

Article

Quantitative Structure–Property Relationship Analysis in Molecular Graphs of Some Anticancer Drugs with Temperature Indices Approach

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Abstract: The most important application of anticancer drugs in various forms (alkylating agents, hormones agents, and antimetabolites) is the treatment of malignant diseases. Topological indices are widely used in the field of chemical and medical sciences, especially in studying the chemical, biological, clinical, and therapeutic aspects of drugs. In this article, the temperature indices in anticancer drugs molecular graphs such as Carmustine, Convolutamine F, Raloxifene, Tambjamine K, and Pterocellin B were calculated and then analyzed based on physical and chemical properties. The analysis was performed by identifying the best regression models based on temperature indices for six physical and chemical features of anticancer drugs. The results indicated that temperature indices were essential topological indices that predict the properties of anticancer drugs, such as boiling point, flash point, enthalpy, molar refractivity, molar volume, and polarizability. It was also observed that the *r* value of the regression model was more than 0.6, and the *p* value was less than 0.05.

Keywords: temperature indices; molecular graph; anticancer drugs; QSPR analysis**MSC:** 05C92

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1. Introduction

The rapid growth of abnormal cells in the human body causes cancer. The drugs used to treat cancer usually include alkylates and metabolites. Making and researching primary drugs for cancer treatment are of interest to doctors, but the drug discovery process, from identifying novel chemical entities to establishing regulatory approval is complex, costly, and time consuming. Traditional methods often suffer from inefficiencies in compound synthesis and biological screening, which prompts the scientific community to seek faster and more efficient ways to discover lead compounds.

Graph theory of chemistry is an interdisciplinary science that is used to study molecular structures and create correlations between different activities, properties, and events.

The molecular graph is related to the structural formula of a chemical compound, and the vertices and edges of the graph correspond to the atoms and chemical bonds of the compound, respectively. Chemical graph theory has provided creative and unique tools for the study of chemical structures, among which topological indices can be mentioned.

The topological index is used as the descriptor to study the structure and some properties of a molecular graph and is expressed as a real number [1–3]. The scarcity and expensiveness of anticancer drugs and the production of more effective drugs lead to studies on drug structures, especially using topological indices.

Many studies were conducted on molecular graphs, especially nanotubes, and pharmaceutical structures, using topological indices [4–10]. Lokesha et al. studied the temperature

indices of certain Archimedean Lattices [11]. Adnan et al. investigated the degree-based indices on some anticancer drugs and found a high correlation between the indices and the physical–chemical properties of the drugs [12]. Hayat et al. used temperature indices to predict the physicochemical properties of polycyclic aromatic hydrocarbons and benzenoid hydrocarbons as well as investigate the π -electron energy of benzenoid hydrocarbons [13–15].

One of the most important methods of studying the relationship between the physical–chemical properties and topological indices of a material is the application of QSPR (quantitative structure–property relationship analysis) models. In the QSPR model, the curve regression method is used as a tool to analyze the relationship between physical and chemical properties and topological indices. Various QSAR studies using topological indices have been performed on multiple drug structures [16,17].

In this article, different temperature indices are investigated on some anticancer drugs to be used for researchers to understand the physical characteristics and chemical reactions related to them.

2. Preliminaries

In the molecular graph G , the degree of arbitrary vertex s is denoted by d_s , and the connection of two vertices z and w is expressed by $zw \in E(G)$.

Definition 1. The temperature of a vertex $s \in E(G)$ is defined as follows [18]:

$$T_s = \frac{d_s}{n - d_s}, \quad (1)$$

where n is the number of graph vertices.

Using vertex temperature, temperature indices were introduced (see Table 1) [19].

Table 1. Temperature-based topological indices of G .

Temperature Index Name	Definition
(a, b)-temperature index [19]	$T_{a,b}(G) = \sum_{rs \in E(G)} (T_r^a T_s^b + T_r^b T_s^a),$
Sum connectivity temperature index [19]	$ST(G) = \sum_{rs \in E(G)} \frac{1}{\sqrt{T_r + T_s}}$
Product connectivity temperature index [19]	$PT(G) = \sum_{rs \in E(G)} \frac{1}{\sqrt{T_r \cdot T_s}}$
Symmetric division temperature index [19]	$SDT(G) = \sum_{rs \in E(G)} \left(\frac{T_r}{T_s} + \frac{T_s}{T_r} \right)$
Temperature Sombor index [20]	$TSO(G) = \sum_{rs \in E(G)} \sqrt{T_r^2 + T_s^2}$

Recently, studies have been conducted on temperature indices [21,22].

3. Results

In this section, after introducing the molecular graphs of Carmustine, Convolutamine F, Raloxifene, Tambjamine K, Pterocellin B and obtaining the temperature of the vertices, the temperature indices are calculated.

