Research Article

Degree-Based Molecular Descriptors and QSPR Analysis of Breast Cancer Drugs

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Received 7 April 2022; Accepted 22 April 2022; Published 23 May 2022

Academic Editor: Hassan Raza

The disease that involves abnormal cell growth and spreads through the surrounding tissues damaging other parts of the body is cancer. Breast cancer is the most common one out of many types. Women are affected by breast cancer either by hormonal changes or genetic changes that occur in DNA. As breast cancer is a life-threatening disease, it is necessary for further studies to gear up in fighting the deadliest disease. In this work, a detailed study is made on the occurrence, symptoms, and the drugs involved in its treatment. For this purpose, the quantitative structure-property relationship (QSPR) analysis is made using 21 drugs used in the treatment of breast cancer. The drugs considered in the study are modelled as molecular graphs using their molecular structures, and 11 topological indices are computed. The QSPR analysis is carried out for these drugs, and conclusions are drawn based on the analysis.

1. Introduction

The human body is made up of trillions of cells. Cell division is a natural phenomenon in all living beings. If the division of cells happens uncontrollably and spreads to surrounding tissues to form lumps, it results in cancer. Cancer can affect any part of the human body. It is the most life-threatening disease, even though a lot of research is happening to cure this disease. Nowadays, the recovery rates in patients have considerably improved. Cancer occurs because of hormonal changes or genetic changes in DNA.

Irrespective of age, cancer occurs in human beings starting from infants to old age and more commonly in adults. If an extra growth or lump or tumour appears in the body, it is necessary to check for biopsy and confirm the diagnosis. Tumours may be malignant or benign. Benign tumours are non-cancerous and do not spread to surrounding tissues. However, some benign tumours may be life threatening, if grown in the brain.

The risk of contracting cancer may be prevented by various factors such as maintaining a healthy lifestyle, avoiding food that causes cancer, and by taking vaccines that can prevent cancer from further development. The substances that cause cancer are usage of tobacco, exposure to carcinogen, and cooking with Teflon-coated vessels that have the ability to cause the deadliest disease [1–3].

Cancer occurs in human beings, irrespective of gender. In common, women are affected especially by breast cancer and cervical cancer. According to the statistics available in the year 2020, 2.3 million women were affected by breast cancer globally out of which 685000 lost their battle against the deadliest disease. It usually develops in the lining of milk ducts and lobules that supply milk to these ducts. There are more than 18 types of breast cancer. Early detection of breast cancer is done by mammograms. The treatment includes clinical trials, immune therapy, hormone therapy, targeted therapy, and surgery with chemotherapy and radiation therapy [4, 5].
Breast cancer is classified based on grading systems influenced by prognosis. There are several factors in describing the type of cancer and its response. They are histopathology, grade, stage, receptor status, and DNA assays. Histopathology deals with the confirmation and analysis of the report produced by pathologist, and grade is a type of category based on the appearance of breast and primarily confirms the malignant cells in the ducts or lobules. This also includes stages starting from 0 to 4. Stage 0 is called the precancerous stage, stages 1–3 refer to cancer within the breasts or lymph nodes, and stage 4 is called metastatic cancer since it would have spread throughout the breast.

1.1. Topological Index Significance and Applications. A numerical descriptor is a mathematical tool pertaining to the structure of the chemical compound used to analyse and investigate physicochemical properties of a molecule, thereby avoiding exorbitant and time-consuming laboratory experiments. It is a real number that stores/gives a lot of valuable information of a chemical compound. There are different types of topological indices (TI’s) such as degree-based, neighbourhood degree-based, distance-based, and eigenvalue-based indices. The property and activity-based models with indices are used that correlate with biological activities and other properties of the corresponding chemical structures [6, 9–17].

To manufacture any drug, the pharmacists collect the properties of molecular structure identified from quantitative structure-property relationship/quantitative structure-activity relationship (QSPR/QSAR) modelling and topological indices [18]. The results obtained helps in knowing that new product is consumable or not by the living beings. Various numerical descriptors are applied to foresee the properties of anticancer drugs, as there is an interrelation between anticancer drugs and characteristics of alkanes [3, 19–21].

In designing any new drug, properties of the molecular structure are required. Such properties are obtained using QSPR models with topological indices. To assist chemists, a detailed study of 21 drugs is carried out and various topological indices are computed.

1.2. Motivation for the Indices Used. There have been many topological indices introduced since 1947 till date. In this work, topological indices chosen have high correlation between them and various drugs used in breast cancer treatment. The application of the considered topological indices is discussed below.

