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On the Temperature Indices of Fuzzy Graphs and its Application for QSPR analysis on Autism drugs

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Abstract

In this work, we introduce the concept of fuzzy temperature indices and rigorously compute them for fundamental fuzzy graph structures as well as their standard operators, including Cartesian products and compositions. Utilizing a graph-theoretical modeling approach, fuzzy graphs are constructed for a selection of pharmaceutical compounds commonly prescribed for Autism Spectrum Disorders (ASD), specifically Aripiprazole, Haloperidol, Risperidone, Sertraline, Venlafaxine, and Ziprasidone. The fuzzy temperature indices are then derived based on the underlying physicochemical descriptors of these compounds. Linear regression analyses are performed to explore the predictive capacity of the fuzzy topological indices in relation to drug properties. The findings highlight the significance of fuzzy temperature indices as robust mathematical invariants, providing valuable insights into the structural and functional profiling of ASD medications, and opening new avenues for the application of fuzzy graph theory in pharmaceutical sciences and computational drug design.

Keywords: Temperature indices, Fuzzy graph, Autism drugs, QSPR analysis.

1|Introduction

Fuzzy graph theory is rapidly expanding in many fields, especially chemical-mathematical, due to its unique properties and closeness to the more realistic model. Many topological indices exist only in the crisp state, but are new in the fuzzy graph environment. Fuzzy topological indices are one of the mathematical approaches performed for many technological, engineering and real-world problems such as telecommunications, social networks, traffic light control, maritime, neural networks, Internet routing and wireless sensor network [11].

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Graph theory is an attractive field for study in the field of discrete mathematics, and its findings are widely used in many scientific fields, especially chemistry, to display and analyze the structure and properties of chemical compounds [1, 2, 3, 4].

Fuzzy graph is one of the most versatile tools in the field of mathematics, which allows the user to easily describe the fuzzy relationship between any object. With the approach of fuzzy relation, Kauffman presented fuzzy Graph [10]. Various studies have been done on fuzzy graphs. Also, some topological indices have been investigated on fuzzy graphs and their application in mathematical chemistry has been stated [7, 8, 9].

One of the most important methods of studying the relationship between physical-chemical properties and topological indicators of a material is the use of QSPR models (Quantitative Structure-Property Analysis). In the QSPR model, the regression curve method is used as a tool to analyse the relationship between physical and chemical properties and topological indicators. Various QSAR studies using topological indices have been performed on multiple drug structures [5, 6]. In this article, the limits of the first fuzzy Temperature index for the fuzzy graphs of path, cycle, star, complete graph, Cartesian multiplication, Join graph and the combination and union of two graphs are calculated and relations are expressed. In the following, after introducing the fuzzy graph of Autism drugs, the fuzzy Temperature indices are obtained for them and the results are expressed by examining the linear regression.

2|Preliminary

Here some necessary definitions required to develop our results are given as following which most of them can be found in [14]. For any universal set X, with a membership function $\mu : X \to [0,1]$, the pair $S = (X, \mu)$ is named a fuzzy set S. The triple $G = (V, \sigma, \mu)$ consists of a nonempty set V, and two mappings $\mu : V \times V \longrightarrow [0,1]$ and $\sigma : V \longrightarrow [0,1]$ is called a fuzzy graph if

$$\mu(x,y) \leq \sigma(x) \wedge \sigma(y) \text{ for all } x, y \in V.$$

Here μ is symmetry and so, we use symbole xy instead (x,y). Also, $\mu^* = \{uv \in V \times V : \mu(uv) > 0\}$ and $\sigma^* = \{u \in V : \sigma(u) > 0\}$, are deputing the supports of μ and σ respectively, signed by $Supp(\mu)$ and $Supp(\sigma)$.

A sequence of different vertices $v_1, v_2, \cdots, v_n$ that $\mu(v_i v_{i+1}) > 0; i = 1, ..., n$ is named a path P of the lenth n in a fuzzy graph $G = (V, \sigma, \mu)$ and the successive pairs $(v_i v_{i+1})$ are considered as edges of the path.

Let $G = (V, \sigma, \mu)$ be a fuzzy graph, then:

(i) if $(Supp(\sigma), Supp(\mu))$ is a cycle, then G is named a cycle.

(ii) if $\nexists$ unique $uv \in Supp(\mu)$ such that $\mu(uv) = \wedge\{\mu(xy) | xy \in Supp(\mu)\}$,

and $(Supp(\sigma), Supp(\mu))$ is a cycle, then G is named a fuzzy cycle.

A fuzzy graph $G = (V, \sigma, \mu)$ is named a complete fuzzy graph (CFG) if $\mu(uv) = \sigma(u) \wedge \sigma(v)$, for all $u, v \in V$.

Let G is a graph and v is a vertex of G, The set of vertices adjacent to v is called the neighborhood of v, denoted $N(v)$.

For all edges incident at a vertex v in a fuzzy graph G, the sum of their membership values represented by $\sum\limits_{u \in N(v)} \mu(uv)$ is called the degree of v.

