# On Analysis of Temperature Based Topological Indices of Anti-Cancer Drugs

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## ABSTRACT

*Cancer is a life-threatening illness. For the treatment of various forms of cancer, there is currently no medicine. To combat this condition, new medication studies are being carried out. HDAC-based multitarget medicines are one of them. The characteristics of the molecular graph can be expressed numerically using topological indices. Topological indices can be utilized to offer details on the physicochemical characteristics and biological properties of molecules in investigations of the structure-property relationship (QSPR) and structure-activity relationship. Theoretical and statistical research on drug-like molecules helps drug design and discovery by rationalising lead identification, immediate judgment, and mechanisms of action comprehension. In this paper, we calculate temperature-based topological indices using the analytically closed formulae of various molecular structures of anti-cancer medications such as vorinostat, tucidinostat, triciferol, CUDC-101, and CUDC-907.*

**Mathematics Subject Classification**: 05C07, 05C35, 05C40.

**Keywords**: Molecular structure, cancer, drugs, Temperature Indices, topological index.

## 1. Introduction

Cancer is a serious condition with no cure and, in certain situations, a deadly outcome. Numerous research are being done to treat cancer patients and prevent the illness. Finding new medicines is one of these investigations. Drug development is a time-consuming, expensive, and complicated process. Computerized drug design is crucial to this procedure for this reason. The target candidates' electrical, drug-like, pharmacokinetic, 3D structure-activity relationship (QSAR), and physicochemical properties are all predicted in this drug design. Topological indices(TIs) are highlighted by chemical graph theory. Real numbers that are derived from the molecule or molecular compound are utilised as TIs to forecast the physicochemical characteristics and biological activities of the chemical structure. Topological indices were first used to determine the physicochemical properties of alkenes [24].

Since 1947, many TIs have been formally defined (see, [25, 26, 27, 28, 31]). These indices are categorised in accordance with the structural characteristics of the graph, including its vertex degree, the separation between adjacent vertices, and its eigenvalues. The boiling, melting, and enthalpy properties of alkenes, as well as other properties, are shown to have a continuous connection with the chemical structures of anticancer medicines [12]. To anticipate the characteristics of anticancer medications in this context, many TIs have been applied.

For the physical characteristics (boiling point, melting point, enthalpy, flashpoint, and molar refraction [MR]) of 17 anticancer medicines, from Amathaspiramide-E to Tambjamine-K, Shanmukha [12] produced QSPR models employing 13 degree-based TIs.

Degree-based TIs of the molecular structure of the Hyaluronic Acid-Paclitaxel conjugates used to treat cancer were calculated by Zheng et al. [13] and Jahanbani et al. [14]. Hyaluronic acid-curcumin conjugates degree-based TIs and polynomials were determined by Ali et al. [15]. Hyaluronic acid Tis were calculated by Wang [16].

According to recent research, dual-target medications will be a significant advance in the fight against cancer (see, [17, 18, 30]). Dual-target medications, particularly those that target HDAC, have been found to be crucial in the treatment of cancer. Additionally, it was discovered that the HDAC-based CUDC-101 and CUDC-907 dualtarget medicines were more effective cancer treatments than each of their parent compounds alone or when combined [17]. HDAC has been the subject of several recent pharmacological research (see, [19, 20, 21, 22, 23]).

A significant contribution to the development of the chemical sciences has come from the field of mathematical chemistry known as chemical graph theory. In the field of chemistry, numerous graph indices have application, particularly in QSPR/QSAR research (see, [1, 3, 4, 5, 6, 7, 10, 29]).

In 1988, Fajtlowicz [2] established the concept of a vertex u temperature for a connected graph *G*.

Defined as: $$T(u) = \frac{d(u)}{n - d(u)},$$

*d(u)* denotes the degree of vertex *u* and $|V(G)| = n$.

Recently, various novel temperature indices for a graph G, such as the general first and second temperature index, the general temperature index and the $(\alpha, \beta)$ − temperature index, the sum connectivity and F-temperature index, were developed and investigated by V. R. Kulli (see, [8, 9]).

In this work, we calculated these recently discovered temperature indices for the chemical structures of the HDAC inhibitors tucidinostat and vorinostat, the dual-target medicines CUDC-907, CUDC-101, and triciferol, which are used to treat cancer patients. In 2019, Kulli [9] introduced the following topological indices (see Table 1):

| | |
|---|---|
| Sum connectivity temperature index | $ST(G) = \sum_{uv \in \hat{u}(G)} \frac{1}{\sqrt{T(u)+T(v)}}$ |
| Product connectivity temperature index | $PT(G) = \sum_{uv \in \hat{u}(G)} \frac{1}{\sqrt{T(u)\times T(v)}}$ |
| Symmetric division temperature index | $ST(G) = \sum_{uv \in \hat{u}(G)} \left(\frac{T(u)}{T(v)} + \frac{T(v)}{T(u)}\right)$ |
| General first temperature index | $T_1^{\alpha}(G) = \sum_{uv \in \hat{u}(G)} \left(T(u)+T(v)\right)^{\alpha}$ |
| General second temperature index | $T_2^{\alpha}(G) = \sum_{uv \in \hat{u}(G)} \left(T(u)\times T(v)\right)^{\alpha}$ |
| General second temperature index | $FT(G) = \sum_{uv \in \hat{u}(G)} \left(T(u)^2 + T(v)^2\right)$ |

| | |
|---|---|
| General temperature index | $T_\alpha(G) = \sum_{uv \in \hat{u}(G)} \left(T(u)^\alpha + T(v)^\alpha\right)$ |
| $(\alpha, \beta)$ − temperature index | $T_{\alpha,\beta}(G) = \sum_{uv \in \hat{u}(G)} \left(T(u)^\alpha T(v)^\beta + T(u)^\beta T(v)^\alpha\right)$ |

Table 1: Temperature-based topological indices of $G$

# 2. Main Results

The main discoveries and computations in this work are centered on topological indices, such as the general first and second temperature index, the general temperature index, the (α, β)-temperature 2 index, the sum connectivity and F−temperature index, and so on of a graph G. Pharmacology, chemical, biological, and pharmacological aspects of molecular structure are critical in drug manufacture and design in medical research. These qualities can be investigated by computing topological indices.

**Theorem 2.1.** *Let $G_1$ be a molecular graph of CUDC-907. Then the temperature index of the CUDC-907 graph are given,*

1. The general first temperature index

$$T_1^\alpha(G_1) = 2\left(\frac{52}{595}\right)^\alpha + 2\left(\frac{46}{385}\right)^\alpha + 8\left(\frac{2}{17}\right)^\alpha + 22\left(\frac{28}{187}\right)^\alpha + 6\left(\frac{2}{11}\right)^\alpha.$$

2. The general second temperature index

$$T_2^\alpha(G_1) = 2\left(\frac{1}{595}\right)^\alpha + 2\left(\frac{1}{385}\right)^\alpha + 8\left(\frac{1}{289}\right)^\alpha + 22\left(\frac{1}{187}\right)^\alpha + 6\left(\frac{1}{121}\right)^\alpha.$$

3. The general temperature index

$$T_\alpha(G_1) = 4\left(\frac{1}{35}\right)^\alpha + 40\left(\frac{1}{17}\right)^\alpha + 36\left(\frac{1}{11}\right)^\alpha.$$

4. The (α, β) temperature index

$$T_{\alpha,\beta}(G_1) = 2\left(\left(\frac{1}{35}\right)^\alpha\left(\frac{1}{17}\right)^\beta + \left(\frac{1}{35}\right)^\beta\left(\frac{1}{17}\right)^\alpha\right) + 2\left(\left(\frac{1}{35}\right)^\alpha\left(\frac{1}{11}\right)^\beta + \left(\frac{1}{35}\right)^\beta\left(\frac{1}{11}\right)^\alpha\right)$$
$$+16\left(\frac{1}{17}\right)^{\alpha+\beta} + 22\left(\left(\frac{1}{17}\right)^\alpha\left(\frac{1}{11}\right)^\beta + \left(\frac{1}{17}\right)^\beta\left(\frac{1}{11}\right)^\alpha\right) + 12\left(\frac{1}{11}\right)^{\alpha+\beta}.$$