Figure 1 shows the molecular graph of Carmustine.

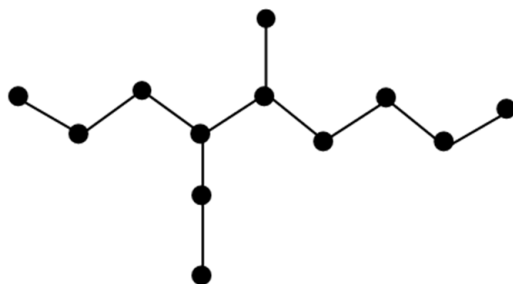


Figure 1. Molecular graph of Carmustine.

The molecular graph of Carmustine is represented by C . There are five types of edges in C as follows:

$$\begin{aligned} E_1 &= \left\{ rs \in E(C) \mid T_r = \frac{1}{5}, T_s = \frac{1}{11} \right\}, & E_2 &= \left\{ rs \in E(C) \mid T_r = \frac{1}{11}, T_s = \frac{1}{3} \right\}, \\ E_3 &= \left\{ rs \in E(C) \mid T_r = \frac{1}{5}, T_s = \frac{1}{5} \right\}, & E_4 &= \left\{ rs \in E(C) \mid T_r = \frac{1}{5}, T_s = \frac{1}{3} \right\}, \\ E_5 &= \left\{ rs \in E(C) \mid T_r = \frac{1}{3}, T_s = \frac{1}{3} \right\}. \end{aligned}$$

The study of the edges in C is shown in Table 2.

Table 2. Edge partition of C .

$(T_r, T_s) \setminus rs \in E(C)$	Number of Edges
$(\frac{1}{5}, \frac{1}{11})$	3
$(\frac{1}{11}, \frac{1}{3})$	1
$(\frac{1}{5}, \frac{1}{5})$	3
$(\frac{1}{5}, \frac{1}{3})$	3
$(\frac{1}{3}, \frac{1}{3})$	1

Using Tables 1 and 2, we can calculate the following topological indices for C :

- $T_{a,b}(G)$ index;
- $ST(G)$ index;
- $PT(G)$ index;
- $SDT(G)$ index;
- $TSO(G)$ index.

Theorem 1. Assume that C is the molecular graph of Carmustine. Then, the temperature indices of C are computed as follows:

$$\begin{aligned} 1. T_{a,b}(C) &= 3\left(\left(\frac{1}{11}\right)^a \left(\frac{1}{5}\right)^b + \left(\frac{1}{11}\right)^b \left(\frac{1}{5}\right)^a\right) + \left(\left(\frac{1}{11}\right)^a \left(\frac{1}{3}\right)^b + \left(\frac{1}{11}\right)^b \left(\frac{1}{3}\right)^a\right) + 3\left(\left(\frac{1}{5}\right)^a \left(\frac{1}{5}\right)^b + \left(\frac{1}{5}\right)^b \left(\frac{1}{5}\right)^a\right) \\ &\quad + 3\left(\left(\frac{1}{5}\right)^a \left(\frac{1}{3}\right)^b + \left(\frac{1}{5}\right)^b \left(\frac{1}{3}\right)^a\right) + 1\left(\left(\frac{1}{3}\right)^a \left(\frac{1}{3}\right)^b + \left(\frac{1}{3}\right)^b \left(\frac{1}{3}\right)^a\right), \\ 2. ST(C) &= 17.17, \\ 3. PT(C) &= 57.61, \\ 4. SDT(C) &= 26.70, \\ 5. TSO(C) &= 3.49. \end{aligned}$$

Proof of Theorem 1. By using the relations in Table 2 and placing them in Table 1, we have the following equations:

$$\begin{aligned}
1. T_{a,b}(C) &= \sum_{rs \in E(G)} (T_r^a T_s^b + T_r^b T_s^a) \\
&= \sum_{rs \in E_1} (T_r^a T_s^b + T_r^b T_s^a) + \sum_{rs \in E_2} (T_r^a T_s^b + T_r^b T_s^a) + \sum_{rs \in E_3} (T_r^a T_s^b + T_r^b T_s^a) \\
&\quad + \sum_{rs \in E_4} (T_r^a T_s^b + T_r^b T_s^a) + \sum_{rs \in E_5} (T_r^a T_s^b + T_r^b T_s^a) \\
&= 3\left(\left(\frac{1}{11}\right)^a \left(\frac{1}{5}\right)^b + \left(\frac{1}{11}\right)^b \left(\frac{1}{5}\right)^a\right) + \left(\left(\frac{1}{11}\right)^a \left(\frac{1}{3}\right)^b + \left(\frac{1}{11}\right)^b \left(\frac{1}{3}\right)^a\right) + 3\left(\left(\frac{1}{5}\right)^a \left(\frac{1}{5}\right)^b + \left(\frac{1}{5}\right)^b \left(\frac{1}{5}\right)^a\right) \\
&\quad + 3\left(\left(\frac{1}{5}\right)^a \left(\frac{1}{3}\right)^b + \left(\frac{1}{5}\right)^b \left(\frac{1}{3}\right)^a\right) + 1\left(\left(\frac{1}{3}\right)^a \left(\frac{1}{3}\right)^b + \left(\frac{1}{3}\right)^b \left(\frac{1}{3}\right)^a\right), \\
2. ST(C) &= \sum_{rs \in E(G)} \frac{1}{\sqrt{T_r + T_s}} = 3\left(\frac{1}{\sqrt{\frac{1}{11} + \frac{1}{5}}}\right) + 1\left(\frac{1}{\sqrt{\frac{1}{11} + \frac{1}{3}}}\right) + 3\left(\frac{1}{\sqrt{\frac{1}{5} + \frac{1}{5}}}\right) + 3\left(\frac{1}{\sqrt{\frac{1}{5} + \frac{1}{3}}}\right) + 1\left(\frac{1}{\sqrt{\frac{1}{3} + \frac{1}{3}}}\right) \\
&= 17.17, \\
3. PT(C) &= \sum_{rs \in E(G)} \frac{1}{\sqrt{T_r \cdot T_s}} = 3\left(\frac{1}{\sqrt{\frac{1}{11} \cdot \frac{1}{5}}}\right) + 1\left(\frac{1}{\sqrt{\frac{1}{11} \cdot \frac{1}{3}}}\right) + 3\left(\frac{1}{\sqrt{\frac{1}{5} \cdot \frac{1}{5}}}\right) + 3\left(\frac{1}{\sqrt{\frac{1}{5} \cdot \frac{1}{3}}}\right) + 1\left(\frac{1}{\sqrt{\frac{1}{3} \cdot \frac{1}{3}}}\right) = 57.61, \\
4. SDT(C) &= \sum_{rs \in E(G)} \left(\frac{T_s}{T_r} + \frac{T_r}{T_s}\right) = 3\left(\frac{\frac{1}{11}}{\frac{1}{5}} + \frac{\frac{1}{5}}{\frac{1}{11}}\right) + 1\left(\frac{\frac{1}{11}}{\frac{1}{3}} + \frac{\frac{1}{3}}{\frac{1}{11}}\right) + 3\left(\frac{\frac{1}{5}}{\frac{1}{5}} + \frac{\frac{1}{5}}{\frac{1}{5}}\right) + 3\left(\frac{\frac{1}{5}}{\frac{1}{3}} + \frac{\frac{1}{3}}{\frac{1}{5}}\right) + 1\left(\frac{\frac{1}{3}}{\frac{1}{3}} + \frac{\frac{1}{3}}{\frac{1}{3}}\right) \\
&= 26.70, \\
5. TSO(C) &= \sum_{rs \in E(G)} \sqrt{T_r^2 + T_s^2} = 3\left(\sqrt{\left(\frac{1}{11}\right)^2 + \left(\frac{1}{5}\right)^2}\right) + 1\left(\sqrt{\left(\frac{1}{11}\right)^2 + \left(\frac{1}{3}\right)^2}\right) + 3\left(\sqrt{\left(\frac{1}{5}\right)^2 + \left(\frac{1}{5}\right)^2}\right) \\
&\quad + 3\left(\sqrt{\left(\frac{1}{5}\right)^2 + \left(\frac{1}{3}\right)^2}\right) + 1\left(\sqrt{\left(\frac{1}{3}\right)^2 + \left(\frac{1}{3}\right)^2}\right) = 3.49.
\end{aligned}$$

□

The molecular graph of Raloxifene (Figure 2) is represented by R . There are four types of edges in R as follows:

$$\begin{aligned}
E'_1 &= \left\{ rs \in E(R) \mid T_r = \frac{1}{33}, T_s = \frac{3}{31} \right\}, & E'_2 &= \left\{ rs \in E(R) \mid T_r = \frac{1}{16}, T_s = \frac{1}{16} \right\}, \\
E'_3 &= \left\{ rs \in E(R) \mid T_r = \frac{1}{16}, T_s = \frac{3}{31} \right\}, & E'_4 &= \left\{ rs \in E(R) \mid T_r = \frac{3}{31}, T_s = \frac{3}{31} \right\}.
\end{aligned}$$

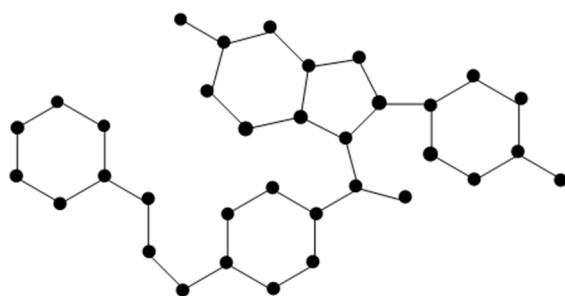


Figure 2. Molecular of Raloxifene.

