Degree-based topological indices on anticancer drugs with QSPR analysis

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Abstract

From last two to three decades, the world is facing the threat of finding treatment for Cancer. This disease is striking almost ten million people every year throughout the world. Anticancer drugs are those which are used to cure malignant disease i.e. Cancer. These anticancer drugs are available in different forms including alkalyting agents, hormones and anti metabolites. Various examinations reveals that, there will be a adjacent relationship between the characteristics of alkanes and the anticancer drugs viz. Boiling point, melting point, enthalpy etc. with their chemical structures. In this proposed work, various topological indices are defined on some anticancer drugs to help the researchers to know the physical characteristics and chemical reaction associated with them. We also discuss the QSPR analysis of thirteen degree based topological indices. Further, we showcase that the characteristics have good correlation with physico-chemical characteristics of anticancer drugs.

1. Introduction and terminologies

Cancer is the rapid growth of abnormal cells in the human body. Carcinogens are the substances that causes cancer. A carcinogen is a chemical substance with certain molecules in tobacco smoke. It has a potential to spread to other parts of the body. Some of the symptoms of this disease includes lump, abnormal bleeding, prolonger cough, weight loss etc. Main causes for this malignant disease are chewing tobacco, obesity, bad diet, laziness, more intake of alcohol. This dangerous disease can be cured by several treatments like surgery, radiotherapy, chemotherapy, hormone therapy, targeted therapy and more. Anticancer drugs are those which are used to cure the disease so called cancer, which includes alkylates and metabolites. The chemical graph theory is a discipline of mathematical chemistry that deals with the chemical graphs which shows chemical system. The chemical graph theory offers defining topological indices on anticancer drugs. In this work, several drugs are taken and using the degree based calculations, few topological indices are defined on various anticancer drugs to determine physical characteristics and chemical reactions associated with them [1,2,3].

Topological indices are the important attributes to analyse the physico-chemical characteristics of chemical compound structures. There are five different types of topological indices: Degree, distance, eigenvalue, matching and mixed. In this work degree based topological indices are stated on anticancer drugs. Generally, the chemical compound is represented as a graph where the elements denote vertices and the bonds connecting them denote edges. In a similar fashion, these anticancer drugs under this study are considered as chemical compounds and the said topological indices are defined. Graph theory offers some tools like QSAR, QSPR and QSTR where chemists or pharmacists use these data for further research work.

In this work, further we discuss QSPR analysis of said topological indices. We also show that the characteristics obtained are highly correlated with the characteristics of anticancer drugs using linear regression [4,5,6,7,8,9].

In theoretical chemistry drugs are represented as molecular graphs where vertex represents an atom and each edge represents link between the two atoms. Consider G (V, E) be a molecular graph with vertex and edge set respectively. The graphs considered are simple graphs with no cycle formation and multiple edges [4,10,11,12].

Definition 1.1. Estrada et al. in [13] proposed degree-based topological index ABC and defined as

\[ \text{ABC}(G) = \sum_{e=uv \in E(G)} \sqrt{d_u + d_v - 2 \over d_u d_v} \]

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Definition 1.2. Ghorbani et al. in [14] proposed ABC4 index and can be stated as,

\[ ABC_4(G) = \sum_{e=uv \in G} \sqrt{s_u + s_v - \frac{2}{s_u s_v}} \]

Definition 1.3. The Randic index [15] proposed by Milan Randic and can be stated as

\[ \chi(G) = \sum_{e=uv \in G} \sqrt{\frac{1}{d_u d_v}} \]

Definition 1.4. The sum-connectivity index is proposed by Zhou and Trinjistic [16], and is defined as

\[ S(G) = \sum_{e=uv \in G} \sqrt{\frac{1}{d_u + d_v}} \]

Definition 1.5. The GA index is proposed by Vukicevic et al. [17] as

\[ GA(G) = \sum_{e=uv \in G} \frac{2 \sqrt{d_u d_v}}{d_u + d_v} \]