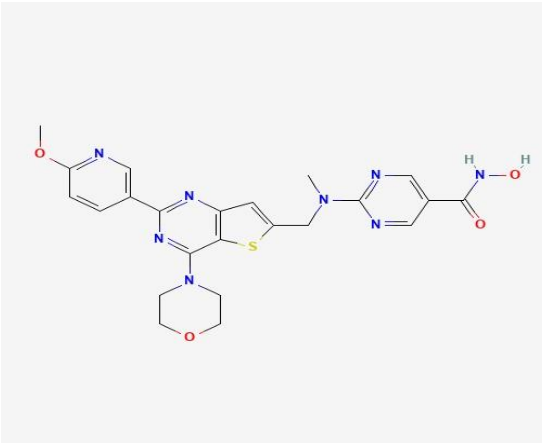
***Proof.*** Let $G_1$ be the molecular graph of CUDC-907, which has 36 vertices and 40 edges as shown in Figure 1a. We have the following three vertex partitions, $V_{\{1\}} = \{u \in V(G_1) \mid d(u) = 1\}$, $V_{\{2\}} = \{u \in V(G_1) \mid d(u) = 2\}$, $V_{\{3\}} = \{u \in V(G_1) \mid d(u) = 3\}$. Therefore, there are 5 edge partitions of $G_1$, which can be written as follows:

$$\mathcal{E}_{1,2} = \{uv \in \mathcal{E}(G_1) \mid d(u) = 1 \text{ and } d(v) = 2\},$$
$$\mathcal{E}_{1,3} = \{uv \in \mathcal{E}(G_1) \mid d(u) = 1 \text{ and } d(v) = 3\},$$
$$\mathcal{E}_{2,2} = \{uv \in \mathcal{E}(G_1) \mid d(u) = 2 \text{ and } d(v) = 2\},$$
$$\mathcal{E}_{2,3} = \{uv \in \mathcal{E}(G_1) \mid d(u) = 2 \text{ and } d(v) = 3\},$$
$$\mathcal{E}_{3,3} = \{uv \in \mathcal{E}(G_1) \mid d(u) = 3 \text{ and } d(v) = 3\},$$

We can see that $|\mathcal{E}_{1,2}|=2$, $|\mathcal{E}_{1,3}|=2$, $|\mathcal{E}_{2,2}|=8$, $|\mathcal{E}_{2,3}|=22$, $|\mathcal{E}_{3,3}|=6$, from the molecular graph of $G_1$.

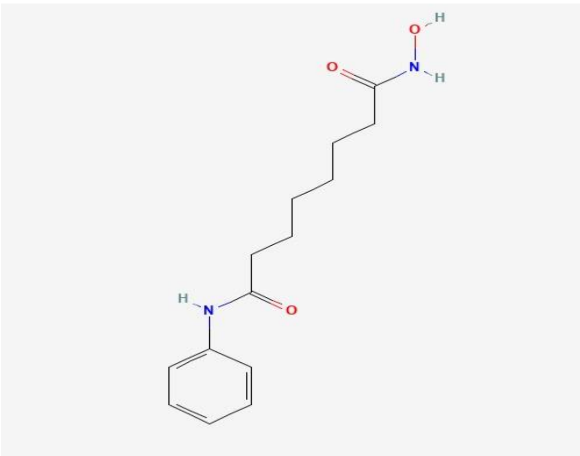
1. The general first temperature index of $G_1$ is

$$T_1^{\alpha}(G_1)=\sum_{uv\in \hat{u}(G_1)}\left(T(u)+T(v)\right)^{\alpha}$$

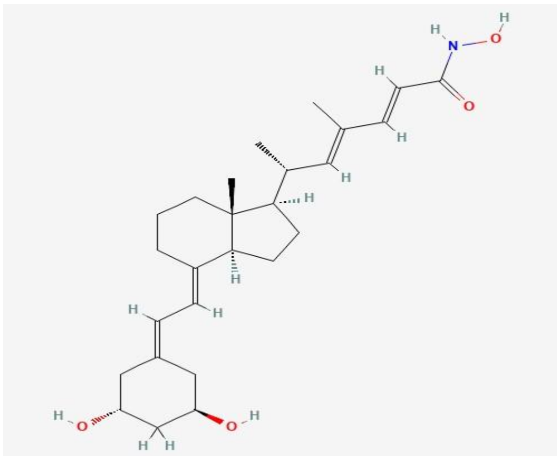


(a) CUDC-907

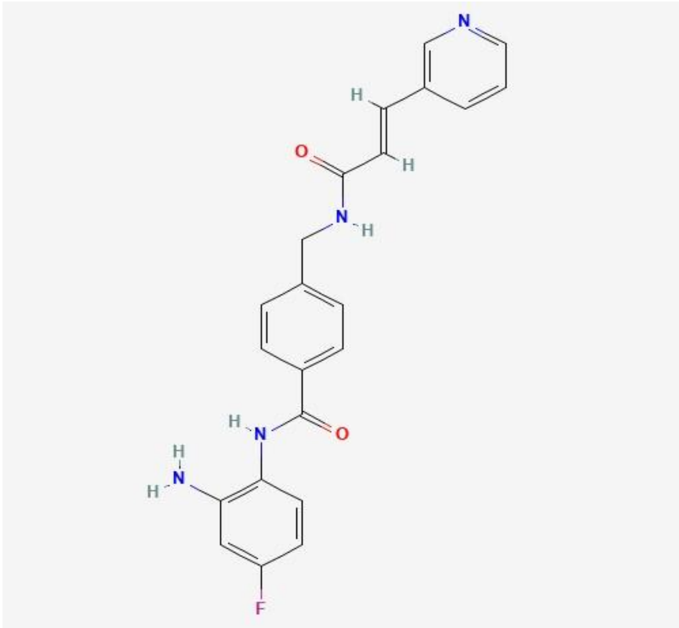
(b) CUDC-101



(c) Triciferol



(d) Vorinostat



(e) Tucidinostat

Figure 1: Molecular structure of Cancer drugs [11].

(a) CUDC – 907. (b) CUDC – 101. (c) Triciferol. (d) Vorinostat. (e) Tucidinostat

$$
\begin{aligned}
&= 2\left(\frac{1}{36-1}+\frac{2}{36-2}\right)^{\alpha} + 2\left(\frac{1}{36-1}+\frac{3}{36-3}\right)^{\alpha} \\
&+8\left(\frac{2}{36-2}+\frac{2}{36-2}\right)^{\alpha} + 22\left(\frac{2}{36-2}+\frac{3}{36-3}\right)^{\alpha} \\
&+6\left(\frac{3}{36-3}+\frac{3}{36-3}\right)^{\alpha} \\
&= 2\left(\frac{52}{595}\right)^{\alpha} + 2\left(\frac{46}{385}\right)^{\alpha} + 8\left(\frac{2}{17}\right)^{\alpha} \\
&+22\left(\frac{28}{187}\right)^{\alpha} + 6\left(\frac{2}{11}\right)^{\alpha}.
\end{aligned}
$$

2. The general second temperature index of $G_1$ is

$$
T_2^{\alpha}(G_1) = \sum_{uv\in \hat{u}(G_1)} \left(T(u)\times T(v)\right)^{\alpha}
$$

$$
\begin{aligned}
&= 2\left(\frac{1}{36-1}\times\frac{2}{36-2}\right)^{\alpha} + 2\left(\frac{1}{36-1}\times\frac{3}{36-3}\right)^{\alpha} \\
&+8\left(\frac{2}{36-2}\times\frac{2}{36-2}\right)^{\alpha} + 22\left(\frac{2}{36-2}\times\frac{3}{36-3}\right)^{\alpha} \\
&+6\left(\frac{3}{36-3}\times\frac{3}{36-3}\right)^{\alpha}
\end{aligned}
$$

$$= 2\left(\frac{1}{595}\right)^{\alpha} + 2\left(\frac{1}{385}\right)^{\alpha} + 8\left(\frac{1}{289}\right)^{\alpha}$$
$$+22\left(\frac{1}{187}\right)^{\alpha} + 6\left(\frac{1}{121}\right)^{\alpha}.$$