The study of the edges in R is shown in Table 3.

Table 3. Edge partition of R .

$(T_r, T_s) \setminus rs \in E(R)$	Number of Edges
$\left(\frac{1}{33}, \frac{3}{31}\right)$	3
$\left(\frac{1}{16}, \frac{1}{16}\right)$	11
$\left(\frac{1}{16}, \frac{3}{31}\right)$	18
$\left(\frac{3}{31}, \frac{3}{31}\right)$	6

Theorem 2. Assume that R is the molecular graph of Raloxifene. Then, the temperature indices of R are computed as follows:

$$\begin{aligned} 1. T_{a,b}(R) &= 3\left(\left(\frac{1}{33}\right)^a \left(\frac{3}{31}\right)^b + \left(\frac{1}{33}\right)^b \left(\frac{3}{31}\right)^a\right) + 11\left(\left(\frac{1}{16}\right)^a \left(\frac{1}{16}\right)^b + \left(\frac{1}{16}\right)^b \left(\frac{1}{16}\right)^a\right) \\ &\quad + 18\left(\left(\frac{1}{16}\right)^a \left(\frac{3}{31}\right)^b + \left(\frac{1}{16}\right)^b \left(\frac{3}{31}\right)^a\right) + 6\left(\left(\frac{3}{31}\right)^a \left(\frac{3}{31}\right)^b + \left(\frac{3}{31}\right)^b \left(\frac{3}{31}\right)^a\right), \\ 2. ST(R) &= 98.27, \\ 3. PT(R) &= 524.85, \\ 4. SDT(R) &= 84.02, \\ 5. TSO(R) &= 4.17. \end{aligned}$$

Proof of Theorem 2. By using the relations in Table 3 and placing them in Table 1, the proof is complete. $\square$

The molecular graph of Tambjamine K (Figure 3) is represented by T . There are five types of edges in T as follows:

$$\begin{aligned} E''_1 &= \left\{ rs \in E(T) \mid T_r = \frac{1}{18}, T_s = \frac{2}{17} \right\}, \quad E''_2 = \left\{ rs \in E(T) \mid T_r = \frac{1}{18}, T_s = \frac{3}{16} \right\}, \\ E''_3 &= \left\{ rs \in E(T) \mid T_r = \frac{2}{17}, T_s = \frac{2}{17} \right\}, \quad E''_4 = \left\{ rs \in E(T) \mid T_r = \frac{2}{17}, T_s = \frac{3}{16} \right\}, \\ E''_5 &= \left\{ rs \in E(T) \mid T_r = \frac{3}{16}, T_s = \frac{3}{16} \right\}. \end{aligned}$$

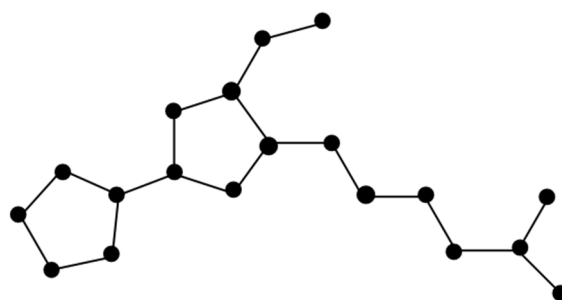


Figure 3. Molecular of Tambjamine K.

The study of the edges in T is shown in Table 4.

Table 4. Edge partition of T .

$(T_r, T_s) \mid rs \in E(T)$	Number of Edges
$\left(\frac{1}{18}, \frac{2}{17}\right)$	1
$\left(\frac{1}{18}, \frac{3}{16}\right)$	2
$\left(\frac{2}{17}, \frac{2}{17}\right)$	6
$\left(\frac{2}{17}, \frac{3}{16}\right)$	9
$\left(\frac{3}{16}, \frac{3}{16}\right)$	2