Definition 1.6. The GA5 index proposed by Graovac et al. [18] and is stated as

\[ GA_5(G) = \sum_{e=uv \in G} \frac{2 \sqrt{s_u s_v}}{s_u + s_v} \]

Definition 1.7. The first and second Zagreb indices are proposed by Gutman and Trinjistic [19], as

\[ M_1(G) = \sum_{e=uv \in G} (d_u + d_v) \]
\[ M_2(G) = \sum_{e=uv \in G} (d_u d_v) \]

Definition 1.8. Fajtlowicz proposed Harmonic index in [20] as,

\[ H(G) = \sum_{e=uv \in G} \frac{2}{d_u + d_v} \]

Definition 1.9. Shirdel et al. in [21] proposed the hyper Zagreb index and is stated as,

\[ HM(G) = \sum_{e=uv \in G} (d_u + d_v)^2 \]

Definition 1.10. Fath-Tabar et al. in [22] proposed the third Zagreb index as

\[ ZG_3(G) = \sum_{e=uv \in G} |d_u - d_v| \]

Definition 1.11. Furtula et al. in [23] proposed the forgotten topological index and is stated as

\[ F(G) = \sum_{e=uv \in G} [(d_u)^2 + (d_v)^2] \]

Definition 1.12. In chemical graph theory, there are some new degree-based graph types, which play an important role in finding total surface area and heat-formation of various chemical compounds. These graphs types are as follow Symmetric division index [24],

\[ SSD(G) = \sum_{e=uv \in G} \left[ \frac{P}{Q} \right] \]

where, \( P = \min \{d_u(v), d_v(w)\} \) and \( Q = \max \{d_u(v), d_v(w)\} \)

2. Degree based topological indices in QSAR studies

Here we defined 13° based topological indices, Atom-bond connectivity index ABC(G), Fourth atom-bond connectivity index ABC4(G), Randic index \( \chi(G) \), Sum-connectivity index S(G), Geometric-arithmetic index GA(G), Fifth Geometric arithmetic index GA5(G), First Zagreb index \( M_1(G) \), Second Zagreb index \( M_2(G) \), Harmonic index H(G), Hyper Zagreb index HM(G), Third Zagreb index ZG_3(G), Forgotten index F(G), Symmetric division index SSD(G) for modelling Five representative physical properties [Boiling point (BP), Melting point (MP), Enthalpy (E), Flash point (FP), Molar refraction (MR)] of the 17 anticancer drugs from Amathaspipiramide-E to Tambjamine-K. The values for these properties are taken from Chem Spider. The above mentioned degree based topological indices and the experimental values for the physical and chemical properties of 17 anticancer drugs (Figure 1) are represented in Tables 1, 2, and 3 respectively.

From the data of above Tables 2 and 3, it has been found that all the data values are normally distributed. Hence the regression model is suitable test to adopt and analyse the data.

3. Regression models

The above table data shows normally distributed values. Hence the study used regression analysis for the calculation purpose. Here we have checked the linear regression model as below

\[ P = A + B(TI) \]  

where \( P \) is the Physical property of anticancer drug, \( A \) is a constant and \( B \) is the regression coefficient and \( TI \) represents the topological index. These were calculated using SPSS software for the values of five physical properties and the thirteen topological indices of seventeen anticancer drugs.

Using (1), we can get the different linear models for the defined degree based topological indices, which are as follows.