Here, δ and Δ represents the minimum and maximum degree of G and $\sigma_{max} = max\{\sigma(u) : u \in V\}$, $\sigma_{min} = min\{\sigma(u) : u \in V\}$ and $\mu_{max} = max\{\mu(uv) : uv \in E(G)\}$, $\mu_{min} = min\{\mu(uv) : uv \in E(G)\}$. Throughout this article, the FG, $G_1 = (V_1, \sigma_1, \mu_1)$ has n_1-vertices, m_1-edges, edge set $E(G_1)$, $\sigma_{max_1} = max\{\sigma_1(u) : u \in V_1\}$, $\sigma_{min_1} = min\{\sigma_1(u) : u \in V\}$ and $G_2 = (V_2, \sigma_2, \mu_2)$ has n_2-vertices, m_2-edges, edge set $E(G_2)$, $\sigma_{max_2} = max\{\sigma_2(u) : u \in V_2\}$, $\sigma_{min_2} = min\{\sigma_2(u) : u \in V_2\}$ and $\Delta_1 = \Delta(G_1), \Delta_2 = \Delta(G_2), \delta_1 = \delta(G_1), \delta_2 = \delta(G_2)$.

If $G_1 = (V_1, \sigma_1, \mu_1)$, $G_2 = (V_2, \sigma_2, \mu_2)$ are 2 FGs, then $G_1 \times G_2 = (V, \sigma, \mu)$ named the Cartesian product of G_1 and G_2, is an FG too, in which $V = V_1 \times V_2$, $\sigma(u,v) = \wedge\{\sigma_1(u), \sigma_2(v)\}$ for all $(u,v) \in V$ and for every $(u_1, v_1), (u_2, v_2) \in V$ we have

TABLE 1. Temperature topological indices of G.

Temperature Index name	**Definition**
First Temperature index	$T_1 = \sum_{uv\in E(G)} (T_u + T_v)$
Second Temperature index	$T_2 = \sum_{uv\in E(G)} (T_u.T_v)$
The modified second Temperature index	$MT_2 = \sum_{uv\in E(G)} \frac{1}{T_u.T_v}$
The modified third Temperature index	$MT_3(G) = \sum_{uv\in E(G)} \frac{1}{T_u + T_v}$
Sum connectivity Temperature index	$ST = \sum_{uv\in E(G)} \frac{1}{\sqrt{T_u + T_v}}$
Product connectivity Temperature index	$PT = \sum_{uv\in E(G)} \frac{1}{\sqrt{T_u.T_v}}$

$$\mu((u_1,v_1)(u_2,v_2)) = \begin{cases} \wedge\{\sigma_1(u_1),\mu_2(v_1v_2)\} & if \quad u_1 = u_2, v_1v_2 \in E(G_2) \\ \wedge\{\sigma_2(v_1),\mu_1(u_1u_2)\} & if \quad v_1 = v_2, u_1u_2 \in E(G_1) \\ 0 & otherwise \end{cases}$$

If $G_1 = (V_1, \sigma_1, \mu_1)$, $G_2 = (V_2, \sigma_2, \mu_2)$ are 2 FGs, then $G_1[G_2] = (V, \sigma, \mu)$ named the composition of G_1 and G_2, is an FG too, in which $V = V_1 \times V_2$, $\sigma(u, v) = \wedge\{\sigma_1(u), \sigma_2(v)\}$ for all $(u, v) \in V$ and for every $(u_1, v_1), (u_2, v_2) \in V$ we have

$$\mu((u_1,v_1)(u_2,v_2)) = \begin{cases} \wedge\{\sigma_1(u_1),\mu_2(v_1v_2)\} & if \quad u_1 = u_2, v_1v_2 \in E(G_2) \\ \wedge\{\sigma_2(v_1),\sigma_2(v_2),\mu_1(u_1u_2)\} & if \quad u_1u_2 \in E(G_1) \\ 0 & otherwise \end{cases}$$

3|The fuzzified Temperature indices

Recently, Temperature indices have been used for studying the crisp graph modelling for molecular structure of Covid19 drugs [15]. In this section we introduce a new definition of Temperature indices for fuzzy graphs, and then we calculate the bounds for first Temperature index; T_1, through proving some theorems, with explicit examples. Other Temperature indices for fuzzy graphs can be obtained simply from the fuzzified form of T_1. But the first we should have a review on the previous definition of Temperature indices for crisp graphs.

Let $G = (V, E)$ be a graph. For a vertex $u \in V(G)$, the Temperature degree of u is defined as follows [12]:

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

where n is the number of vertices, $d(u)$ is the degree of u. Using this Temperature degree, the Temperature indices were introduced (see Table 1) [12, 13].

Now we define Temperature indices for a fuzzy graph as follows: For a fuzzy graph $G = (V, \sigma, \mu)$, the Temperature degree of a vertex $u \in V(G)$ is defined as follows:

$$T_u = \frac{d(u)}{n - d(u)} \tag{1}$$

where n is the number of vertices of G. According to definition we can define the Temperature indices for a fuzzy graph as Table 2. Let $G = (V, \sigma, \mu)$ be a fuzzy graph with m edges and n vertices. Then we have:

$$2m\sigma_{min}\frac{\delta}{n-\delta} \le T_1(G) \le 2m\sigma_{max}\frac{\Delta}{n-\Delta}.$$

Table 2. Temperature topological indices of FG.