Theorem 3. Assume that T is the molecular graph of Tambjamine K. Then, the temperature indices of T are computed as follows:

$$\begin{aligned} 1. T_{a,b}(T) &= \left(\left(\frac{1}{18}\right)^a \left(\frac{2}{17}\right)^b + \left(\frac{1}{18}\right)^b \left(\frac{2}{17}\right)^a\right) + 2\left(\left(\frac{1}{18}\right)^a \left(\frac{3}{16}\right)^b + \left(\frac{1}{18}\right)^b \left(\frac{3}{16}\right)^a\right) \\ &\quad + 6\left(\left(\frac{2}{17}\right)^a \left(\frac{2}{17}\right)^b + \left(\frac{2}{17}\right)^b \left(\frac{2}{17}\right)^a\right) + 9\left(\left(\frac{2}{17}\right)^a \left(\frac{3}{16}\right)^b + \left(\frac{2}{17}\right)^b \left(\frac{3}{16}\right)^a\right) \\ &\quad + 2\left(\left(\frac{3}{16}\right)^a \left(\frac{3}{16}\right)^b + \left(\frac{3}{16}\right)^b \left(\frac{3}{16}\right)^a\right), \\ 2. ST(T) &= 38.39, \\ 3. PT(T) &= 154.23, \\ 4. SDT(T) &= 45.92, \\ 5. TSO(T) &= 4.04. \end{aligned}$$

Proof of Theorem 3. By using the relations in Table 4 and placing them in Table 1, the proof is complete. $\square$

The molecular graph of Pterocellin B (Figure 4) is represented by P . There are five types of edges in P as follows:

$$\begin{aligned}\bar{E}_1 &= \left\{ rs \in E(P) \mid T_r = \frac{1}{23}, T_s = \frac{2}{22} \right\}, & \bar{E}_2 &= \left\{ rs \in E(P) \mid T_r = \frac{1}{23}, T_s = \frac{3}{21} \right\}, \\ \bar{E}_3 &= \left\{ rs \in E(P) \mid T_r = \frac{2}{22}, T_s = \frac{2}{22} \right\}, & \bar{E}_4 &= \left\{ rs \in E(P) \mid T_r = \frac{2}{22}, T_s = \frac{3}{21} \right\}, \\ \bar{E}_5 &= \left\{ rs \in E(P) \mid T_r = \frac{3}{21}, T_s = \frac{3}{21} \right\}.\end{aligned}$$

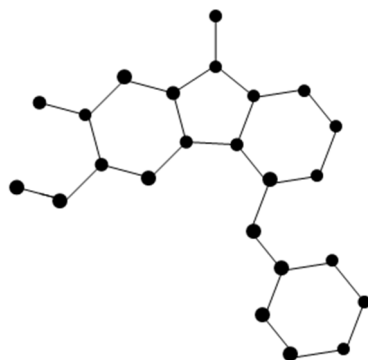


Figure 4. Molecular of Pterocellin B.

The study of the edges in P is shown in Table 5.

Table 5. Edge partition of P .

$(T_r, T_s) \setminus rs \in E(P)$	Number of Edges
$(\frac{1}{23}, \frac{2}{22})$	1
$(\frac{1}{23}, \frac{3}{21})$	2
$(\frac{2}{22}, \frac{2}{22})$	6
$(\frac{2}{22}, \frac{3}{21})$	12
$(\frac{3}{21}, \frac{3}{21})$	5

Theorem 4. Assume that P is the molecular graph of Pterocellin B. Then, the temperature indices of P are computed as follows:

$$\begin{aligned}1. T_{a,b}(P) &= ((\frac{1}{23})^a (\frac{2}{22})^b + (\frac{1}{23})^b (\frac{2}{22})^a) + 2((\frac{1}{23})^a (\frac{3}{21})^b + (\frac{1}{23})^b (\frac{3}{21})^a) + 6((\frac{2}{22})^a (\frac{2}{22})^b \\ &\quad + (\frac{2}{22})^b (\frac{2}{22})^a) + 12((\frac{2}{22})^a (\frac{3}{21})^b + (\frac{2}{22})^b (\frac{3}{21})^a) + 5((\frac{3}{21})^a (\frac{3}{21})^b + (\frac{3}{21})^b (\frac{3}{21})^a), \\ 2. ST(P) &= 55.61, \\ 3. PT(P) &= 247.58, \\ 4. SDT(P) &= 58.24, \\ 5. TSO(P) &= 4.21.\end{aligned}$$

Proof of Theorem 4. By using the relations in Table 5 and placing them in Table 1, the proof is complete. $\square$

The molecular graph of Convolutamine F (Figure 5) is represented by F . There are five types of edges in F as follows:

$$\begin{aligned}\tilde{E}_1 &= \left\{ rs \in E(F) \mid T_r = \frac{1}{14}, T_s = \frac{2}{13} \right\}, & \tilde{E}_2 &= \left\{ rs \in E(F) \mid T_r = \frac{1}{14}, T_s = \frac{3}{12} \right\}, \\ \tilde{E}_3 &= \left\{ rs \in E(F) \mid T_r = \frac{2}{13}, T_s = \frac{2}{13} \right\}, & \tilde{E}_4 &= \left\{ rs \in E(F) \mid T_r = \frac{2}{13}, T_s = \frac{3}{13} \right\}, \\ \tilde{E}_5 &= \left\{ rs \in E(F) \mid T_r = \frac{3}{13}, T_s = \frac{3}{13} \right\}.\end{aligned}$$