3. The general temperature index of $G_1$ is

$$T_{\alpha}(G_1) = \sum_{uv \in \hat{u}(G_1)} \left(T(u)^{\alpha} + T(v)^{\alpha}\right)$$

$$= 2\left(\left(\frac{1}{36-1}\right)^{\alpha} + \left(\frac{2}{36-2}\right)^{\alpha}\right) + 2\left(\left(\frac{1}{36-1}\right)^{\alpha} + \left(\frac{3}{36-3}\right)^{\alpha}\right)$$
$$+8\left(\left(\frac{2}{36-2}\right)^{\alpha} + \left(\frac{2}{36-2}\right)^{\alpha}\right) + 22\left(\left(\frac{2}{36-2}\right)^{\alpha} + \left(\frac{3}{36-3}\right)^{\alpha}\right)$$
$$+6\left(\left(\frac{3}{36-3}\right)^{\alpha} + \left(\frac{3}{36-3}\right)^{\alpha}\right)$$

$$= 4\left(\frac{1}{35}\right)^{\alpha} + 40\left(\frac{1}{17}\right)^{\alpha} + 36\left(\frac{1}{11}\right)^{\alpha}.$$

4. The $(\alpha, \beta)$ - temperature index of $G_1$ is

$$T_{\alpha,\beta}(G_1) = \sum_{uv \in \hat{u}(G_1)} \left(T(u)^{\alpha} T(v)^{\alpha} + T(u)^{\beta} T(v)^{\alpha}\right)$$

$$= 2\left(\left(\frac{1}{36-1}\right)^{\alpha}\left(\frac{2}{36-2}\right)^{\beta} + \left(\frac{1}{36-1}\right)^{\beta}\left(\frac{2}{36-2}\right)^{\alpha}\right)$$
$$+2\left(\left(\frac{1}{36-1}\right)^{\alpha}\left(\frac{3}{36-3}\right)^{\beta} + \left(\frac{1}{36-1}\right)^{\beta}\left(\frac{3}{36-3}\right)^{\alpha}\right)$$
$$+8\left(\left(\frac{2}{36-2}\right)^{\alpha}\left(\frac{2}{36-2}\right)^{\beta} + \left(\frac{2}{36-2}\right)^{\beta}\left(\frac{2}{36-2}\right)^{\alpha}\right)$$
$$+22\left(\left(\frac{2}{36-2}\right)^{\alpha}\left(\frac{3}{36-3}\right)^{\beta} + \left(\frac{2}{36-2}\right)^{\beta}\left(\frac{3}{36-3}\right)^{\alpha}\right)$$
$$+6\left(\left(\frac{3}{36-3}\right)^{\alpha}\left(\frac{3}{36-3}\right)^{\beta} + \left(\frac{3}{36-3}\right)^{\beta}\left(\frac{3}{36-3}\right)^{\alpha}\right)$$

$$= 2\left(\left(\frac{1}{35}\right)^{\alpha}\left(\frac{1}{17}\right)^{\beta} + \left(\frac{1}{35}\right)^{\beta}\left(\frac{1}{17}\right)^{\alpha}\right) + 2\left(\left(\frac{1}{35}\right)^{\alpha}\left(\frac{1}{11}\right)^{\beta} + \left(\frac{1}{35}\right)^{\beta}\left(\frac{1}{11}\right)^{\alpha}\right)$$
$$+16\left(\frac{1}{17}\right)^{\alpha+\beta} + 22\left(\left(\frac{1}{17}\right)^{\alpha}\left(\frac{1}{11}\right)^{\beta} + \left(\frac{1}{17}\right)^{\beta}\left(\frac{1}{11}\right)^{\alpha}\right) + 12\left(\frac{1}{11}\right)^{\alpha+\beta}.$$

**Corollary 2.2.** *Let $G_1$ be a molecular graph of CUDC-907. Then by Theorem 2.1, we have*

1. The sum connectivity temperature index

$$ST(G_1) = 106.801$$

by taking $\alpha$ = (- ½) in $T_1^{\alpha}(G_1)$.

2. The product connectivity temperature index

$$PT(G_1) = 590.874$$

by taking $\alpha$ = (- ½) in $T_2^{\alpha}(G_1)$.

3. The F-temperature index

$$FT(G_1) = 0.349$$

by taking α = 2 in $T_{\alpha}^{\alpha}(G_1)$.

4. Symmetric division temperature index

$$SDT(G_1) = 88.317$$

by taking α, β = 1 and -1 in $T_{\alpha,\beta}(G_1)$.

**Theorem 2.3.** *Let $G_2$ be a molecular graph of CUDC-101. Then the temperature index of the CUDC-101graph are given,*

1. The general first temperature index

$$T_1^{\alpha}(G_2) = 3\left(\frac{46}{465}\right)^{\alpha} + \left(\frac{122}{899}\right)^{\alpha} + 10\left(\frac{2}{15}\right)^{\alpha} + 17\left(\frac{74}{435}\right)^{\alpha} + 3\left(\frac{6}{29}\right)^{\alpha}.$$

2. The general second temperature index

$$T_2^{\alpha}(G_2) = 3\left(\frac{1}{465}\right)^{\alpha} + \left(\frac{3}{899}\right)^{\alpha} + 10\left(\frac{1}{225}\right)^{\alpha} + 17\left(\frac{3}{435}\right)^{\alpha} + 3\left(\frac{9}{841}\right)^{\alpha}.$$

3. The general temperature index

$$T_{\alpha}(G_2) = 4\left(\frac{1}{31}\right)^{\alpha} + 40\left(\frac{1}{15}\right)^{\alpha} + 24\left(\frac{3}{29}\right)^{\alpha}.$$

4. The (α, β) temperature index

$$T_{\alpha,\beta}(G_2) = 3\left(\left(\frac{1}{31}\right)^{\alpha}\left(\frac{1}{15}\right)^{\beta} + \left(\frac{1}{31}\right)^{\beta}\left(\frac{1}{15}\right)^{\alpha}\right) + \left(\left(\frac{1}{31}\right)^{\alpha}\left(\frac{3}{29}\right)^{\beta} + \left(\frac{1}{31}\right)^{\beta}\left(\frac{3}{29}\right)^{\alpha}\right)$$
$$+20\left(\frac{1}{15}\right)^{\alpha+\beta} + 17\left(\left(\frac{1}{15}\right)^{\alpha}\left(\frac{3}{29}\right)^{\beta} + \left(\frac{1}{15}\right)^{\beta}\left(\frac{3}{29}\right)^{\alpha}\right) + 6\left(\frac{3}{29}\right)^{\alpha+\beta}.$$

***Proof.*** Let $G_2$ be the molecular graph of CUDC-101, which has 32 vertices and 34 edges as shown in Figure 1b. We have the following three vertex partitions, $V_{\{1\}} = \{u \in V(G_2) \mid d(u) = 1\}$, $V_{\{2\}} = \{u \in V(G_2) \mid d(u) = 2\}$, $V_{\{3\}} = \{u \in V(G_2) \mid d(u) = 3\}$. Therefore, there are 5 edge partitions of $G_2$, which can be written as follows:

$$\mathcal{E}_{1,2} = \{uv \in \mathcal{E}(G_2) \mid d(u) = 1 \text{ and } d(v) = 2\},$$
$$\mathcal{E}_{1,3} = \{uv \in \mathcal{E}(G_2) \mid d(u) = 1 \text{ and } d(v) = 3\},$$
$$\mathcal{E}_{2,2} = \{uv \in \mathcal{E}(G_2) \mid d(u) = 2 \text{ and } d(v) = 2\},$$
$$\mathcal{E}_{2,3} = \{uv \in \mathcal{E}(G_2) \mid d(u) = 2 \text{ and } d(v) = 3\},$$

$$\mathcal{E}_{3,3} = \{uv \in \mathcal{E}(G_2) \mid d(u) = 3 \text{ and } d(v) = 3\},$$

We can see that $|\mathcal{E}_{1,2}|=3$, $|\mathcal{E}_{1,3}|=1$, $|\mathcal{E}_{2,2}|=10$, $|\mathcal{E}_{2,3}|=17$, $|\mathcal{E}_{3,3}|=3$, from the molecular graph of $G_2$.