Temperature Index name	**Definition**
First Temperature index	$T_1 = \sum_{uv\in E(G)} (\sigma_u T_u + \sigma_v T_v)$
Second Temperature index	$T_2 = \sum_{uv\in E(G)} (\sigma_u T_u . \sigma_v T_v)$
The modified second Temperature index	$MT_2 = \sum_{uv\in E(G)} \frac{1}{\sigma_u T_u . \sigma_v T_v}$
The modified third Temperature index	$MT_3(G) = \sum_{uv\in E(G)} \frac{1}{\sigma_u T_u + \sigma_v T_v}$
Sum connectivity Temperature index	$ST = \sum_{uv\in E(G)} \frac{1}{\sqrt{\sigma_u T_u + \sigma_v T_v}}$
Product connectivity Temperature index	$PT = \sum_{uv\in E(G)} \frac{1}{\sqrt{\sigma_u T_u . \sigma_v T_v}}$

Proof: According to relation (1), we have

$$T_u = \frac{d(u)}{n - d(u)} \leq \frac{\Delta}{n - \Delta}. \tag{2}$$

Therefore

$$T_1 = \sum_{uv\in E(G)} (\sigma(u)T_u + \sigma(v)T_v) \leq 2m\sigma_{max} \frac{\Delta}{n - \Delta}.$$

Similarly $T_1 \geq 2m\sigma_{min} \frac{\delta}{n - \delta}$ □

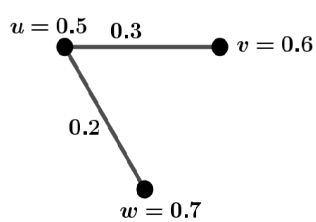

Figure 1. A fuzzy graph

Suppose G is the FG shown in Figure 1. Then we have the Temperature degree of vertices as Table 3.

Table 3. Temperature degree of vertices.

vertex	**Temperature degree**
u	$T_u = \frac{0.5}{3 - 0.5} = 0.2$
v	$T_v = \frac{0.3}{3 - 0.3} = 0.11$
w	$T_w = \frac{0.2}{3 - 0.2} = 0.07$

Therefore for $T_1(G)$, we have:

(1) $T_1(G) = \sum_{uv\in E(G)} (\sigma(u)T_u + \sigma(v)T_v) = (0.5 \times 0.2 + 0.6 \times 0.11) + (0.7 \times 0.07 + 0.5 \times 0.2) = 0.315$

(2) $2m\sigma_{max}\dfrac{\Delta}{n-\Delta} = 2 \times 2 \times 0.7 \times \dfrac{0.5}{3-0.5} \simeq 0.56$

(3) $2m\sigma_{min}\dfrac{\delta}{n-\delta} = 2 \times 2 \times 0.5 \times \dfrac{0.2}{3-0.2} \simeq 0.14.$

Clearly $0.14 \leq T_1(G) \leq 0.56$. For a fuzzy path $P = (\sigma, \mu) : (v_1, v_2, \cdots, v_n)$, we have:

$$T_1(P) \leq \sigma_{max}(\frac{2\mu_{max}}{n-\mu_{max}} + \frac{(4n-8)\mu_{max}}{n-2\mu_{max}}).$$

Proof: As P is a path, $d(v_1) = \mu_1$, $d(v_n) = \mu_{n-1}$ and $d(v_i) = \mu_{i-1} + \mu_i$ for $i = 2, 3, ..., n-1$, where $\sigma(v_i) = \sigma_i$ and $\mu(v_iv_{i+1}) = \mu_i$ for $i = 1, 2, 3, ..., n$. Therefore

$$\begin{aligned}
T_1(P) =&(\sigma_1\frac{\mu_1}{n-\mu_1} + \sigma_2\frac{\mu_1+\mu_2}{n-(\mu_1+\mu_2)}) + \sum_{i=2}^{n-2}(\sigma_i\frac{\mu_{i-1}+\mu_i}{n-(\mu_{i-1}+\mu_i)}) + (\sigma_{i+1}\frac{\mu_i+\mu_{i+1}}{n-(\mu_i+\mu_{i+1})})\\
&+(\sigma_{n-1}\frac{\mu_{n-2}+\mu_{n-1}}{n-(\mu_{n-2}+\mu_{n-1})} + \sigma_n\frac{\mu_{n-1}}{n-\mu_{n-1}})\\
\leq& 2\sigma_{max}\frac{\mu_{max}}{n-\mu_{max}} + 2\sigma_{max}\frac{2\mu_{max}}{n-2\mu_{max}} + 2(n-3)(\sigma_{max}\frac{2\mu_{max}}{n-2\mu_{max}})\\
=&\sigma_{max}(\frac{2\mu_{max}}{n-\mu_{max}} + \frac{(4n-8)\mu_{max}}{n-2\mu_{max}}).
\end{aligned}$$

□

For a fuzzy cycle $C = (\sigma, \mu) : (v_1, v_2, \cdots, v_n)$, we have $T_1(C) \leq \dfrac{4n\sigma_{max}\mu_{max}}{n-2\mu_{max}}$.

Proof: As $C(v_1, v_2, \cdots, v_n)$ is a cycle, then $d(v_1) = \mu_1 + \mu_n$ and $d(v_i) = \mu_{i-1} + \mu_i$ for $i = 2, 3, ..., n$, where $\sigma(v_i) = \sigma_i$ and $\mu(v_iv_{i+1}) = \mu_i$ for $i = 1, 2, 3, ..., n$. Therefore

$$\begin{aligned}
T_1(C) =&(\sigma_1\frac{\mu_1+\mu_n}{n-(\mu_1+\mu_n)} + \sigma_2\frac{\mu_1+\mu_2}{n-(\mu_1+\mu_2)}) + \sum_{i=2}^{n-1}(\sigma_i\frac{\mu_{i-1}+\mu_{i+1}}{n-(\mu_{i-1}+\mu_i)} + \sigma_{i+1}\frac{\mu_i+\mu_{i+1}}{n-(\mu_i+\mu_{i+1})})\\
&+(\sigma_n\frac{\mu_{n-1}+\mu_n}{n-(\mu_{n-1}+\mu_n)} + \sigma_1\frac{\mu_1+\mu_n}{n-(\mu_1+\mu_n)})\\
\leq& 4\sigma_{max}\frac{2\mu_{max}}{n-2\mu_{max}} + 2(n-2)\sigma_{max}\frac{2\mu_{max}}{n-2\mu_{max}}\\
=&\frac{4n\sigma_{max}\mu_{max}}{n-2\mu_{max}}.
\end{aligned}$$