1. Atom-bond Connectivity index ABC(G):

\[ \begin{align*} 
BP &= 232.702 + 18.457 [ABC(G)] \\
MP &= 97.481 + 6.385 [ABC(G)] \\
E &= 46.017 + 2.385 [ABC(G)] \\
FP &= 105.864 + 9.791 [ABC(G)] \\
MR &= 27.349 + 3.590 [ABC(G)] 
\end{align*} \]

2. Fourth Atom-bond Connectivity index ABC4(G):

\[ \begin{align*} 
BP &= 242.956 + 24.290 [ABC_4(G)] \\
MP &= 84.818 + 9.517 [ABC_4(G)] \\
E &= 46.834 + 3.081 [ABC_4(G)] \\
FP &= 114.955 + 12.640 [ABC_4(G)] \\
MR &= 27.134 + 4.889 [ABC_4(G)] 
\end{align*} \]

3. Randic index \( \chi(G) \):

\[ \begin{align*} 
BP &= 207.524 + 31.676 [\chi(G)] \\
MP &= 75.233 + 12.437 [\chi(G)] \\
E &= 42.806 + 3.966 [\chi(G)] \\
FP &= 89.052 + 17.119 [\chi(G)] \\
MR &= 19.758 + 6.397 [\chi(G)] 
\end{align*} \]

4. Sum-Connectivity index S(G):

\[ \begin{align*} 
BP &= 219.568 + 29.619 [S(G)] \\
\end{align*} \]
Figure 1. Molecular structures of anticancer drugs.
Table 1. Various Anticancer drugs with its physico-chemical properties.

| S.No. | Drugs            | BP   | MP   | E    | FP   | MR   |
|-------|------------------|------|------|------|------|------|
| 1     | Amathaspiramide E| 572.7| 209.72| 90.3 | 300.2| 89.4 |
| 2     | Aminopterin      | 782.27| 344.45|      |      | 114  |
| 3     | Aspidostomide E  | 798.8| 116.2| 436.9| 116  |
| 4     | Carmustine       | 309.6| 120.99| 63.8 | 141  |
| 5     | Caulibugulone E  | 373  | 129.46| 62   | 179.4| 52.2 |
| 6     | Convolutamide A  | 629.9| 97.9 | 334.7| 130.1|
| 7     | Convolutamine F  | 387.7| 128.67| 63.7 | 188.3| 73.8 |
| 8     | Convolutamidine A| 504.9| 199.2| 81.6 | 259.2| 68.2 |
| 9     | Daunorubicin      | 770  | 208.5| 117.6| 419.5| 130  |
| 10    | Deguelin         | 560.1| 213.39| 84.3 | 244.8| 105.1|
| 11    | Melatonin        | 512.8| 182.51| 7.84 | 264  |
| 12    | Minocycline      | 803.3| 326.3| 122.5| 439.6| 116  |
| 13    | Perfragilin A    | 431.5| 187.62| 68.7 | 214.8| 63.6 |
| 14    | Podophyllotoxin  | 597.9| 235.86| 93.6 | 210.2| 104.3|
| 15    | Pterocellin B    | 521.6| 199.88| 79.5 | 269.2| 87.4 |
| 16    | Raloxifene       | 728.2| 289.58| 110.1| 394.2| 136.6|
| 17    | Tambjamine K     | 391.7| 64.1 | 3190.7| 76.6 |

MP = 86.175 + 11.026 [S(G)]  
E = 45.580 + 3.682 [S(G)]  
FP = 97.414 + 15.829 [S(G)]  
MR = 22.568 + 5.950 [S(G)]

5. Geometric-Arithmetic index GA(G):

BP = 276.572 + 12.115 [GA(G)]  
MP = 90.640 + 5.053 [GA(G)]  
E = 51.708 + 1.5 [GA(G)]  
FP = 134.852 + 6.163 [GA(G)]  
MR = 31.169 + 2.552 [GA(G)]

6. Fifth Geometric-Arithmetic index GA5(G):

BP = 226.669 + 14.157 [GA5(G)]  
MP = 81.299 + 5.563 [GA5(G)]  
E = 51.953 + 1.175 [GA5(G)]  
FP = 109.675 + 6.163 [GA5(G)]  
MR = 31.169 + 2.552 [GA5(G)]

Table 2. Various Anticancer drugs with Topological Indices values.