5. The general first temperature index of $G_2$ is

$$T_1^{\alpha}(G_2) = \sum_{uv\in \hat{u}(G_2)} \left(T(u)+T(v)\right)^{\alpha}$$

$$= 3\left(\frac{1}{32-1}+\frac{2}{32-2}\right)^{\alpha} + \left(\frac{1}{32-1}+\frac{3}{32-3}\right)^{\alpha}$$

$$+10\left(\frac{2}{32-2}+\frac{2}{32-2}\right)^{\alpha} +17\left(\frac{2}{32-2}+\frac{3}{32-3}\right)^{\alpha}$$

$$+3\left(\frac{3}{32-3}+\frac{3}{32-3}\right)^{\alpha}$$

$$= 3\left(\frac{46}{465}\right)^{\alpha} + \left(\frac{122}{899}\right)^{\alpha} +10\left(\frac{2}{15}\right)^{\alpha}$$

$$+17\left(\frac{74}{435}\right)^{\alpha} +3\left(\frac{6}{29}\right)^{\alpha}.$$

6. The general second temperature index of $G_3$ is

$$T_1^{\alpha}(G_2) = \sum_{uv\in \hat{u}(G_2)} \left(T(u)\times T(v)\right)^{\alpha}$$

$$= 3\left(\frac{1}{32-1}\times\frac{2}{32-2}\right)^{\alpha} + \left(\frac{1}{32-1}\times\frac{3}{32-3}\right)^{\alpha}$$

$$+10\left(\frac{2}{32-2}\times\frac{2}{32-2}\right)^{\alpha} +17\left(\frac{2}{32-2}\times\frac{3}{32-3}\right)^{\alpha}$$

$$+3\left(\frac{3}{32-3}\times\frac{3}{32-3}\right)^{\alpha}$$

$$= 3\left(\frac{1}{465}\right)^{\alpha} + \left(\frac{3}{899}\right)^{\alpha} +10\left(\frac{1}{225}\right)^{\alpha}$$

$$+17\left(\frac{3}{435}\right)^{\alpha} +3\left(\frac{9}{841}\right)^{\alpha}.$$

7. The general temperature index of $G_2$ is

$$T_{\alpha}(G_2) = \sum_{uv\in \hat{u}(G_2)} \left(T(u)^{\alpha}+T(v)^{\alpha}\right)$$

$$= 3\left(\left(\frac{1}{32-1}\right)^{\alpha} + \left(\frac{2}{32-2}\right)^{\alpha}\right) + \left(\left(\frac{1}{32-1}\right)^{\alpha} + \left(\frac{3}{32-3}\right)^{\alpha}\right)$$

$$+10\left(\left(\frac{2}{32-2}\right)^{\alpha} + \left(\frac{2}{32-2}\right)^{\alpha}\right) +17\left(\left(\frac{2}{32-2}\right)^{\alpha} + \left(\frac{3}{32-3}\right)^{\alpha}\right)$$

$$+3\left(\left(\frac{3}{32-3}\right)^{\alpha} + \left(\frac{3}{32-3}\right)^{\alpha}\right)$$

$$=4\left(\frac{1}{31}\right)^{\alpha}+40\left(\frac{1}{15}\right)^{\alpha}+24\left(\frac{3}{29}\right)^{\alpha}.$$

8. The $(\alpha, \beta)$ - temperature index of $G_3$ is

$$T_{\alpha,\beta}(G_2)=\sum_{uv\in \hat{u}(G_2)}\left(T(u)^{\alpha}T(v)^{\alpha}+T(u)^{\beta}T(v)^{\alpha}\right)$$

$$=3\left(\left(\frac{1}{32-1}\right)^{\alpha}\left(\frac{2}{32-2}\right)^{\beta}+\left(\frac{1}{32-1}\right)^{\beta}\left(\frac{2}{32-2}\right)^{\alpha}\right)$$
$$+\left(\left(\frac{1}{32-1}\right)^{\alpha}\left(\frac{3}{32-3}\right)^{\beta}+\left(\frac{1}{32-1}\right)^{\beta}\left(\frac{3}{32-3}\right)^{\alpha}\right)$$
$$+10\left(\left(\frac{2}{32-2}\right)^{\alpha}\left(\frac{2}{32-2}\right)^{\beta}+\left(\frac{2}{32-2}\right)^{\beta}\left(\frac{2}{32-2}\right)^{\alpha}\right)$$
$$+17\left(\left(\frac{2}{32-2}\right)^{\alpha}\left(\frac{3}{32-3}\right)^{\beta}+\left(\frac{2}{32-2}\right)^{\beta}\left(\frac{3}{32-3}\right)^{\alpha}\right)$$
$$+3\left(\left(\frac{3}{32-3}\right)^{\alpha}\left(\frac{3}{32-3}\right)^{\beta}+\left(\frac{3}{32-3}\right)^{\beta}\left(\frac{3}{32-3}\right)^{\alpha}\right)$$

$$=3\left(\left(\frac{1}{31}\right)^{\alpha}\left(\frac{1}{15}\right)^{\beta}+\left(\frac{1}{31}\right)^{\beta}\left(\frac{1}{15}\right)^{\alpha}\right)+\left(\left(\frac{1}{31}\right)^{\alpha}\left(\frac{3}{29}\right)^{\beta}+\left(\frac{1}{31}\right)^{\beta}\left(\frac{3}{29}\right)^{\alpha}\right)$$
$$+20\left(\frac{1}{15}\right)^{\alpha+\beta}+17\left(\left(\frac{1}{15}\right)^{\alpha}\left(\frac{3}{29}\right)^{\beta}+\left(\frac{1}{15}\right)^{\beta}\left(\frac{3}{29}\right)^{\alpha}\right)+6\left(\frac{3}{29}\right)^{\alpha+\beta}.$$

**Corollary 2.4.** *Let $G_2$ be a molecular graph of CUDC-101. Then by Theorem 2.3, we have*

1. The sum connectivity temperature index

   $$ST(G_2) = 87.452$$

   by taking α = (- ½) in $T_1^{\alpha}(G_2)$.

2. The product connectivity temperature index

   $$PT(G_2) = 465.710$$

   by taking α = (- ½) in $T_2^{\alpha}(G_2)$.

3. The $F$ - temperature index

   $$FT(G_2) = 0.439$$

   by taking α = 2 in $T_{\alpha}^{\alpha}(G_2)$.

4. Symmetric division temperature index

   $$SDT(G_2) = 73.619$$

   by taking α, β = 1 and -1 in $T_{\alpha,\beta}(G_2)$.