□

Let $G = (V, \sigma, \mu)$ be a complete fuzzy graph with vertex set $V = \{v_1, \cdots, v_n\}$ such that $\sigma_1 \leq \sigma_2 \leq \cdots \leq \sigma_n$, in which $\sigma(v_i) = \sigma_i$ for $i = 1, 2, 3, ..., n$. Then $T_1(G) = n(n-1)\sum_{i=1}^{n}\sigma_i\dfrac{(n-i)\sigma_i + \sum_{t=1}^{i-1}\sigma_t}{n-[(n-i)\sigma_i + \sum_{t=1}^{i-1}\sigma_t]}$.

Proof: As G is a CFG, then $d(v_i) = (n-i)\sigma_i + \sum_{j=1}^{i-1}\sigma_j$. Therefore

$$T_1(G) = \sum_{1\leq i\leq j\leq n} (\sigma_i \frac{(n-i)\sigma_i + \sum_{t=1}^{i-1}\sigma_t}{n-[(n-i)\sigma_i + \sum_{t=1}^{i-1}\sigma_t]} + \sigma_j \frac{(n-j)\sigma_j + \sum_{t=1}^{j-1}\sigma_t}{n-[(n-j)\sigma_j + \sum_{t=1}^{j-1}\sigma_t]})$$
$$= n(n-1)\sum_{i=1}^{n} \sigma_i \frac{(n-i)\sigma_i + \sum_{t=1}^{i-1}\sigma_t}{n-[(n-i)\sigma_i + \sum_{t=1}^{i-1}\sigma_t]}.$$

□

Let $G = (V, \sigma, \mu)$ be a complete fuzzy graph with vertex set $V = \{v_1, \cdots, v_n\}$ such that $\sigma_1 \leq \sigma_2 \leq \cdots \leq \sigma_n$, in which $\sigma(v_i) = \sigma_i$ for $i = 1, 2, 3, ..., n$. Then $T_1(G) \leq n(n-1)^2(\frac{\sigma_n^2}{n-(n-1)\sigma_n})$.

Proof: As G is a CFG, then $d(v_i) = (n-i)\sigma_i + \sum_{j=1}^{i-1}\sigma_j$. Therefore

$$T_1(G) = \sum_{1\leq i\leq j\leq n} (\sigma_i \frac{(n-i)\sigma_i + \sum_{t=1}^{i-1}\sigma_t}{n-[(n-i)\sigma_i + \sum_{t=1}^{i-1}\sigma_t]} + \sigma_j \frac{(n-j)\sigma_j + \sum_{t=1}^{j-1}\sigma_t}{n-[(n-j)\sigma_j + \sum_{t=1}^{j-1}\sigma_t]})$$
$$\leq \frac{n(n-1)}{2}[\sigma_n \frac{(n-i)\sigma_n + (i-1)\sigma_n}{n-[(n-i)\sigma_n + (i-1)\sigma_n]} + \sigma_n \frac{(n-j)\sigma_n + (j-1)\sigma_n}{n-(n-1)\sigma_n}]$$
$$= \frac{n(n-1)}{2}(2\sigma_n^2 \frac{n-1}{n-(n-1)\sigma_n}) = n(n-1)^2 \frac{\sigma_n^2}{n-(n-1)\sigma_n}.$$

□

For two fuzzy graphs $G_1 = (V_1, \sigma_1, \mu_1)$, $G_2 = (V_2, \sigma_2, \mu_2)$ and their Cartesian product $G = G_1 \times G_2 = (V, \sigma, \mu)$, such that G_i have n_i vertices and m_i edges for $i = 1, 2$, we have

$$T_1(G_1 \times G_2) \leq (2m_1n_2 + 2m_2n_1)[\frac{\Delta}{n-\Delta}(\wedge\{\sigma_{1max}(u_2), \sigma_{2max}(v_1)\})].$$

Proof: Using the definition of the Cartesian product of G_1 and G_2 we have:

$\sigma(u, v) = \wedge\{\sigma_1(u), \sigma_2(v)\}, \forall (u, v) \in V$,

$$\mu((u_1, v_1)(u_2, v_2)) = \begin{cases} \wedge\{\sigma_1(u_1), \mu_2(v_1v_2)\} & if \quad u_1 = u_2, v_1v_2 \in E(G_2) \\ \wedge\{\sigma_2(v_1), \mu_1(u_1u_2)\} & if \quad v_1 = v_2, u_1u_2 \in E(G_1) \\ 0 & otherwise \end{cases}, \quad \forall (u_1, v_1), (u_2, v_2) \in V. \quad \text{Then}$$

$$d_{G_1\times G_2}(u, v) = \sum_{vv_i\in E(G_2)} \mu((u, v)(u, v_i)) + \sum_{uu_i\in E(G_1)} \mu((u, v)(u_i, v))$$
$$= \sum_{vv_i\in E(G_2)} \wedge\{\sigma_1(u), \mu_2(vv_i)\} + \sum_{uu_i\in E(G_1)} \wedge\{\sigma_2(v), \mu_1(uu_i)\}$$
$$\leq \sum_{vv_i\in E(G_2)} \mu_2(vv_i) + \sum_{uu_i\in E(G_1)} \mu_1(uu_i) = d_{G_1}(u) + d_{G_2}(v)$$