The first and second Zagreb indices help in determining the total $\pi$-electron energy of molecules [22]. Randic introduced a topological index for computing the extent of branching of carbon atoms of saturated hydrocarbons which is named as Randic index [23]. The reciprocal Randic index helps in studying the chemical and physical properties of compounds with alkanes [24]. The harmonic index is another variant of Randic index first introduced by Fajtlowicz [8]. The heat of formation of heptanes and octanes is studied using the ABC index [7]. The heat of formation of alkanes is anticipated using augmented Zagreb index [25]. Furtula and Gutman [26] proposed forgotten TI, used to test various properties of drugs. Zhao et al. [27] proposed SS index and studied the physicochemical properties of 67 alkane isomers. It was found that SS index has good correlation with five properties, that is, boiling point (BP), melting point (MP), molar refraction (MR), heat of vaporization (HV), and critical pressure (CP), of which molar refraction (MR) was found to be having highest correlation of 0.99. Also, the SS index has good correlation for four various dendrimer structures. It was observed that the correlation coefficient of porphyrin dendrimer was perfect positive ($r = 1$). The Sombor index was recently introduced by Gutman [28], and its chemical applicability was checked by Redzepovic [29]. It was found that there was a reasonable correlation between the Sombor index and entropy. The Sombor index is used in forecasting the entropy of octanes. The total surface area of octane isomers is forecasted using the inverse sum indeg index [30].

In chemical graph theory (CGT), the molecular structure of drug is expressed as molecular graph such that an atom denotes a vertex and the bond connecting two atoms denotes an edge. For standard graph notations and terminologies, see [31–34].

**Definition 1.** Gutman et al. [22] introduced

$$M_1 (G) = \sum_{v \in V (G)} (d_v + d_w),$$

**Definition 2.** Estrada et al. in [7] introduced

$$ABC(G) = \sum_{v \in V (G)} \frac{d_v + d_w - 2}{d_v d_w}$$

**Definition 3.** Vukicevic et al. [30] introduced

$$IS(G) = \sum_{v \in V (G)} \frac{d_v d_w}{d_v + d_w}$$

**Definition 4.** Recently, Zhao et al. [27] formulated the SS index which is defined as

$$ SS(G) = \sum_{v \in V (G)} \frac{d_v d_w}{d_v + d_w} $$

**Definition 5.** Recently, Gutman [28] formulated the Sombor index which is defined as

$$ SO(G) = \sum_{v \in V (G)} \sqrt{(d_v)^2 + (d_w)^2}. $$
(a) 

(b) 

(c) 

(d) 

(e) 

(f) 

(g) 

(h) 

Figure 1: Continued.
Figure 1: Continued.
Definition 6. Furtula et al. in [25] proposed the augmented Zagreb index given by

\[ A(G) = \sum_{vu \in E(G)} \left( \frac{d_v d_w}{d_v + d_w - 2} \right)^3. \]  

Definition 7. Randić [23] introduced

\[ R(G) = \sum_{vu \in E(G)} \frac{1}{\sqrt{d_v d_w}}. \]  

Definition 8. The reciprocal Randić index [24] formulated by Gutman et al. is given by

\[ F(G) = \sum_{vu \in E(G)} (d_v^{-2} + d_w^{-2}). \]  

Definition 9. Harmonic index [8] is given by

\[ H(G) = \sum_{vu \in E(G)} \frac{2}{d_v + d_w}. \]  

Definition 10. Furtula et al. in [26] introduced

\[ RR(G) = \sum_{vu \in E(G)} \sqrt{d_v d_w}. \]
2. Results and Discussion

In this work, topological indices are computed for chemical structures of drugs used in the treatment of breast cancer. The QSAR analysis of indices considered in the study is discussed, and it is shown that the correlation coefficient between the indices and physical properties of drugs is highly correlated.

The drugs considered in this work are alpelisib, azacitidine, cytarabine, daunorubicin, dexmethasone, docetaxel, doxorubicin, glasdegib, gilteritinib, ivosidenib, midostaurin, olaparib, palbociclib, pamidronate, prednisonie, ribociclib, tioguanine, tucatinib, and venetoclax. The molecular structure of these drugs is represented in Figure 1.