| Drugs       | ABC(G) | ABCa(G) | χ(G) | S(G) | GA(G) | GAa(G) | M1(G) |
|-------------|--------|---------|------|------|-------|--------|-------|
| Amathaspiramide E | 10.773 | 9.079  | 7.112| 7.076| 14.403| 11.748 | 70    |
| Aminopterin  | 24.65 | 18.96  | 15.23| 15.68| 32.700| 33.650 | 162   |
| Aspidostomide E | 18.813| 11.346| 12.35| 13.00| 17.548| 26.906 | 148   |
| Carmustine   | 7.847 | 6.775  | 5.757| 5.482| 10.634| 10.738 | 46    |
| Caulibugulone E | 10.664| 8.342  | 6.736| 6.946| 14.574| 18.966 | 72    |
| Convolutamide A | 24.463| 19.369| 17.93| 17.74| 35.702| 34.208 | 167   |
| Convolutamine F | 10.773| 8.616  | 7.113| 7.077| 14.403| 14.599 | 70    |
| Convolutamidine A | 12.016| 8.962  | 7.93 | 7.544| 16.273| 15.753 | 88    |
| Daunorubicin  | 32.295| 22.564| 17.89| 18.89| 40.190| 33.116| 216   |
| Deguelin     | 23.398| 17.507| 15.19| 14.80| 31.954| 32.526| 168   |
| Melatonin    | 12.865| 9.676  | 8.203| 8.419| 17.493| 17.809 | 84    |
| Minocycline  | 26.081| 19.093| 15.54| 16.12| 34.271| 35.014| 184   |
| Perfragilin A | 12.992| 9.836  | 7.968| 8.171| 17.172| 17.491| 90    |
| Podophyllotoxin | 22.02 | 16.42  | 12.95| 13.86| 30.909| 30.53  | 158   |
| Pterocellin B | 19.027| 11.250| 11.69| 12.93| 26.452| 20.788| 132   |
| Raloxifene   | 26.956| 20.862| 16.58| 17.5 | 37.234| 37.684| 182   |
| Tambjamine K | 14.28 | 9.654  | 9.203| 9.419| 19.493| 19.774| 92    |
FP = 116.671 + 1.115 [M2(G)]  
MR = 34.562 + 0.391 [M2(G)]  

**9. Harmonic index H(G):**

BP = 218.618 + 32.191 [H(G)]  
MP = 79.495 + 12.656 [H(G)]  
E = 44.375 + 32.191 [H(G)]  
FP = 96.112 + 17.286 [H(G)]  
MR = 20.814 + 6.610 [H(G)]

**10. Hyper Zagreb index HM(G):**

BP = 242.453 + 0.508 [HM(G)]  
MP = 109.795 + 0.161 [HM(G)]  
E = 47.108 + 20.087 [HM(G)]  
FP = 111.462 + 0.267 [HM(G)]  
MR = 30.608 + 0.097 [HM(G)]

**11. Third Zagreb index ZG3(G):**

BP = 247.098 + 16.151 [ZG3(G)]  
MP = 105.646 + 5.462 [ZG3(G)]  
E = 47.108 + 20.087 [ZG3(G)]  
FP = 109.841 + 8.890 [ZG3(G)]  
MR = 38.887 + 2.703 [ZG3(G)]