**Theorem 2.5.** *Let $G_3$ be a molecular graph triciferol. Then the temperature index of the triciferol graph are given,*

1. The general first temperature index

$$T_1^{\alpha}(G_3)=\left(\frac{89}{870}\right)^{\alpha}+5\left(\frac{59}{420}\right)^{\alpha}+\left(\frac{147}{810}\right)^{\alpha}+5\left(\frac{4}{29}\right)^{\alpha}+16\left(\frac{143}{812}\right)^{\alpha}+\left(\frac{170}{783}\right)^{\alpha}+2\left(\frac{3}{14}\right)^{\alpha}+2\left(\frac{193}{756}\right)^{\alpha}.$$

2. The general second temperature index

$$T_2^{\alpha}(G_3)=\left(\frac{1}{435}\right)^{\alpha}+5\left(\frac{1}{280}\right)^{\alpha}+\left(\frac{2}{405}\right)^{\alpha}+5\left(\frac{4}{841}\right)^{\alpha}+16\left(\frac{3}{406}\right)^{\alpha}+\left(\frac{8}{783}\right)^{\alpha}+2\left(\frac{9}{784}\right)^{\alpha}+2\left(\frac{3}{189}\right)^{\alpha}.$$

3. The general temperature index

$$T_{\alpha}(G_3)=7\left(\frac{1}{30}\right)^{\alpha}+28\left(\frac{2}{29}\right)^{\alpha}+27\left(\frac{3}{28}\right)^{\alpha}+4\left(\frac{4}{27}\right)^{\alpha}.$$

4. The (α, β) - temperature index

$$\begin{aligned}T_{\alpha,\beta}(G_3)=&\left(\left(\frac{1}{30}\right)^{\alpha}\left(\frac{2}{29}\right)^{\beta}+\left(\frac{1}{30}\right)^{\beta}\left(\frac{2}{29}\right)^{\alpha}\right)+5\left(\left(\frac{1}{30}\right)^{\alpha}\left(\frac{3}{28}\right)^{\beta}+\left(\frac{1}{30}\right)^{\beta}\left(\frac{3}{28}\right)^{\alpha}\right)\\&+\left(\left(\frac{1}{30}\right)^{\alpha}\left(\frac{2}{27}\right)^{\beta}+\left(\frac{1}{30}\right)^{\beta}\left(\frac{4}{27}\right)^{\alpha}\right)+10\left(\frac{2}{29}\right)^{\alpha+\beta}+16\left(\left(\frac{2}{29}\right)^{\alpha}\left(\frac{3}{28}\right)^{\beta}\right.\\&\left.+\left(\frac{2}{29}\right)^{\beta}\left(\frac{3}{28}\right)^{\alpha}\right)+\left(\left(\frac{2}{29}\right)^{\alpha}\left(\frac{4}{27}\right)^{\beta}+\left(\frac{2}{29}\right)^{\beta}\left(\frac{4}{27}\right)^{\alpha}\right)+4\left(\frac{3}{28}\right)^{\alpha+\beta}\\&+2\left(\left(\frac{3}{28}\right)^{\alpha}\left(\frac{4}{27}\right)^{\beta}+\left(\frac{3}{28}\right)^{\beta}\left(\frac{4}{27}\right)^{\alpha}\right).\end{aligned}$$

***Proof.*** Let $G_3$ be the molecular graph of triciferol, which has 31 vertices and 33 edges as shown in Figure 1c. We have the following four vertex partitions, $V_{\{1\}} = \{u \in V(G_3) \mid d(u) = 1\}$, $V_{\{2\}} = \{u \in V(G_3) \mid d(u) = 2\}$, $V_{\{3\}} = \{u \in V(G_3) \mid d(u) = 3\}$, $V_{\{4\}} = \{u \in V(G_3) \mid d(u) = 4\}$. Therefore, there are 8 edge partitions of $G_3$, which can be written as follows:

$\mathcal{E}_{1,2} = \{uv \in \mathcal{E}(G_3) \mid d(u) = 1 \text{ and } d(v) = 2\}$,

$\mathcal{E}_{1,3} = \{uv \in \mathcal{E}(G_3) \mid d(u) = 1 \text{ and } d(v) = 3\}$,

$\mathcal{E}_{1,4} = \{uv \in \mathcal{E}(G_3) \mid d(u) = 1 \text{ and } d(v) = 4\}$,

$\mathcal{E}_{2,2} = \{uv \in \mathcal{E}(G_3) \mid d(u) = 2 \text{ and } d(v) = 2\}$,

$\mathcal{E}_{2,3} = \{uv \in \mathcal{E}(G_3) \mid d(u) = 2 \text{ and } d(v) = 3\}$,

$\mathcal{E}_{2,4} = \{uv \in \mathcal{E}(G_3) \mid d(u) = 2 \text{ and } d(v) = 4\}$,

$\mathcal{E}_{3,3} = \{uv \in \mathcal{E}(G_3) \mid d(u) = 3 \text{ and } d(v) = 3\}$,

$\mathcal{E}_{3,4} = \{uv \in \mathcal{E}(G_3) \mid d(u) = 3 \text{ and } d(v) = 4\}$.

We can see that $|\mathcal{E}_{1,2}|=1$, $|\mathcal{E}_{1,3}|=5$, $|\mathcal{E}_{1,4}|=1$, $|\mathcal{E}_{2,2}|=5$, $|\mathcal{E}_{2,3}|=16$, $|\mathcal{E}_{2,4}|=1$, $|\mathcal{E}_{3,3}|=2$, $|\mathcal{E}_{3,4}|=2$ from the molecular graph of $G_3$.

1. The general first temperature index of $G_3$ is

$$T_1^{\alpha}(G_3)=\sum_{uv\in \mathcal{E}(G_3)}\left(T(u)+T(v)\right)^{\alpha}$$

$$=\left(\frac{1}{31-1}+\frac{2}{31-2}\right)^{\alpha}+5\left(\frac{1}{31-1}+\frac{3}{31-3}\right)^{\alpha}+\left(\frac{1}{31-1}+\frac{4}{31-4}\right)^{\alpha}$$
$$+5\left(\frac{2}{31-2}+\frac{2}{31-2}\right)^{\alpha}+16\left(\frac{2}{31-2}+\frac{3}{31-3}\right)^{\alpha}+\left(\frac{2}{31-2}+\frac{4}{31-4}\right)^{\alpha}$$
$$+2\left(\frac{3}{31-3}+\frac{3}{31-3}\right)^{\alpha}+2\left(\frac{3}{31-3}+\frac{4}{31-4}\right)^{\alpha}$$
$$=\left(\frac{89}{870}\right)^{\alpha}+5\left(\frac{59}{420}\right)^{\alpha}+\left(\frac{147}{810}\right)^{\alpha}+5\left(\frac{4}{29}\right)^{\alpha}$$
$$+16\left(\frac{143}{812}\right)^{\alpha}+\left(\frac{170}{783}\right)^{\alpha}+2\left(\frac{3}{14}\right)^{\alpha}+2\left(\frac{193}{756}\right)^{\alpha}.$$

2. The general second temperature index of $G_3$ is

$$T_2^{\alpha}(G_3)=\sum_{uv\in \hat{\mathrm{u}}(G_3)}\left(T(u)\times T(v)\right)^{\alpha}$$
$$=\left(\frac{1}{31-1}\times\frac{2}{31-2}\right)^{\alpha}+5\left(\frac{1}{31-1}\times\frac{3}{31-3}\right)^{\alpha}+\left(\frac{1}{31-1}\times\frac{4}{31-4}\right)^{\alpha}$$
$$+5\left(\frac{2}{31-2}\times\frac{2}{31-2}\right)^{\alpha}+16\left(\frac{2}{31-2}\times\frac{3}{31-3}\right)^{\alpha}+\left(\frac{2}{31-2}\times\frac{4}{31-4}\right)^{\alpha}$$
$$+2\left(\frac{3}{31-3}\times\frac{3}{31-3}\right)^{\alpha}+2\left(\frac{3}{31-3}\times\frac{4}{31-4}\right)^{\alpha}$$
$$=\left(\frac{1}{435}\right)^{\alpha}+5\left(\frac{1}{280}\right)^{\alpha}+\left(\frac{2}{405}\right)^{\alpha}+5\left(\frac{4}{841}\right)^{\alpha}$$
$$+16\left(\frac{3}{406}\right)^{\alpha}+\left(\frac{8}{783}\right)^{\alpha}+2\left(\frac{9}{784}\right)^{\alpha}+2\left(\frac{3}{189}\right)^{\alpha}.$$