Now first Temperature index of $G_1 \times G_2$ is:

$$\begin{aligned} T_1(G_1 \times G_2) = &\sum_{u_1u_2 \in E_1, v_1 \in V_2} (\sigma(u_1, v_1)T_{(u_1,v_1)} + \sigma(u_2, v_1)T_{(u_2,v_1)}) \\ &+ \sum_{u_1 \in V_1, v_1v_2 \in E_2} (\sigma(u_1, v_1)T_{(u_1,v_1)} + \sigma(u_1, v_2)T_{(u_1,v_2)}) \\ &= K_1 + K_2 \end{aligned}$$

where $K_1 = \sum_{u_1u_2 \in E_1, v_1 \in V_2} (\sigma(u_1, v_1)T_{(u_1,v_1)} + \sigma(u_2, v_1)T_{(u_2,v_1)})$ and

$K_2 = \sum_{u_1 \in V_1, v_1v_2 \in E_2} (\sigma(u_1, v_1)T_{(u_1,v_1)} + \sigma(u_1, v_2)T_{(u_1,v_2)})$. Now

$$\begin{aligned} K_1 \leq &\sum_{u_1u_2 \in E_1, v \in V_2} (\wedge\{\sigma_1(u_1), \sigma_2(v_1)\}T_{(u_1,v_1)} + \wedge\{\sigma_1(u_2), \sigma_2(v_1)\}T_{(u_2,v_1)} \\ \leq &\sum_{u_1u_2 \in E_1, v \in V_2} (\wedge\{\sigma_{1max}(u_1), \sigma_{2max}(v_1)\}T_{(u_1,v_1)} + \wedge\{\sigma_{1max}(u_2), \sigma_{2max}(v_1)\}T_{(u_2,v_1)} \\ = &\wedge \{\sigma_{1max}(u_2), \sigma_{2max}(v_1)\} \sum_{u_1u_2 \in E_1, v \in V_2} (T_{(u_1,v_1)} + T_{(u_2,v_1)}) \\ \leq &2m_1n_2 \frac{\Delta}{n - \Delta} (\wedge\{\sigma_{1max}(u_2), \sigma_{2max}(v_1)\}) \end{aligned}$$

Similarly we can get $K_2 \leq 2m_2n_1(\wedge\{\sigma_{1max}(u_2), \sigma_{2max}(v_1)\})(\frac{\Delta}{n - \Delta})$. Therefore

$T_1(G_1 \times G_2) \leq (2m_1n_2 + 2m_2n_1)[\frac{\Delta}{n - \Delta}(\wedge\{\sigma_{1max}(u_2), \sigma_{2max}(v_1)\})]$. □

Suppose $G_1 \times G_2$ is the fuzzy graph shown in Figure 2. Then we have the Temperature degree of vertices as

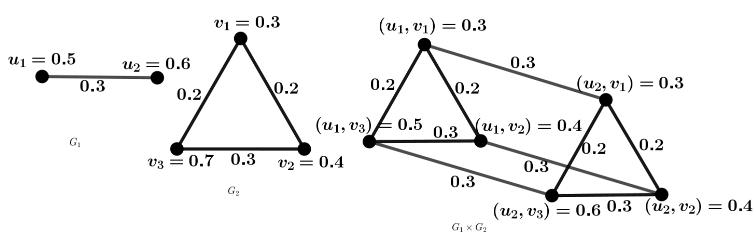

FIGURE 2. The cartesian product of fuzzy graph's G_1 and G_2

Table 4.

Therefore for $T_1(G_1 \times G_2)$, we have:

(1) $T_1(G_1 \times G_2) = (0.3 \times 0.13 + 0.3 \times 0.13) + (0.3 \times 0.13 + 0.4 \times 0.15) + (0.4 times 0.15 + 0.5 \times 0.15) + (0.5 \times 0.15 + 0.3 \times 0.13) + (0.5 \times 0.15 \times 0.6 \times 0.15) + (0.4 \times 0.15 + 0.4 \times 0.13) + (0.3 \times 0.13 + 0.4 \times 0.13) + (0.4 \times 0.13 + 0.6 \times 0.15) + (0.6 \times 0.15 + 0.3 \times 0.13) = 1.065$

(2) $(2m_1n_1 + 2m_2n_1)[\frac{\Delta}{n - \Delta}(\wedge\{\sigma_{1max}(u_2), \sigma_{2max}(v_1)\})] = 1.6$.

Clearly $T_1(G_1 \times G_2) \leq 1.6$. Let $G_1[G_2] = (V, \sigma, \mu)$ be the composition of G_1 and G_2. Then

$$T_1(G_1[G_2]) \leq 2(m_2n_1 + m_1n_2)(\sigma_{1max} + \sigma_{2max})(\frac{\Delta}{n - \Delta}).$$

Proof: As $G_1[G_2] = (V, \sigma, \mu)$ is the composition of $G_1 = (V_1, \sigma_1, \mu_1)$ and $G_2 = (V_2, \sigma_2, \mu_2)$ where $V = V_1 \times V_2$ and $\sigma(u, v) = \wedge\{\sigma_1(u), \sigma_2(v)\}, \forall(u, v) \in V$,

TABLE 4. Temperature degree of vertices.

