum_{uv\in E(G)} \left(T(u) + T(v)\right)^x$$

$$= \sum_{uv\in E_1(G)} \left(T(u) + T(v)\right)^x + \sum_{uv\in E(G)} \left(T(u) + T(v)\right)^x$$

$$+ \sum_{uv\in E_3(G)} \left(T(u) + T(v)\right)^x + \sum_{uv\in E(G)} \left(T(u) + T(v)\right)^x$$

$$= 4\left(\frac{1}{11-1} + \frac{3}{11-3}\right)^x + \left(\frac{2}{11-2} + \frac{3}{11-2}\right)^x$$

$$+ 4\left(\frac{2}{11-1} + \frac{3}{11-3}\right)^x + 4\left(\frac{3}{11-3} + \frac{3}{11-3}\right)^x$$

$$= \left(\frac{4}{9}\right)^x + 2\left(\frac{3}{4}\right)^x + 4\left(\frac{19}{43}\right)^x + 4\left(\frac{43}{72}\right)^x$$

The following conclusion may get by setting $x = 2$ in theorem 1.

Corollary 1.1. As a chemical graph, the first hyper temperature index of favipiravir f is HT_1 (F) = 3.651728395

The following conclusion may get by setting $x = \frac{-1}{2}$ in theorem 1.

Corollary 1.2. As a chemical graph, the sum connectivity temperature index of favipiravir f is ST(F) = 14.78918419

Theorem 2. The chemical graph of favipiravir F has a general second temperature index of

$$T_2^x = \left(\frac{4}{81}\right)^x + \left(\frac{9}{64}\right)^x + \left(\frac{1}{12}\right)^x + \left(\frac{3}{80}\right)^x$$

There is also proof. The general second temperature index of F by defining it.

$$T_1^x = \sum_{uv\in E_1(G)} \left(T(u) \times T(v)\right)^x$$

$$= \sum_{uv\in E_2(G)} \left(T(u) \times T(v)^x\right) + \sum_{uv\in E(G)} \left(T(u) \times T(v)^x\right)$$

$$+ \sum_{uv\in E_3(G)} \left(T(u) \times T(v)^x\right) \sum_{uv\in E_4(G)} \left(T(u) \times T(v)^x\right)$$

$$= 4\left(\frac{1}{11-1} \times \frac{3}{11-3}\right)^x + \left(\frac{2}{11-2} \times \frac{3}{11-2}\right)^x$$

$$+ 4\left(\frac{2}{11-1} \times \frac{3}{11-3}\right)^x + 4\left(\frac{3}{11-3} \times \frac{3}{11-3}\right)^x$$

$$= \left(\frac{4}{81}\right)^x + \left(\frac{9}{64}\right)^x + \left(\frac{1}{12}\right)^x + \left(\frac{3}{80}\right)^x$$

The following conclusion may get by setting x = 2 in Theorem 2.

Corollary 2.2. As a chemical graph, the product connectivity temperature index of favipiravir f is = PT(F) = 44.34565097

The following conclusion mey get by setting $x = \frac{1}{2}$ in Theorem 2.

Corollary 2.3. As a chemical graph, the Reciprocal product connectivity temperature index of favipiravir f is RPT (F) = 2.90151943

In the next theorem:

Theorem 3: The chemical graph of favipiravir F has a general temperature index of

$$4=\left(\frac{1}{10}\right)^x + 6\left(\frac{2}{9}\right)^x + 12\left(\frac{3}{8}\right)^x$$

Proof. The general temperature index of favipiravir F by describing it.

$$T_1^x = \sum_{uv\in E(G)} \left(T(u) + T(v)^x\right)$$

$$= \sum_{uv\in E_1(G)} \left(T(v) + T(v)^x\right) + \sum_{uv\in E_2(G)} \left(T(v)^x + T(v)^x\right)$$

$$+ \sum_{uv\in E_3(G)} \left(T(v)^x + T(v)^x\right) + \sum_{uv\in E_4(G)} \left(T(v)^x + T(v)^x\right)$$

$$4\left[\left(\frac{1}{11-1}\right)^x + \left(\frac{3}{11-3}\right)^x\right]$$

$$+\left[\left(\frac{2}{11-2}\right)^x + \left(\frac{2}{11-2}\right)^x\right]$$

$$+4\left[\left(\frac{2}{11-2}\right)^x + \left(\frac{2}{11-2}\right)^x\right]$$

$$+4\left[\left(\frac{3}{11-3}\right)^x + \left(\frac{3}{11-3}\right)^x\right]$$

$$=\left(\frac{4}{9}\right)^x + 2\left(\frac{3}{4}\right)^x + 4\left(\frac{19}{40}\right)^x + 4\left(\frac{43}{72}\right)^x$$

$$=4\left(\frac{1}{10}\right)^x + 6\left(\frac{2}{9}\right)^x + 12\left(\frac{3}{8}\right)^x$$

The following statement is obtained by setting x = 2 in Theorem 3.