3. The general temperature index of $G_3$ is

$$T_{\alpha}(G_3)=\sum_{uv\in \hat{\mathrm{u}}(G_3)}\left(T(u)^{\alpha}+T(v)^{\alpha}\right)$$
$$=\left(\left(\frac{1}{31-1}\right)^{\alpha}+\left(\frac{2}{31-2}\right)^{\alpha}\right)+5\left(\left(\frac{1}{31-1}\right)^{\alpha}+\left(\frac{3}{31-3}\right)^{\alpha}\right)+\left(\left(\frac{1}{31-1}\right)^{\alpha}+\left(\frac{4}{31-4}\right)^{\alpha}\right)$$
$$+5\left(\left(\frac{2}{31-2}\right)^{\alpha}+\left(\frac{2}{31-2}\right)^{\alpha}\right)+16\left(\left(\frac{2}{31-2}\right)^{\alpha}+\left(\frac{3}{31-3}\right)^{\alpha}\right)+\left(\left(\frac{2}{31-2}\right)^{\alpha}+\left(\frac{4}{31-4}\right)^{\alpha}\right)$$
$$+2\left(\left(\frac{3}{31-3}\right)^{\alpha}+\left(\frac{3}{31-3}\right)^{\alpha}\right)+2\left(\left(\frac{3}{31-3}\right)^{\alpha}+\left(\frac{4}{31-4}\right)^{\alpha}\right)$$
$$=7\left(\frac{1}{30}\right)^{\alpha}+28\left(\frac{2}{29}\right)^{\alpha}+27\left(\frac{3}{28}\right)^{\alpha}+4\left(\frac{4}{27}\right)^{\alpha}.$$

4. The $(\alpha, \beta)$ - temperature index of $G_3$ is

$$T_{\alpha,\beta}(G_3)=\sum_{uv\in \hat{u}(G_3)}\left(T(u)^{\alpha}T(v)^{\alpha}+T(u)^{\beta}T(v)^{\alpha}\right)$$

$$=\left(\left(\frac{1}{31-1}\right)^{\alpha}\left(\frac{2}{31-2}\right)^{\beta}+\left(\frac{1}{31-1}\right)^{\beta}\left(\frac{2}{31-2}\right)^{\alpha}\right)$$

$$+5\left(\left(\frac{1}{31-1}\right)^{\alpha}\left(\frac{3}{31-3}\right)^{\beta}+\left(\frac{1}{31-1}\right)^{\beta}\left(\frac{3}{31-3}\right)^{\alpha}\right)$$

$$+\left(\left(\frac{1}{31-1}\right)^{\alpha}\left(\frac{4}{31-4}\right)^{\beta}+\left(\frac{1}{31-1}\right)^{\beta}\left(\frac{4}{31-4}\right)^{\alpha}\right)$$

$$+5\left(\left(\frac{2}{31-2}\right)^{\alpha}\left(\frac{2}{31-2}\right)^{\beta}+\left(\frac{2}{31-2}\right)^{\beta}\left(\frac{2}{31-2}\right)^{\alpha}\right)$$

$$+16\left(\left(\frac{2}{31-2}\right)^{\alpha}\left(\frac{3}{31-3}\right)^{\beta}+\left(\frac{2}{31-2}\right)^{\beta}\left(\frac{3}{31-3}\right)^{\alpha}\right)$$

$$+\left(\left(\frac{2}{31-2}\right)^{\alpha}\left(\frac{4}{31-4}\right)^{\beta}+\left(\frac{2}{31-2}\right)^{\beta}\left(\frac{4}{31-4}\right)^{\alpha}\right)$$

$$+2\left(\left(\frac{3}{31-3}\right)^{\alpha}\left(\frac{3}{31-3}\right)^{\beta}+\left(\frac{3}{31-3}\right)^{\beta}\left(\frac{3}{31-3}\right)^{\alpha}\right)$$

$$+2\left(\left(\frac{3}{31-3}\right)^{\alpha}\left(\frac{4}{31-4}\right)^{\beta}+\left(\frac{3}{31-3}\right)^{\beta}\left(\frac{4}{31-4}\right)^{\alpha}\right)$$

$$=\left(\left(\frac{1}{30}\right)^{\alpha}\left(\frac{2}{29}\right)^{\beta}+\left(\frac{1}{30}\right)^{\beta}\left(\frac{2}{29}\right)^{\alpha}\right)+5\left(\left(\frac{1}{30}\right)^{\alpha}\left(\frac{3}{28}\right)^{\beta}+\left(\frac{1}{30}\right)^{\beta}\left(\frac{3}{28}\right)^{\alpha}\right)$$

$$+\left(\left(\frac{1}{30}\right)^{\alpha}\left(\frac{4}{2}\right)^{\beta}+\left(\frac{1}{30}\right)^{\beta}\left(\frac{4}{27}\right)^{\alpha}\right)+10\left(\frac{2}{29}\right)^{\alpha+\beta}+16\left(\left(\frac{2}{29}\right)^{\alpha}\left(\frac{3}{28}\right)^{\beta}+\left(\frac{2}{29}\right)^{\beta}\left(\frac{3}{28}\right)^{\alpha}\right)$$

$$+\left(\left(\frac{2}{29}\right)^{\alpha}\left(\frac{4}{27}\right)^{\beta}+\left(\frac{2}{29}\right)^{\beta}\left(\frac{4}{27}\right)^{\alpha}\right)+4\left(\frac{3}{28}\right)^{\alpha+\beta}+2\left(\left(\frac{3}{28}\right)^{\alpha}\left(\frac{4}{27}\right)^{\beta}+\left(\frac{3}{28}\right)^{\beta}\left(\frac{4}{27}\right)^{\alpha}\right).$$

**Corollary 2.6.** *Let $G_3$ be a molecular graph of triciferol. Then by Theorem 2.5, we have*

1. The sum connectivity temperature index

$$ST(G_3) = 80.829$$

by taking α = (- ½) in $T_1^{\alpha}(G_3)$.

2. The product connectivity temperature index

$$PT(G_3) = 421.819$$

by taking α = (- ½) in $T_2^{\alpha}(G_3)$.

3. The *F* - connectivity temperature index

$$FT(G_3) = 0.539$$

by taking α = 2 in $T_{\alpha}^{\alpha}(G_3)$.

4. Symmetric division temperature index

$$SDT(G_3) = 80.830$$

by taking α, β = 1 and – 1 in $T_{\alpha,\beta}(G_3)$.

**Theorem 2.7.** *Let $G_4$ be a molecular graph vorinostat. Then the temperature index of the vorinostat graph are given,*

1. The general first temperature index

$$T_1^{\alpha}(G_4)=\left(\frac{53}{306}\right)^{\alpha}+2\left(\frac{70}{288}\right)^{\alpha}+9\left(\frac{4}{17}\right)^{\alpha}+7\left(\frac{83}{272}\right)^{\alpha}.$$

2. The general second temperature index

$$T_2^{\alpha}(G_4)=\left(\frac{2}{306}\right)^{\alpha}+2\left(\frac{1}{96}\right)^{\alpha}+9\left(\frac{4}{289}\right)^{\alpha}+7\left(\frac{3}{136}\right)^{\alpha}.$$

3. The general temperature index

$$T_{\alpha}(G_4)=3\left(\frac{1}{18}\right)^{\alpha}+26\left(\frac{2}{17}\right)^{\alpha}+9\left(\frac{3}{16}\right)^{\alpha}.$$

4. The (*α, β*) temperature index

$$T_{\alpha,\beta}(G_4)=\left(\left(\frac{1}{18}\right)^{\alpha}\left(\frac{2}{17}\right)^{\beta}+\left(\frac{1}{18}\right)^{\beta}\left(\frac{2}{17}\right)^{\alpha}\right)+2\left(\left(\frac{1}{18}\right)^{\alpha}\left(\frac{3}{16}\right)^{\beta}+\left(\frac{1}{18}\right)^{\beta}\left(\frac{3}{16}\right)^{\alpha}\right)$$
$$+18\left(\frac{2}{17}\right)^{\alpha+\beta}+7\left(\left(\frac{2}{17}\right)^{\alpha}\left(\frac{3}{16}\right)^{\beta}+\left(\frac{2}{17}\right)^{\beta}\left(\frac{3}{16}\right)^{\alpha}\right).$$

***Proof.*** Let $G_4$ be the molecular graph of *vorinostat*, which has 19 vertices and 19 edges as shown in Figure 1d. We have the following three vertex partitions, $V_{\{1\}} = \{u \in V(G_4) \mid d(u) = 1\}$, $V_{\{2\}} = \{u \in V(G_4) \mid d(u) = 3\}$, $V_{\{3\}} = \{u \in V(G_4) \mid d(u) = 3\}$. Therefore, there are 4 edge partitions of $G_4$, which can be written as follows:

$$\mathcal{E}_{1,2} = \{uv \in \mathcal{E}(G_4) \mid d(u) = 1 \text{ and } d(v) = 2\},$$
$$\mathcal{E}_{1,3} = \{uv \in \mathcal{E}(G_4) \mid d(u) = 1 \text{ and } d(v) = 3\},$$
$$\mathcal{E}_{2,2} = \{uv \in \mathcal{E}(G_4) \mid d(u) = 2 \text{ and } d(v) = 2\},$$
$$\mathcal{E}_{2,3} = \{uv \in \mathcal{E}(G_3) \mid d(u) = 2 \text{ and } d(v) = 3\},$$

We can see that $|\mathcal{E}_{1,2}|=1$, $|\mathcal{E}_{1,3}|=2$, $\mathcal{E}_{2,2}|=9$, $|\mathcal{E}_{2,3}|=7$ from the molecular graph of $G_4$.