vertex	Temperature degree
(u_1,v_1)	$T_{(u_1,v_1)}=\frac{0.7}{6-0.7}=0.13$
(u_1,v_2)	$T_{(u_1,v_2)}=\frac{0.8}{6-0.8}=0.15$
(u_1,v_3)	$T_{(u_1,v_3)}=\frac{0.8}{6-0.8}=0.15$
(u_2,v_1)	$T_{(u_2,v_1)}=\frac{0.7}{6-0.7}=0.13$
(u_2,v_2)	$T_{(u_2,v_2)}=\frac{0.7}{6-0.7}=0.13$
(u_2,v_3)	$T_{(u_2,v_3)}=\frac{0.8}{6-0.8}=0.15$

$$\mu((u_1,v_1)(u_2,v_2))=\begin{cases}\wedge\{\sigma_1(u_1),\mu_2(v_1v_2)\} & if \quad u_1=u_2, v_1v_2\in E(G_2)\\ \wedge\{\sigma_2(v_1),\sigma_2(v_2),\mu_1(u_1u_2)\} & if \quad u_1u_2\in E(G_1)\\ 0 & otherwise\end{cases} \qquad \forall (u_1,v_1),(u_2,v_2)\in V,$$

we have

$$\begin{aligned} d_{G_1[G_2]}(u,v) &= \sum_{v_iv\in E(G_2)}\mu((u,v)(u_1,v_1)) + \sum_{u_iu\in E(G_1),v_j\in V_2}\mu((u,v)(u_i,v_j)\\ &= \sum_{v_iv\in E(G_2)}\wedge\{\sigma_1(u),\mu_2(vv_i)\} + \sum_{u_iu\in E(G_1),v_j\in V_2}\wedge\{\sigma_2(v),\sigma_2(v_j),\mu_1(uu_i)\}\\ &\le \sum_{v_iv\in E(G_2)}\mu_2(vv_i) + \sum_{u_iu\in E(G_1),v_j\in V_2}\mu_1(uu_i)\\ &= n_2d_{G_1}(u)+d_{G_2}(v). \end{aligned}$$

Hence

$$\begin{aligned} T_1(G_1[G_2]) &= \sum_{u_1\in V_1,v_1v_2\in E_2}(\sigma(u_1,v_1)T_{(u_1,v_1)}+\sigma(u_1,v_2)T_{(u_1,v_2)})\\ &+ \sum_{u_1u_2\in E_1,v_1,v_2\in V_2}(\sigma(u_1,v_1)T_{(u_1,v_1)}+\sigma(u_2,v_2)T_{(u_2,v_2)})\\ &= K_1+K_2, \end{aligned}$$

where $K_1=\sum_{u_1\in V_1,v_1v_2\in E_2}(\sigma(u_1,v_1)T_{(u_1,v_1)}+\sigma(u_1,v_2)T_{(u_1,v_2)})$ and

$K_2=\sum_{u_1u_2\in E_1,v_1,v_2\in V_2}(\sigma(u_1,v_1)T_{(u_1,v_1)}+\sigma(u_2,v_2)T_{(u_2,v_2)})$.

Now we get

$$\begin{aligned} K_1 &\le \sum_{u_1\in V_1,v_1v_2\in E_2}(\wedge\{\sigma_1(u_1),\sigma_2(v_1)\}T_{(u_1,v_1)}+\wedge\{\sigma_1(u_1),\sigma_2(v_2)\}T_{(u_1,v_2)})\\ &\le \sum_{u_1\in V_1,v_1v_2\in E_2}(2\sigma_{1max}\times\frac{\Delta}{n-\Delta}+2\sigma_{2max}\times\frac{\Delta}{n-\Delta})\\ &= 2m_1n_2(\sigma_{1max}+\sigma_{2max})\times\frac{\Delta}{n-\Delta}. \end{aligned}$$

Similarly we can get $K_2\le 2m_2n_1(\sigma_{1max}+\sigma_{2max})\times\frac{\Delta}{n-\Delta}$. Therefore,

$$T_1(G_1[G_2]) \leq 2(m_2n_1 + m_1n_2)(\sigma_{1max} + \sigma_{2max})(\frac{\Delta}{n - \Delta}).$$

□

4|Application of fuzzified Temperature indices for chemical compounds

In this section, we applied the Temperature indices of fuzzy molecular graphs for Autism drugs. Since the correlation between any topological index with some physico-chemical characteristics of a chemical compound, should be checked in order to verify that index's efficiency (according to the regulations suggested by International Academy of Mathematical Chemistry), hence in this article the correlation between physico-chemical features of Autism drugs and the Temperature indices, is investigated through QSPR calculations.

4.1 A review on Autism's drugs

The six most prevalent Autism's drugs; including Ziprasidone, Aripiprazole, Haloperidol, Sertraline, Risperidone, Venlafaxine, are studied in this research. The molecular structure of these drug are shown in Figure (3). Furthermore, the values of eight physico-chemical factors (Boiling Point, Enthalpy, Flash point, Molar Refractivity, Polarizability, Molar Volume, Surface tension, Polar surface area) for all of these drugs are studied in Table (5).