**Table 3. Various Anticancer drugs with Topological Indices values.**

| Drugs               | M2(G) | H(G)  | HM(G) | ZG3(G) | F(G)  | SSD(G) |
|---------------------|-------|-------|-------|--------|-------|--------|
| Amathaspiramide E   | 81    | 6.767 | 343   | 12     | 180   | 35.667 |
| Aminopterin         | 185   | 14.53 | 786   | 32     | 416   | 80.33  |
| Aspidostomide E     | 186   | 11.767| 778   | 22     | 406   | 55     |
| Carmustine          | 48    | 5.533 | 202   | 8      | 106   | 25.331 |
| Cauhibugulone E     | 86    | 6.5   | 358   | 10     | 186   | 29.5   |
| Convolutamide A     | 167   | 17.265| 793   | 21     | 419   | 86.583 |
| Convolutamine F     | 81    | 6.767 | 522   | 12     | 432   | 29.167 |
| Convolutamydine A   | 109   | 6.738 | 666   | 20     | 250   | 40.083 |
| Daunorubicin        | 270   | 16.919| 1146  | 98     | 606   | 101.666|
| Deguelin            | 208   | 13.4  | 878   | 28     | 462   | 76.166 |
| Melatonin           | 96    | 7.933 | 402   | 14     | 210   | 40.666 |
| Minocycline         | 229   | 14.567| 970   | 30     | 512   | 89     |
| Pefragilin A        | 110   | 7.5   | 466   | 16     | 246   | 44     |
| Podophyllotoxin     | 198   | 12.47 | 824   | 22     | 428   | 70.66  |
| Pierocellin B       | 161   | 11.4  | 664   | 16     | 342   | 58.999 |
| Raloxifene          | 215   | 16.2  | 890   | 24     | 460   | 83     |
| Tambjamine K        | 104   | 8.933 | 434   | 14     | 226   | 44.667 |

**Table 4. Correlation coefficients.**

| Index              | ABC(G) | ABC4(G) | χ(G) | S(G) | GA(G) | GA5(G) | M1(G) | M2(G) | HM(G) | ZG3(G) | F(G) | SSD(G) |
|--------------------|--------|---------|------|------|-------|--------|-------|-------|-------|--------|------|--------|
| Boiling Point      | 0.826  | 0.789   | 0.819| 0.821| 0.728  | 0.794  | 0.849 | 0.844| 0.827| 0.837  | 0.744| 0.815  |
| Melting Point      | 0.726  | 0.762   | 0.767| 0.747| 0.745  | 0.779  | 0.727 | 0.698| 0.663| 0.837  | 0.559| 0.767  |
| Enthalpy           | 0.810  | 0.777   | 0.804| 0.802| 0.708  | 0.761  | 0.836 | 0.686| 0.818| 0.749  | 0.730| 0.804  |
| Flash Point        | 0.733  | 0.679   | 0.740| 0.735| 0.620  | 0.672  | 0.754 | 0.749| 0.737| 0.877  | 0.664| 0.720  |
| Molar Refraction   | 0.913  | 0.903   | 0.941| 0.938| 0.872  | 0.889  | 0.919 | 0.877| 0.941| 0.895  | 0.841| 0.904  |

The significance of bold numbers denote highest correlation value.
Table 5. Statistical parameters for the linear QSPR model for ABC(G).

| Physical Properties       | N  | A   | b   | r   | F   | p      | Indicator   |
|---------------------------|----|-----|-----|-----|-----|--------|-------------|
| Boiling Point             | 17 | 232.702 | 18.457 | 0.826 | 32.119 | 0.000   | significant |
| Melting Point             | 15 | 97.481 | 6.385 | 0.726 | 13.381 | 0.003   | significant |
| Enthalpy                  | 16 | 46.017 | 2.307 | 0.810 | 26.772 | 0.000   | significant |
| Flash Point               | 16 | 105.864 | 9.791 | 0.733 | 16.221 | 0.001   | significant |
| Molar Refraction          | 17 | 27.349 | 3.590 | 0.913 | 75.573 | 0.000   | significant |

The significance of bold numbers denote highest correlation value.

Table 6. Statistical parameters for the linear QSPR model for ABC4(G).

| Physical Properties       | N  | A   | b   | r   | F   | p      | Indicator   |
|---------------------------|----|-----|-----|-----|-----|--------|-------------|
| Boiling Point             | 17 | 242.956 | 24.290 | 0.789 | 24.649 | 0.000   | significant |
| Melting Point             | 15 | 84.818 | 9.517 | 0.762 | 16.580 | 0.002   | significant |
| Enthalpy                  | 16 | 46.834 | 3.081 | 0.777 | 21.267 | 0.000   | significant |
| Flash Point               | 16 | 114.955 | 12.646 | 0.679 | 11.977 | 0.004   | significant |
| Molar Refraction          | 17 | 27.134 | 4.889 | 0.903 | 66.079 | 0.000   | significant |