Corollary 3.1. As a chemical graph, the f-temperature index of favipiravir f is FT (G) = 2.023796296

Theorem 4. The chemical graph of favipiravir f has (x,y)- temperature index of

$$T_{x.y(f)} = \left(\frac{1}{9}\right)^{x+y} + 2\left(\frac{1}{8}\right)^{x+y} + 4\left(\frac{1}{10}\right)^{x+y}$$

$$+4\left[\left(\frac{1}{9}\right)^x \left(\frac{1}{8}\right)^y + \left(\frac{1}{10}\right)^y \left(\frac{3}{8}\right)^x\right.$$

$$\left.+\left(\frac{2}{9}\right)^x \left(\frac{3}{8}\right)^y + \left(\frac{3}{8}\right)^y \left(\frac{2}{9}\right)\right]$$

$$T_{xy} = \sum_{uv\in E(G)} \left[\left(T(x)^x (T(x)^y + T(x)^x (T(x)^y\right)\right]$$

Proof. The (x,y) temperature index of favipiravir f by describing it.

$$= \sum_{uv\in E_1(G)} \left[\left(T(x)^x (T(x)^y + T(x)^x (T(x)^y\right)\right]$$

$$+ \sum_{uv\in E_2(G)} \left[\left(T(x)^x (T(x)^y + T(x)^x (T(x)^y\right)\right]$$

$$+ \sum_{uv\in E_3(G)} \left[\left(T(x)^x (T(x)^y + T(x)^x (T(x)^y\right)\right]$$

$$+ \sum_{uv\in E_4(G)} \left[\left(T(x)^x (T(x)^y + T(x)^x (T(x)^y\right)\right]$$

$$=4\left[\left(\frac{1}{11-1}\right)^x + \left(\frac{3}{11-3}\right)^y\right.$$

$$\left.+\left(\frac{1}{11-1}\right)^y + \left(\frac{3}{11-3}\right)^x\right]$$

$$+\left[\left(\frac{2}{11-2}\right)^x + \left(\frac{2}{11-2}\right)^y\right.$$

$$\left.+\left(\frac{2}{11-2}\right)^y + \left(\frac{2}{11-2}\right)^x\right]$$

$$+2\left[\left(\frac{3}{11-3}\right)^{x}+\left(\frac{3}{11-3}\right)^{y}+\left(\frac{3}{11-3}\right)^{y}+\left(\frac{3}{11-3}\right)^{x}\right]$$

$$T_{x.y(f)} = \left(\frac{1}{9}\right)^{x+y} + 2\left(\frac{1}{8}\right)^{x+y} 4\left(\frac{1}{10}\right)^{x+y}$$

$$+4\left[\left(\frac{1}{9}\right)^{x}\left(\frac{1}{8}\right)^{y}+\left(\frac{1}{10}\right)^{y}\left(\frac{3}{8}\right)^{x}+\left(\frac{2}{9}\right)^{x}\left(\frac{3}{8}\right)^{y}+\left(\frac{3}{8}\right)^{y}\left(\frac{2}{9}\right)^{x}\right]$$

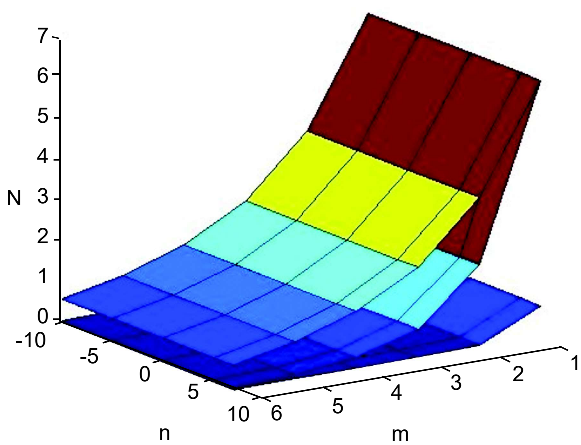

Fig. 2. The graphical representation of theorem 1 to 3.

Conclusion

The computed formulae regarding calculating some specific and topological indices of favipiravir. The concluding outputs of the topology are examined with the help of MATLAB. The results and findings are essential and would contribute significantly to developing and understanding the topology of these necessary structures. Chemical, medical, biochemical and medicinal properties or possession of molecular structure are critical for medicine design in medical research. The topological index calculation might be used to investigate and examine these properties. The first and second hyper temperature indices, sum and product connectivity temperature indices, F-temperature index and overall first and second temperature indices of favipiravir have been computed in the current research paper. These findings and results can be significant assets and helpful to the researchers working in degree-based topological indices to explore new drugs and vaccines to treat COVID-19.

Conflict of Interest. The authors declare that they have no conflict of interest.

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