1. The general first temperature index of $G_4$ is

$$T_1^{\alpha}(G_4)=\sum_{uv\in \hat{\mathrm{u}}(G_4)}\left(T(u)+T(v)\right)^{\alpha}$$
$$=\left(\frac{1}{19-1}+\frac{2}{19-2}\right)^{\alpha}+2\left(\frac{1}{19-1}+\frac{3}{19-3}\right)^{\alpha}$$
$$+9\left(\frac{2}{19-2}+\frac{2}{19-2}\right)^{\alpha}+7\left(\frac{2}{19-2}+\frac{3}{19-2}\right)^{\alpha}$$

$$=\left(\frac{53}{306}\right)^{\alpha}+2\left(\frac{70}{288}\right)^{\alpha}+9\left(\frac{4}{17}\right)^{\alpha}+7\left(\frac{83}{272}\right)^{\alpha}.$$

2. The general second temperature index of $G_4$ is

$$T_2^{\alpha}(G_4)=\sum_{uv\in \hat{\text{u}}(G_4)}\left(T(u)\times T(v)\right)^{\alpha}$$

$$=\left(\frac{1}{19-1}\times\frac{2}{19-2}\right)^{\alpha}+2\left(\frac{1}{19-1}\times\frac{3}{19-3}\right)^{\alpha}$$

$$+9\left(\frac{2}{19-2}\times\frac{2}{19-2}\right)^{\alpha}+7\left(\frac{2}{19-2}\times\frac{3}{19-3}\right)^{\alpha}$$

$$=\left(\frac{2}{306}\right)^{\alpha}+2\left(\frac{1}{96}\right)^{\alpha}+9\left(\frac{4}{289}\right)^{\alpha}+7\left(\frac{3}{136}\right)^{\alpha}.$$

3. The general temperature index of $G_4$ is

$$T_{\alpha}(G_4)=\sum_{uv\in \hat{\text{u}}(G_4)}\left(T(u)^{\alpha}+T(v)^{\alpha}\right)$$

$$=\left(\left(\frac{1}{19-1}\right)^{\alpha}+\left(\frac{2}{19-2}\right)^{\alpha}\right)+2\left(\left(\frac{1}{19-1}\right)^{\alpha}+\left(\frac{3}{19-3}\right)^{\alpha}\right)$$

$$+9\left(\left(\frac{2}{19-2}\right)^{\alpha}+\left(\frac{2}{19-2}\right)^{\alpha}\right)+7\left(\left(\frac{2}{19-2}\right)^{\alpha}+\left(\frac{3}{19-3}\right)^{\alpha}\right)$$

$$=3\left(\frac{1}{18}\right)^{\alpha}+26\left(\frac{2}{17}\right)^{\alpha}+9\left(\frac{3}{16}\right)^{\alpha}.$$

4. The $(\alpha, \beta)$ - temperature index of $G_4$ is

$$T_{\alpha,\beta}(G_4)=\sum_{uv\in \hat{\text{u}}(G_4)}\left(T(u)^{\alpha}T(v)^{\alpha}+T(u)^{\beta}T(v)^{\alpha}\right)$$

$$=\left(\left(\frac{1}{19-1}\right)^{\alpha}\left(\frac{2}{19-2}\right)^{\beta}+\left(\frac{1}{19-1}\right)^{\beta}\left(\frac{2}{19-2}\right)^{\alpha}\right)$$

$$+2\left(\left(\frac{1}{19-1}\right)^{\alpha}\left(\frac{3}{19-3}\right)^{\beta}+\left(\frac{1}{19-1}\right)^{\beta}\left(\frac{3}{19-3}\right)^{\alpha}\right)$$

$$+9\left(\left(\frac{2}{19-2}\right)^{\alpha}\left(\frac{2}{19-2}\right)^{\beta}+\left(\frac{2}{19-2}\right)^{\beta}\left(\frac{2}{19-2}\right)^{\alpha}\right)$$

$$+7\left(\left(\frac{2}{19-2}\right)^{\alpha}\left(\frac{3}{19-3}\right)^{\beta}+\left(\frac{2}{19-2}\right)^{\beta}\left(\frac{3}{19-3}\right)^{\alpha}\right)$$

$$=\left(\left(\frac{1}{18}\right)^{\alpha}\left(\frac{2}{17}\right)^{\beta}+\left(\frac{1}{18}\right)^{\beta}\left(\frac{2}{17}\right)^{\alpha}\right)+2\left(\left(\frac{1}{18}\right)^{\alpha}\left(\frac{3}{16}\right)^{\beta}+\left(\frac{1}{18}\right)^{\beta}\left(\frac{3}{16}\right)^{\alpha}\right)$$
$$+18\left(\frac{2}{17}\right)^{\alpha+\beta}+7\left(\left(\frac{2}{17}\right)^{\alpha}\left(\frac{3}{16}\right)^{\beta}+\left(\frac{2}{17}\right)^{\beta}\left(\frac{3}{16}\right)^{\alpha}\right).$$

**Corollary 2.8.** *Let $G_4$ be a molecular graph of vorinostat. Then by Theorem 2.7, we have*

1. The sum connectivity temperature index

$$ST(G_4) = 37.685$$

by taking α = (- ½) in $T_1^{\alpha}(G_4)$.

2. The product connectivity temperature index

$$PT(G_4) = 155.596$$

by taking α = (- ½) in $T_2^{\alpha}(G_4)$.

3. The $F$ - connectivity temperature index

$$FT(G_4) = 0.686$$

by taking α = 2 in $T_{\alpha}^{\alpha}(G_4)$.

4. Symmetric division temperature index

$$SDT(G_4) = 43.481$$

by taking α, β = 1 and – 1 in $T_{\alpha,\beta}(G_4)$.

**Theorem 2.9.** *Let $G_5$ be a molecular graph tucidinostat. Then the temperature index of the tucidinostat graph are given,*

5. The general first temperature index

$$T_1^{\alpha}(G_5)=4\left(\frac{55}{364}\right)^{\alpha}+9\left(\frac{4}{27}\right)^{\alpha}+16\left(\frac{133}{702}\right)^{\alpha}+2\left(\frac{3}{13}\right)^{\alpha}.$$

6. The general second temperature index

$$T_2^{\alpha}(G_5)=4\left(\frac{3}{728}\right)^{\alpha}+9\left(\frac{4}{729}\right)^{\alpha}+16\left(\frac{1}{117}\right)^{\alpha}+2\left(\frac{9}{676}\right)^{\alpha}.$$

7. The general temperature index

$$T_{\alpha}(G_5)=4\left(\frac{1}{28}\right)^{\alpha}+24\left(\frac{3}{26}\right)^{\alpha}+34\left(\frac{2}{27}\right)^{\alpha}.$$