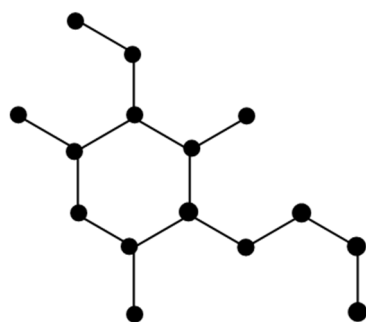


Figure 5. Molecular of Convolutamine F.

The study of the edges in F is shown in Table 6.

Table 6. Edge partition of F .

$(T_r, T_s) \setminus rs \in E(F)$	Number of Edges
$(\frac{1}{14}, \frac{2}{13})$	2
$(\frac{1}{14}, \frac{3}{12})$	1
$(\frac{2}{13}, \frac{2}{13})$	2
$(\frac{2}{13}, \frac{3}{13})$	4
$(\frac{3}{13}, \frac{3}{13})$	4

Theorem 5. Assume that F is the molecular graph of Convolutamine F. Then, the temperature indices of F are computed as follows:

$$\begin{aligned}
 1. T_{a,b}(F) &= 2((\frac{1}{14})^a (\frac{2}{13})^b + (\frac{1}{14})^b (\frac{2}{13})^a) + ((\frac{1}{14})^a (\frac{3}{12})^b + (\frac{1}{14})^b (\frac{3}{12})^a) \\
 &\quad + 2((\frac{2}{13})^a (\frac{2}{13})^b + (\frac{2}{13})^b (\frac{2}{13})^a) + 4((\frac{2}{13})^a (\frac{3}{13})^b + (\frac{2}{13})^b (\frac{3}{13})^a) \\
 &\quad + 4((\frac{3}{13})^a (\frac{3}{13})^b + (\frac{3}{13})^b (\frac{3}{13})^a), \\
 2. ST(F) &= 21.92, \\
 3. PT(F) &= 78.12, \\
 4. SDT(F) &= 29.69, \\
 5. TSO(F) &= 3.45.
 \end{aligned}$$

Proof of Theorem 5. By using the relations in Table 6 and placing them in Table 1, the proof is complete. $\square$

4. Temperature Indices and QSPR

Here, we have four topological indices based on temperature indices such as PT (G), ST (G), SDT (G), and TSO (G) to model five representative physical properties (BP, EN, FP, MR, MV, and PO) with five anticancer drugs: Carmustine, Convolutamine F, Raloxifene, Tambjamine K, and Pterocellin B. The values of these properties are taken from ChemSpider (Table 7). Topological indices based on the above degree and experimental values for the physical and chemical properties of five anticancer drugs are shown in Table 8, respectively. From the data in Table 9, it is clear that all data values are normally distributed. Therefore, a regression model is used for data acceptance and analysis.

The results of Theorems 1–5 are shown in Table 8.

Table 7. Physical properties of drugs used for anticancer drugs.

Drugs	BP	EN	FP	MR	MV	PO
Carmustine	309.60	63.80	141.00	46.60	146.40	18.50
Convolutamine F	728.20	110.10	394.20	136.60	367.30	54.10
Raloxifene	391.70	64.10	190.70	76.60	235.10	30.40
Tambjamine K	521.60	79.50	269.20	87.40	228.30	34.70
Pterocellin B	387.70	63.70	188.30	73.80	220.10	29.20

Table 8. Temperature indices of drugs used for anticancer drugs.

Drugs	PT (G)	ST (G)	SDT (G)	TSO (G)
Carmustine	57.61211	17.17352836	26.7030303	3.490705977
Convolutamine F	78.12000	21.92083073	29.68864469	3.449213296
Raloxifene	524.84617	98.26893994	84.01600684	4.171286646
Tambjamine K	154.23000	38.38737911	45.9232707	4.041993485
Pterocellin B	236.15000	55.60580345	58.24280068	4.212925884

Table 9. Correlation coefficients of physical properties of drugs.

Drugs	BP	EN	FP	MR	MV	PO
PT (G)	0.983	0.983	0.983	0.966	0.941	0.967
ST (G)	0.984	0.971	0.984	0.966	0.936	0.967
SDT (G)	0.959	0.938	0.959	0.974	0.969	0.975
TSO (G)	0.671	0.578	0.670	0.618	0.548	0.621

The significance of bold numbers denotes the highest correlation value.

Regression Models

In this section, the analysis is conducted using the temperature indices calculated in Section 3.