The significance of bold numbers denote highest correlation value.
Table 7. Statistical parameters for the linear QSPR model for $\chi(G)$.

| Physical Properties | N  | A     | b     | r     | F    | p    | Indicator |
|---------------------|----|-------|-------|-------|------|------|-----------|
| Boiling Point       | 17 | 207.524 | 31.676 | 0.819 | 30.638 | 0.000 | significant |
| Melting Point       | 15 | 75.233  | 12.437 | 0.767 | 17.167 | 0.001 | significant |
| Enthalpy            | 16 | 42.806  | 3.966  | 0.804 | 25.674 | 0.000 | significant |
| Flash Point         | 16 | 89.052  | 17.119 | 0.740 | 16.907 | 0.001 | significant |
| Molar Refraction    | 17 | 19.758  | 6.347  | 0.941 | 116.416 | 0.000 | significant |

The significance of bold numbers denote highest correlation value.

Table 8. Statistical parameters for the linear QSPR model for $S(G)$.

| Physical Properties | N  | A     | b     | r     | F    | p    | Indicator |
|---------------------|----|-------|-------|-------|------|------|-----------|
| Boiling Point       | 17 | 219.568 | 29.619 | 0.821 | 31.014 | 0.000 | significant |
| Melting Point       | 15 | 86.175  | 11.026 | 0.747 | 15.172 | 0.002 | significant |
| Enthalpy            | 16 | 45.580  | 1.5    | 0.708 | 14.098 | 0.002 | significant |
| Flash Point         | 16 | 97.414  | 15.829 | 0.735 | 16.448 | 0.001 | significant |
| Molar Refraction    | 17 | 22.568  | 5.950  | 0.938 | 109.935 | 0.000 | significant |

The significance of bold numbers denote highest correlation value.

Table 9. Statistical parameters for the linear QSPR model for $GA(G)$.

| Physical Properties | N  | A     | b     | r     | F    | p    | Indicator |
|---------------------|----|-------|-------|-------|------|------|-----------|
| Boiling Point       | 17 | 276.572 | 12.115 | 0.728 | 16.912 | 0.001 | significant |
| Melting Point       | 15 | 90.640  | 5.053  | 0.745 | 14.93  | 0.002 | significant |
| Enthalpy            | 16 | 51.708  | 1.5    | 0.708 | 14.098 | 0.002 | significant |
| Flash Point         | 16 | 134.852 | 6.163  | 0.620 | 8.735  | 0.010 | Significant |
| Molar Refraction    | 17 | 31.169  | 2.552  | 0.872 | 47.644 | 0.000 | Significant |

The significance of bold numbers denote highest correlation value.

Table 10. Statistical parameters for the linear QSPR model for $GA_5(G)$.

| Physical Properties | N  | A     | b     | r     | F    | p    | Indicator |
|---------------------|----|-------|-------|-------|------|------|-----------|
| Boiling Point       | 17 | 226.669 | 14.157 | 0.794 | 25.640 | 0.000 | Significant |
| Melting Point       | 15 | 100.234 | 0.913  | 0.727 | 13.472 | 0.003 | Significant |
| Enthalpy            | 16 | 45.953  | 1.745  | 0.761 | 19.266 | 0.001 | Significant |
| Flash Point         | 16 | 109.675 | 7.234  | 0.672 | 11.526 | 0.004 | Significant |
| Molar Refraction    | 17 | 25.435  | 2.784  | 0.889 | 56.261 | 0.000 | Significant |

The significance of bold numbers denote highest correlation value.