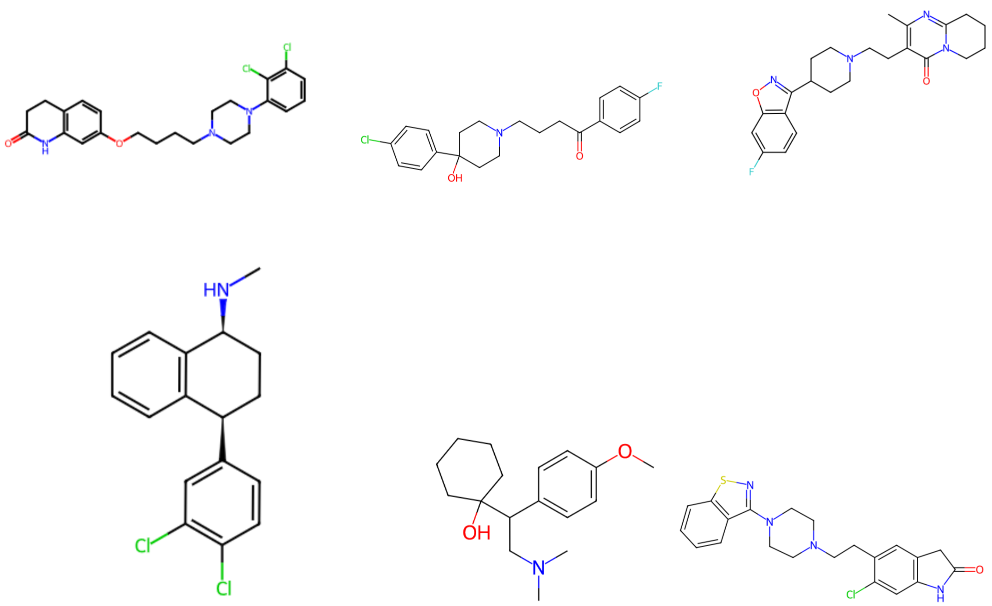

FIGURE 3. Drugs: a:Aripiprazole, b:Haloperidol, c:Risperidone, d:Sertraline, e:Venlafaxine, f:Ziprasidone

Table 5. Physical properties of drugs used for Autism drugs.

Autism drugs	BP	EN	FP	MR	PO	MV	PSA	SUT
iprasidone	554.8	83.6	289.3	114.1	45.2	301.4	77	61.5
Aripiprazole	646.2	95.3	344.6	120.3	47.7	355	45	48.4
Haloperidol	529	84.6	273.8	101	40	303.3	41	47.9
Risperidone	572.4	85.8	300	111.7	44.3	296.8	62	51.1
Venlafaxine	397.6	68.3	194.2	82.6	32.8	261.7	33	41.1
Sertraline	416.3	67	205.6	85.8	34	243.9	12	48.9

4.2 Modelling the molecular structure by fuzzy graphs and Temperature indices

We calculated all ten Temperature indices of Table (2), for each of the six Autism drugs in Table (6). The fuzzified form of the molecular graphs of these six drugs are shown in Figure (4). We fuzzified atomic mass and bond lengths, using the following formula, in order to be used in calculation of the Temperature indices for the molecule of each drug.

$$\sigma(u) = \frac{Atomic\ mass\ of\ u}{Maximum\ atomic\ mass}\ ,\ \ \mu(uv) = \frac{Bond\ Length\ of\ uv}{Maximum\ atomic\ mass\ of\ u, v}.$$

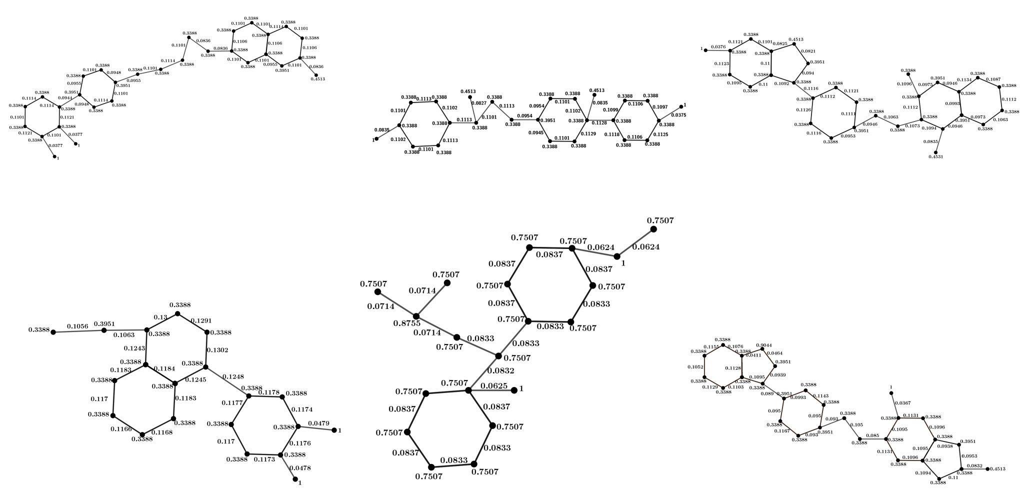

Figure 4. Fuzzy Autism drugs; a: Aripiprazole, b: Haloperidol, c: Risperidone, d: Sertraline, e:Venlafaxine, f:Ziprasidone

Table 6. The values of the Temperature indices of the Autism drugs.

Autism drugs	T_1	T_2	MT_2	MT_3	ST	PT
Ziprasidone	0.205355	0.0003161	3797780.16	5416.775766	421.6397	11046.63
Aripiprazole	0.194705	0.0002802	4467038.1	5833.579	436.8136	11947.88
Haloperidole	0.191148	0.003298	2480437	3914.134	324.0558	8067.35
Risperidone	0.201433	0.0002962	4399434	5884.816	445.885	12036.53
Venlafaxine	0.352379	0.001371	430122.8	1391.316	169.4981	2931.301
Sertraline	0.21265	0.0005206	1115179	2367.794	227.0836	4831.581

4.3 The QSPR analysis of the proposed method

In this section, the quantitative structure property relationship (QSPR) analysis is done for the topological indices calculated for fuzzy molecular graphs in Table (6), in compare with the physico-chemical properties presented in Table (5). The correlation results, obtained through SPSS software, are shown in Table (7). The linear regression model is considered as follows:

$$P = B + A(TI) \tag{3}$$

where P is the Autism drug property, B is the intersept constant, A is the regression coefficient, and TI represents the topological index. This capability is calculated using SPSS 26, for four topological indices ($MT_2(G)$, $MT_3(G)$, ST and PT) and some specific physico-chemical characteristics of six Autism drugs. Different linear models for regression of topological indices and physico-chemical properties of the drugs are obtained through equation (3) as follows.