The analysis includes computing 11 indices such as $M_1(G)$, $M_2(G)$, $R(G)$, $RR(G)$, $H(G)$, $ABC(G)$, $A(G)$, $F(G)$, $SS(G)$, $SO(G)$, and $IS(G)$. These indices are modelled using 6 physical properties (boiling point (BP) °C at 760 mmHg, enthalpy of vaporization (EV) kJ/mol, flash point (FP) °C, molar refractivity (MR) cm$^3$, LogP, molar volume (MV) cm$^3$) for 21 anticancer drugs used in the treatment of breast cancer from alpelisib to venetoclax. The computed values for indices considered in the study and the practical values from the laboratory experiments of 21 drugs are presented in Tables 1 and 2, respectively.

Tables 3–13 display the statistical parameters such as number of drugs considered, constant, regression coefficient, correlation coefficient, Fisher’s statistic, significant value, and standard error denoted by $N$, $A$, $b$, $r$, $F$, $p$, and SE, respectively, for all the considered TI’s and physical properties. In each table, the value of $p$ is less than or equal to 0.001 ($p \leq 0.05$), indicating the significance of the results.

The correlation coefficient of physicochemical properties against TI’s is depicted in Figure 2.

**Theorem 1.** Consider a molecular graph $G$ for doxorubicin; then, $M_1(G) = 220$, $M_2(G) = 275$, $RR(G) = 106.2$, $H(G) = 17.486$, $ABC(G) = 30.771$, $A(G) = 358.054$, $F(G) = 614$, $SS(G) = 46.591$, $SO(G) = 160.401$, and $IS(G) = 51.414$.

**Proof.** From Figure 3, it is obvious that there are 39 vertices and 8 different types of edges counting to 43. They are as follows.

$$E_{1,2} = \{ e = vw \in E(a) | d_v = 1, d_w = 2 \},$$

$$E_{1,3} = \{ e = vw \in E(a) | d_v = 1, d_w = 3 \},$$

$$E_{1,4} = \{ e = vw \in E(a) | d_v = 1, d_w = 4 \},$$

$$E_{2,2} = \{ e = vw \in E(a) | d_v = 2, d_w = 2 \},$$

$$E_{2,3} = \{ e = vw \in E(a) | d_v = 2, d_w = 3 \},$$

$$E_{2,4} = \{ e = vw \in E(a) | d_v = 2, d_w = 4 \},$$

$$E_{3,3} = \{ e = vw \in E(a) | d_v = 3, d_w = 3 \},$$

$$E_{3,4} = \{ e = vw \in E(a) | d_v = 3, d_w = 4 \},$$

(12)
Table 3: Statistical specifications for the linear model of $M_1(G)$.

| Physical properties | N  | A    | b     | r   | $r^2$ | F   | p    | Indicator     | SE  |
|---------------------|----|------|-------|-----|-------|-----|------|---------------|-----|
| BP                  | 16 | 402.789 | 1.616 | 0.895 | 0.8 | 56.103 | 0.000 | Significant | 67.479 |
| EV                  | 16 | 71.022 | 0.204 | 0.845 | 0.713 | 34.823 | 0.000 | Significant | 10.806 |
| FP                  | 16 | 198.864 | 0.974 | 0.898 | 0.807 | 58.472 | 0.000 | Significant | 38.83 |
| MR                  | 21 | 2.517 | 0.648 | 0.977 | 0.955 | 402.526 | 0.000 | Significant | 11.62 |
| LogP                | 21 | –4.399 | 0.036 | 0.797 | 0.635 | 33.009 | 0.000 | Significant | 2.275 |
| MV                  | 21 | –5.607 | 1.816 | 0.956 | 0.913 | 200.581 | 0.000 | Significant | 46.127 |

Table 4: Statistical specifications for the linear model of $M_2(G)$.

| Physical properties | N  | A    | b     | r   | $r^2$ | F   | p    | Indicator     | SE  |
|---------------------|----|------|-------|-----|-------|-----|------|---------------|-----|
| BP                  | 16 | 409.985 | 1.292 | 0.887 | 0.786 | 51.411 | 0.000 | Significant | 69.857 |
| EV                  | 16 | 71.424 | 0.165 | 0.849 | 0.721 | 36.206 | 0.000 | Significant | 10.656 |
| FP                  | 16 | 202.841 | 0.780 | 0.892 | 0.796 | 54.573 | 0.000 | Significant | 40.946 |
| MR                  | 21 | 7.446 | 0.512 | 0.958 | 0.919 | 214.332 | 0.000 | Significant | 15.62 |
| LogP                | 21 | –4.120 | 0.029 | 0.781 | 0.610 | 29.701 | 0.000 | Significant | 2.351 |
| MV                  | 21 | 9.845 | 1.427 | 0.933 | 0.870 | 126.965 | 0.000 | Significant | 56.575 |