8. The ($\alpha$, $\beta$) temperature index

$$T_{\alpha,\beta}(G_5)=4\left(\left(\frac{1}{28}\right)^{\alpha}\left(\frac{3}{26}\right)^{\beta}+\left(\frac{1}{28}\right)^{\beta}\left(\frac{3}{26}\right)^{\alpha}\right)+18\left(\frac{2}{27}\right)^{\alpha+\beta}$$
$$+16\left(\left(\frac{2}{27}\right)^{\alpha}\left(\frac{3}{26}\right)^{\beta}+\left(\frac{2}{27}\right)^{\beta}\left(\frac{3}{26}\right)^{\alpha}\right)+4\left(\frac{3}{26}\right)^{\alpha+\beta}.$$

***Proof.*** Let $G_5$ be the molecular graph of *vorinostat*, which has 29 vertices and 31 edges as shown in Figure 1e. We have the following three vertex partitions, $V_{\{1\}} = \{u \in V(G_5) \mid d(u) = 1\}$, $V_{\{2\}} = \{u \in V(G_5) \mid d(u) = 2\}$, $V_{\{3\}} = \{u \in V(G_5) \mid d(u) = 3\}$. Therefore, there are 4 edge partitions of $G_5$, which can be written as follows:

$$\mathcal{E}_{1,3} = \{uv \in \mathcal{E}(G_5) \mid d(u) = 1 \text{ and } d(v) = 3\},$$
$$\mathcal{E}_{2,2} = \{uv \in \mathcal{E}(G_5) \mid d(u) = 2 \text{ and } d(v) = 2\},$$
$$\mathcal{E}_{2,3} = \{uv \in \mathcal{E}(G_5) \mid d(u) = 2 \text{ and } d(v) = 3\},$$
$$\mathcal{E}_{3,3} = \{uv \in \mathcal{E}(G_5) \mid d(u) = 3 \text{ and } d(v) = 3\},$$

We can see that $|\mathcal{E}_{1,3}|=4$, $|\mathcal{E}_{2,2}|=9$, $\mathcal{E}_{2,3}|=16$, $|\mathcal{E}_{3,3}|=2$ from the molecular graph of $G_5$.

1. The general first temperature index of $G_5$ is

$$T_1^\alpha(G_5) = \sum_{uv\in \hat{u}(G_5)} \left(T(u)+T(v)\right)^\alpha$$
$$= 4\left(\frac{1}{29-1}+\frac{3}{29-3}\right)^\alpha + 9\left(\frac{2}{29-2}+\frac{2}{29-2}\right)^\alpha$$
$$+16\left(\frac{2}{29-2}+\frac{3}{29-3}\right)^\alpha + 2\left(\frac{3}{29-3}+\frac{3}{29-3}\right)^\alpha$$
$$= 4\left(\frac{55}{364}\right)^\alpha + 9\left(\frac{4}{27}\right)^\alpha + 16\left(\frac{133}{702}\right)^\alpha + 2\left(\frac{3}{13}\right)^\alpha.$$

2. The general second temperature index of $G_5$ is

$$T_2^\alpha(G_5) = \sum_{uv\in \hat{u}(G_5)} \left(T(u)\times T(v)\right)^\alpha$$
$$= 4\left(\frac{1}{29-1}\times\frac{3}{29-3}\right)^\alpha + 9\left(\frac{2}{29-2}\times\frac{2}{29-2}\right)^\alpha$$
$$+16\left(\frac{2}{29-2}\times\frac{3}{29-3}\right)^\alpha + 2\left(\frac{3}{29-3}\times\frac{3}{29-3}\right)^\alpha$$
$$= 4\left(\frac{3}{728}\right)^\alpha + 9\left(\frac{4}{729}\right)^\alpha + 16\left(\frac{1}{117}\right)^\alpha + 2\left(\frac{9}{676}\right)^\alpha.$$

3. The general temperature index of $G_5$ is

$$T_\alpha(G_5) = \sum_{uv\in \hat{u}(G_5)} \left(T(u)^\alpha + T(v)^\alpha\right)$$
$$= 4\left(\left(\frac{1}{29-1}\right)^\alpha + \left(\frac{3}{29-3}\right)^\alpha\right) + 9\left(\left(\frac{2}{29-2}\right)^\alpha + \left(\frac{2}{29-2}\right)^\alpha\right)$$
$$+16\left(\left(\frac{2}{29-2}\right)^\alpha + \left(\frac{3}{29-3}\right)^\alpha\right) + 2\left(\left(\frac{3}{29-3}\right)^\alpha + \left(\frac{3}{29-3}\right)^\alpha\right)$$
$$= 4\left(\frac{1}{28}\right)^\alpha + 24\left(\frac{3}{26}\right)^\alpha + 34\left(\frac{2}{27}\right)^\alpha.$$

4. The ($\alpha$, $\beta$) - temperature index of $G_5$ is

$$T_{\alpha,\beta}(G_5)=\sum_{uv\in \hat{U}(G_5)}\left(T(u)^{\alpha}T(v)^{\alpha}+T(u)^{\beta}T(v)^{\alpha}\right)$$

$$=4\left(\left(\frac{1}{29-1}\right)^{\alpha}\left(\frac{3}{29-3}\right)^{\beta}+\left(\frac{1}{29-1}\right)^{\beta}\left(\frac{3}{29-3}\right)^{\alpha}\right)$$

$$+9\left(\left(\frac{2}{29-2}\right)^{\alpha}\left(\frac{2}{29-2}\right)^{\beta}+\left(\frac{2}{29-2}\right)^{\beta}\left(\frac{2}{29-2}\right)^{\alpha}\right)$$

$$+16\left(\left(\frac{2}{29-2}\right)^{\alpha}\left(\frac{3}{29-3}\right)^{\beta}+\left(\frac{2}{29-2}\right)^{\beta}\left(\frac{3}{29-3}\right)^{\alpha}\right)$$

$$+2\left(\left(\frac{3}{29-3}\right)^{\alpha}\left(\frac{3}{29-3}\right)^{\beta}+\left(\frac{3}{29-3}\right)^{\beta}\left(\frac{3}{29-3}\right)^{\alpha}\right)$$

$$=4\left(\left(\frac{1}{28}\right)^{\alpha}\left(\frac{3}{26}\right)^{\beta}+\left(\frac{1}{28}\right)^{\beta}\left(\frac{3}{26}\right)^{\alpha}\right)+18\left(\frac{2}{27}\right)^{\alpha+\beta}$$

$$+16\left(\left(\frac{2}{27}\right)^{\alpha}\left(\frac{3}{26}\right)^{\beta}+\left(\frac{2}{27}\right)^{\beta}\left(\frac{3}{26}\right)^{\alpha}\right)+4\left(\frac{3}{26}\right)^{\alpha+\beta}.$$

**Corollary 2.10.** *Let $G_5$ be a molecular graph of vorinostat. Then by Theorem 2.9, we have*

1. The sum connectivity temperature index

$$ST(G_5) = 74.595$$

by taking α = (- ½) in $T_1^{\alpha}(G_5)$.

2. The product connectivity temperature index

$$PT(G_5) = 374.211$$

by taking α = (- ½) in $T_2^{\alpha}(G_4)$.

3. The *F* - connectivity temperature index

$$FT(G_5) = 0.511$$

by taking α = 2 in $T_{\alpha}^{\alpha}(G_5)$.

4. Symmetric division temperature index

$$SDT(G_5) = 71.356$$

by taking α, β = 1 and – 1 in $T_{\alpha,\beta}(G_5)$.

# 3. Conclusion

The application of topological indices in the evaluation of QSAR antiparasitic drugs has opened up a world of possibilities. QSAR approaches have provided a number of alternatives for detecting drug targets. The creation of a novel product in pharmaceutical drug design depends on the features of the molecular structure. This study uses Topological indices to acquire data on molecular structure topology for the least amount of money and time possible. Calculating the TIs of a chemical structure is more challenging as the number of n grows. The expressions of the temperature based topological indices for a number of potential medications, including triciferol, vorinostat, tucidinostat, HDCA based CUDC-101, and CUCD-907 multi-target pharmaceuticals, are established for these drugs by examining their molecular structure and edge partition method. The boiling point and p-electronic energy of the molecules may be predicted using the vertex-based temperature indices. Additionally, this will be helpful when correlated with docking score and binding affinity.

# 4. Conflict of interest

All authors declare that they have no conflicts of interest.

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