(1) Product connectivity Temperature index $[PT(G)]$

$BP = 0.023[PT(G)] + 321.063$

$EN = 0.003[PT(G)] + 59.062$

$FP = 0.014[PT(G)] + 147.957$

$PO = 0.002[PT(G)] + 27.514$

(2) Modified second Temperature index $[MT_2(G)]$

$BP = 0.0001[MT_2(G)] + 371.637$

$EN = 0.0001[MT_2(G)] + 64.583$

$FP = 0.0001[MT_2(G)] + 178.551$

$PO = 0.0001[MT_2(G)] + 30.923$

(3) Modified third Temperature index $[MT_3(G)]$

$BP = 0.047[MT_3(G)] + 323.210$

$EN = 0.005[MT_3(G)] + 59.333$

$FP = 0.029[MT_3(G)] + 149.256$

$PO = 0.003[MT_3(G)] + 27.639$

(4) Sum connectivity Temperature index $[ST(G)]$

$BP = 0.765[ST(G)] + 261.059$

$EN = 0.084[ST(G)] + 52.563$

$FP = 0.463[ST(G)] + 111.663$

$PO = 0.051[ST(G)] + 23.421$

Table 7. Correlation coefficients of physical properties of drugs.

Temperature indices	BP	EN	FP	MR	PO	MV	PSA	SUT
PT	**0.951**	**0.905**	**0.951**	-0.078	**0.978**	0.8	0.753	0.636
MT_2	**0.959**	**0.913**	**0.959**	-0.089	**0.981**	0.817	0.740	0.596
MT_3	**0.949**	**0.902**	**0.949**	-0.078	**0.978**	0.795	0.752	0.596
ST	**0.942**	**0.895**	**0.943**	-.082	**0.976**	0.786	0.769	0.658

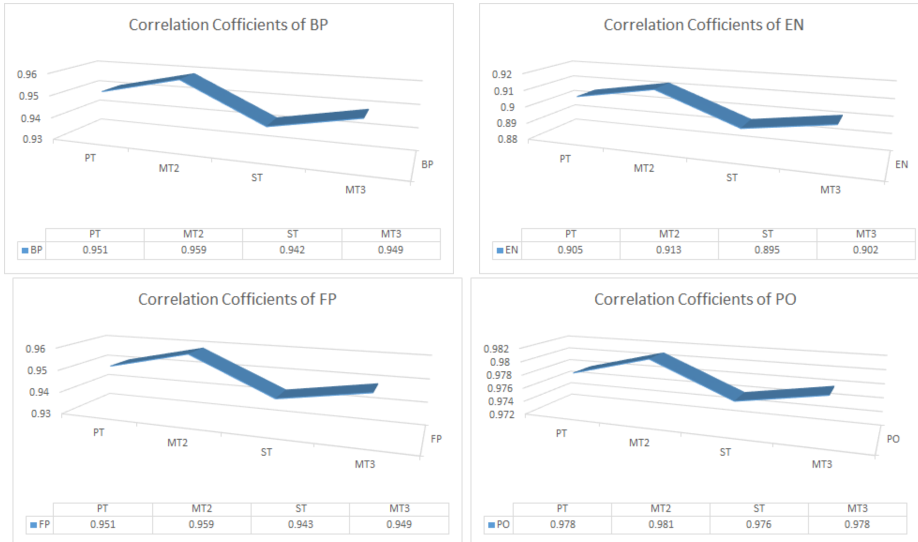

FIGURE 5. Physicochemical properties with Temperature indices

5|Conclusion

The results in Table 7 indicate that the computed property values closely align with the actual values, further validating the predictive accuracy of these indices. Additionally, Figure illustrates the correlation between the physical and chemical properties of Autism drugs and specific topological indices. The modified second Temperature index demonstrates a strong positive correlation with Polarizability, with respective R-values of $(r = 0.981)$. Additionally, the modified third Temperature index and Product connectivity Temperature index shows a significant positive correlation, with a value of $(r = 0.978)$. The study reveals a positive correlation between the physical and chemical properties of Autism drugs and their topological indices (TI). Regression models for various physical and chemical properties, presented in Cases 1, 2, 3 and 4 demonstrate that the p-values are below 0.05, indicating that these predictors are statistically significant in linear regression. Consequently, it can be inferred that all physical and chemical properties are of considerable importance. This underscores the potential relevance of these topological indices in Quantitative Structure-Property Relationship (QSPR) analysis for Autism drugs, with corresponding regression lines plotted. The findings of this study could contribute to the production, development, and enhancement of more effective Autism drugs. Moreover, the methodology used in this research can be applied to investigate the structures of other drugs.

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Author Contribution

M. Sadeghi: software and writing. S.P. Azizi: conceptualization and editing. J.Ramezani: methodology and editing. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest

The authors declare that there is no conflict of interest concerning the reported research findings. Funders played no role in the study's design, in the collection, analysis, or interpretation of the data, in the writing of the manuscript, or in the decision to publish the results.

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