Table 11. Statistical parameters for the linear QSPR model for $M_1(G)$.

| Physical Properties | N  | A     | b     | r     | F    | p    | Indicator |
|---------------------|----|-------|-------|-------|------|------|-----------|
| Boiling Point       | 17 | 232.771 | 2.686  | 0.849 | 38.616 | 0.000 | Significant |
| Melting Point       | 15 | 100.234 | 0.913  | 0.727 | 13.472 | 0.003 | Significant |
| Enthalpy            | 16 | 46.094  | 0.334  | 0.836 | 32.541 | 0.000 | Significant |
| Flash Point         | 16 | 106.537 | 1.414  | 0.754 | 18.503 | 0.001 | Significant |
| Molar Refraction    | 17 | 28.756  | 0.511  | 0.919 | 81.435 | 0.000 | Significant |

The significance of bold numbers denote highest correlation value.

Table 12. Statistical parameters for the linear QSPR model for $M_2(G)$.

| Physical Properties | N  | A     | b     | r     | F    | p    | Indicator |
|---------------------|----|-------|-------|-------|------|------|-----------|
| Boiling Point       | 17 | 250.418 | 2.138  | 0.844 | 37.243 | 0.000 | Significant |
| Melting Point       | 15 | 109.887 | 0.692  | 0.698 | 11.405 | 0.005 | Significant |
| Enthalpy            | 16 | 48.129  | 0.266  | 0.837 | 32.841 | 0.000 | Significant |
| Flash Point         | 16 | 116.671 | 1.115  | 0.749 | 17.849 | 0.001 | Significant |
| Molar Refraction    | 17 | 34.562  | 0.391  | 0.877 | 50.156 | 0.000 | Significant |

The significance of bold numbers denote highest correlation value.
FP = 117.165 + 2.870 [SSD(G)] \hspace{1cm} (65) \\
MR = 31.147 + 1.058 [SSD(G)] \hspace{1cm} (66)

4. Conclusion, study implications, limitations and future study

4.1. Conclusion

The Table 4 and graphs (Figure 2) indicates the correlated values of Physico-chemical properties of anticancer drugs with the defined degree based topological indices. It can be observed that \( M_1(G) = 0.849 \) index shows higher significant positive correlation with Boiling point (BP), when compared with other indices.

Similarly \( G_{5}(G) = 0.779 \) index gives positive correlated value with melting point (MP). In case of enthalpy, \( M_2(G) \) shows highest correlated value i.e. \( r = 0.837 \).

Flashing point (FP) offers highest correlated value of 0.754 from the physico-chemical properties.

Based on molar refraction (MR), \( \chi(G) \) and \( M_2(G) \) indices depicts highest positive correlation value i.e. \( r = 0.941 \).
Hence it can be remarked that all the physical and chemical properties of anticancer drugs are positively correlate with the defined degree based topological indices.

Tables 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, and 17 shows the regression model of various physico-chemical properties. It can be observed that the regression model value $r$ is more than 0.6 and $p$ value shows less than 0.05. Hence it can be concluded that all the physico-chemical properties are highly significant.

4.2. Study implications

The work imply that these anti-cancer drugs may be considered for further study by pharmacists and chemists in designing the drugs using these topological indices values. May be the composition of these drugs, like the combinations may be tried for different ailments based on the range of the topological indices that are determined in the study. As the correlation coefficient has been found for the topological indices, the positively high correlated drugs may be considered for the combination of design of novel drugs.

4.3. Limitations

As the range of topological indices are not published by chemists anywhere in web/internet, the mathematicians may not be able to decide upon the values they obtain for different chemical compounds whether the compounds the researchers chose have future study or not. The best solution for this would be a joint venture of the study in future may be carried out by both mathematicians/statisticians and chemists/pharmacists.

4.4. Future study

In a similar fashion, a study may be carried out for different chemical structures and a conclusion may be given based on their topological indices range. May it be benzene structure or polymers or any chemical compounds can be taken for future study. A multidisciplinary project may be taken up by various disciplines researchers for a better result.

Declarations

Author contribution statement

Shanmukha M C, Basavarajappa N S, Shilpa K C, Usha A: Conceived and designed the experiments; Performed the experiments; Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.

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Competing interest statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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