The linear regression model is considered as follows:

$$P = A + B (TI), \quad (2)$$

where P is the anticancer drug property, A is a constant, B is the regression coefficient, and TI represents the topological index. This capability was calculated using SPSS software for six specific characteristics and four topological indices of five anticancer drugs.

Using equation (1), the different linear models for temperature indices are as follows.

Product connectivity temperature index [PT (G)]

$$BP = 288.656 + 0.852[PT (G)]$$

$$EN = 54.315 + 0.104[PT (G)]$$

$$FP = 128.361 + 0.515[PT (G)]$$

$$MR = 48.899 + 0.168[PT (G)]$$

$$MV = 156.065 + 0.397[PT (G)]$$

$$PO = 19.405 + 0.066[PT (G)]$$

Sum connectivity temperature index [ST (G)]

$$BP = 240.117 + 4.948[ST (G)]$$

$$EN = 48.764 + 0.597[ST (G)]$$

$$FP = 99.006 + 2.992[ST (G)]$$

$$MR = 39.399 + 0.974[ST (G)]$$

$$MV = 134.146 + 2.284[ST (G)]$$

$$PO = 15.641 + 0.386[ST (G)]$$

Symmetric division temperature index [SDT (G)]

$$BP = 166.496 + 6.624[SDT (G)]$$

$$EN = 40.170 + 0.793[SDT (G)]$$

$$FP = 54.473 + 4.007[SDT (G)]$$

$$MR = 22.859 + 1.349[SDT (G)]$$

$$MV = 91.371 + 3.256[SDT (G)]$$

$$PO = 9.097 + 0.534[SDT (G)]$$

Temperature Somber index [TSO (G)]

No topological index displays a satisfactory correlation with TSO (G).

The boiling point (BP) is the temperature at which the addition of heat leads to the conversion of a liquid into its vapor without increasing the temperature. The enthalpy (EN) of a system is equal to the internal energy of the system plus the product of pressure and volume. The flash point (FP) is the lowest temperature at which sufficient flammable vapor is present to support ignition when an ignition source is applied. Molar refractivity (MR) is a measure of the total polarizability of one mole of a substance. The molar volume (MV) of a substance is the ratio of the volume of a substance to the amount of the substance at a given temperature and pressure. Polarizability (PO) usually refers to the tendency of a material in an electric field to acquire a proportional electric dipole moment. The physical properties of drugs used for anticancer drugs are shown in Table 7.

5. Conclusions

Table 9 and the graphs in Figure 6 indicate the correlated values of the physicochemical properties of anticancer drugs with the defined temperature indices. It can be seen that the index ST (G) = 0.984 shows a higher positive and significant correlation with boiling point (BP), and also ST (G) = 0.984 shows a more positive correlation with flash point (FP) than the others. In the case of enthalpy, PT (G) shows the highest correlation value, i.e., 0.983. The SDT (G) index with molar refractivity (MR), molar volume (MV) and polarizability (PO) provides the highest positive correlation with values of 0.974, 0.974 and 0.975 for the physical and chemical properties, respectively.

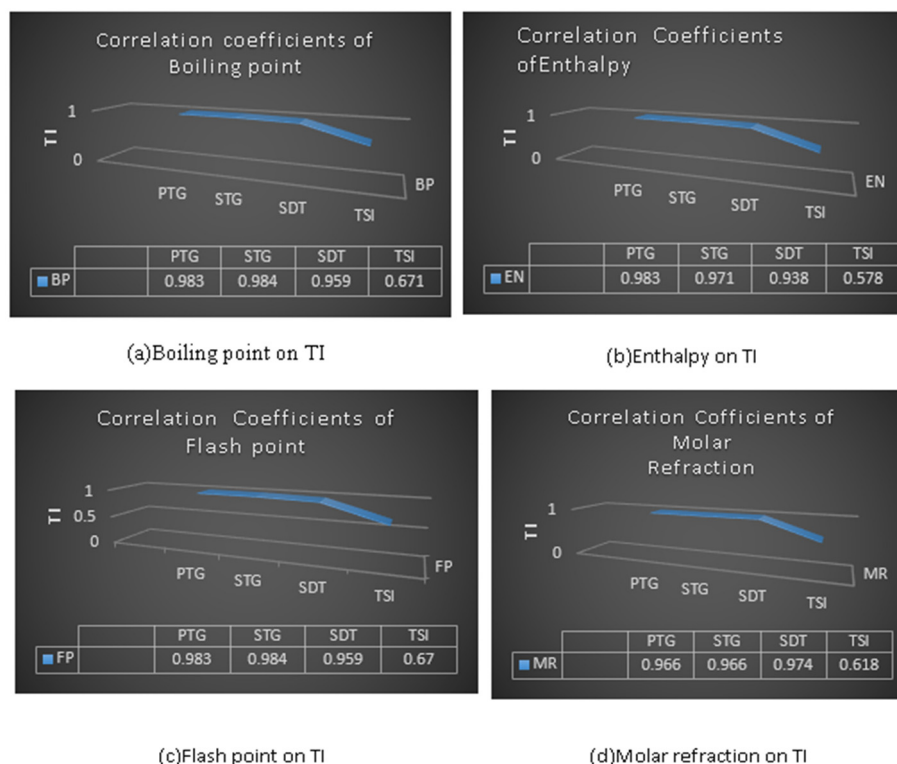


Figure 6. Cont.

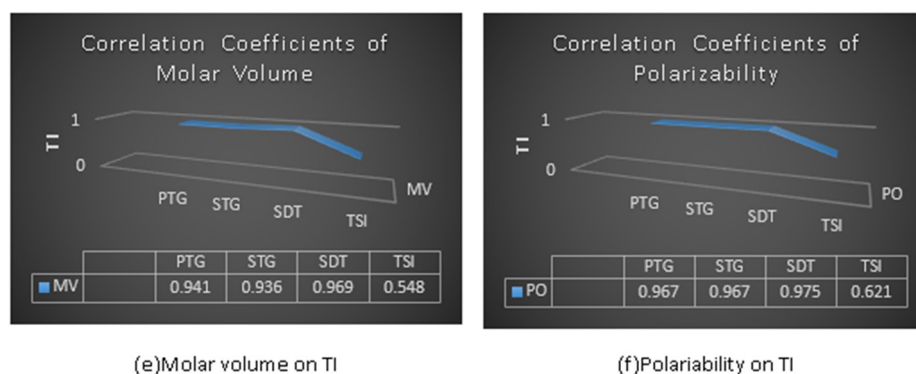


Figure 6. Physicochemical properties with topological indices.

A positive correlation is observed between the physical and chemical properties of anticancer drugs and temperature indices. Tables 10–12 show the regression model of various physicochemical properties. The results show that the regression model value r is more than 0.6, and the p value is less than 0.05. The most reliable predictors for linear regression equations are the min criterion (SE), max (R^2) and max (F). Hence, it can be concluded that all the physicochemical properties are highly significant. This topic shows the potential importance of these topological indicators in the QSPR analysis of anticancer drugs, and the drawn regression line is visible. The results of this study can be used in the production, development, and improvement of more effective anticancer drugs. The method of this article can be used to investigate other pharmaceutical structures as well.

Table 10. Statistical parameters for the linear QSPR model for PT (G).

Physical Properties	N	A	b	R	R ²	SE	F	P	Indicator
BP	5	288.656	0.852	0.983	0.966	35.2010	84.108	0.003	significant
EN	5	54.315	0.104	0.983	0.966	4.27066	85.632	0.003	significant
FP	5	128.361	0.515	0.983	0.966	21.2897	84.102	0.003	significant
MR	5	48.899	0.168	0.966	0.934	9.78020	42.328	0.007	significant
MV	5	156.065	0.397	0.941	0.885	31.29009	23.067	0.017	significant
PO	5	19.405	0.066	0.967	0.935	3.84476	42.922	0.007	significant

The bold numbers denote the highest correlation value.

Table 11. Statistical parameters for the linear QSPR model for ST (G).

Physical Properties	N	A	b	R	R ²	SE	F	P	Indicator
BP	5	240.117	4.948	0.984	0.968	33.7133	91.966	0.002	significant
EN	5	48.764	0.597	0.971	0.942	5.59077	48.717	0.006	significant
FP	5	99.006	2.992	0.984	0.968	20.3959	91.904	0.002	significant
MR	5	39.399	0.974	0.966	0.934	9.78322	42.299	0.007	significant
MV	5	134.146	2.289	0.936	0.876	32.4480	21.240	0.01	significant
PO	5	15.641	0.386	0.967	0.935	3.83327	43.198	0.007	significant

The bold numbers denote the highest correlation value.

Table 12. Statistical parameters for the linear QSPR model for SDT (G).

Physical Properties	N	A	b	R	R ²	SE	F	P	Indicator
BP	5	166.496	6.624	0.959	0.920	53.7884	34.307	0.01	significant
EN	5	40.170	0.793	0.938	0.880	8.03429	22.043	0.018	significant
FP	5	54.473	4.007	0.959	0.920	32.5155	34.341	0.01	significant
MR	5	22.859	1.349	0.974	0.949	8.5775	55.929	0.005	significant
MV	5	91.371	3.256	0.969	0.939	22.6902	46.571	0.006	significant
PO	5	9.097	0.534	0.975	0.939	3.3647	56.957	0.005	significant

The bold numbers denote the highest correlation value.

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