Table 5: Statistical specifications for the linear model of $R(G)$.

| Physical properties | N  | A    | b     | r   | $r^2$ | F   | p    | Indicator     | SE  |
|---------------------|----|------|-------|-----|-------|-----|------|---------------|-----|
| BP                  | 16 | 398.262 | 18.974 | 0.885 | 0.784 | 50.727 | 0.000 | Significant | 70.225 |
| EV                  | 16 | 71.492 | 2.325 | 0.812 | 0.659 | 27.017 | 0.000 | Significant | 11.79 |
| FP                  | 16 | 196.716 | 11.395 | 0.886 | 0.785 | 51.051 | 0.000 | Significant | 42.04 |
| MR                  | 21 | –2.012 | 7.809 | 0.991 | 0.981 | 1000.385 | 0.000 | Significant | 7.475 |
| LogP                | 21 | –4.730 | 0.442 | 0.816 | 0.667 | 37.979 | 0.000 | Significant | 2.173 |
| MV                  | 21 | –19.917 | 21.976 | 0.973 | 0.947 | 342.442 | 0.000 | Significant | 35.923 |

Table 6: Statistical specifications for the linear model of $RR(G)$.

| Physical properties | N  | A    | b     | r   | $r^2$ | F   | p    | Indicator     | SE  |
|---------------------|----|------|-------|-----|-------|-----|------|---------------|-----|
| BP                  | 16 | 403.211 | 3.343 | 0.89 | 0.792 | 53.176 | 0.000 | Significant | 68.933 |
| EV                  | 16 | 71.367 | 0.418 | 0.833 | 0.694 | 31.742 | 0.000 | Significant | 11.164 |
| FP                  | 16 | 199.120 | 2.014 | 0.893 | 0.798 | 55.319 | 0.000 | Significant | 40.725 |
| MR                  | 21 | 2.078 | 1.347 | 0.979 | 0.958 | 428.607 | 0.000 | Significant | 11.28 |
| LogP                | 21 | –4.439 | 0.076 | 0.8 | 0.639 | 33.675 | 0.000 | Significant | 2.260 |
| MV                  | 21 | –6.008 | 3.763 | 0.955 | 0.912 | 195.774 | 0.000 | Significant | 46.640 |

Table 7: Statistical specifications for the linear model of $H(G)$.

| Physical properties | N  | A    | b     | r   | $r^2$ | F   | p    | Indicator     | SE  |
|---------------------|----|------|-------|-----|-------|-----|------|---------------|-----|
| BP                  | 16 | 400.808 | 19.683 | 0.873 | 0.763 | 45.016 | 0.000 | Significant | 73.545 |
| EV                  | 16 | 72.158 | 2.387 | 0.793 | 0.628 | 23.644 | 0.000 | Significant | 12.307 |
| FP                  | 16 | 198.199 | 11.824 | 0.874 | 0.764 | 45.381 | 0.000 | Significant | 44.001 |
| MR                  | 21 | –2.119 | 8.158 | 0.993 | 0.985 | 1272.264 | 0.000 | Significant | 6.641 |
| LogP                | 21 | –4.812 | 0.467 | 0.827 | 0.683 | 41.025 | 0.000 | Significant | 2.117 |
| MV                  | 21 | –19.156 | 22.889 | 0.972 | 0.946 | 329.779 | 0.000 | Significant | 36.6 |
Considering the number of edges and their respective types in the definitions of indices from equations (1)–(11), the following results are obtained.

Similarly, the indices are computed for other drugs considered in the study. NK here results obtained are depicted in Table 1.

From Table 1, it is noticed that the obtained values are normally distributed based on the descriptive statistics analysis, and the kurtosis value lies in between ± 1.96. The normality is also checked with the Shapiro–Wilk test \( (n < 50) \), such that the significance value is greater than 0.05. Hence, we conclude that the values are normally distributed. Therefore, the suitable method used to analyse the data is regression analysis.

\[ E_1,2 = 2, \]
\[ E_{1,a} = 8, \]
\[ E_{1,b} = 1, \]
\[ E_{2,a} = 2, \]
\[ E_{2,b} = 12, \]
\[ E_{2,d} = 2, \]
\[ E_{3,a} = 15, \]
\[ E_{3,d} = 1. \]

\[ |E_{1,a}| = 2, \]
\[ |E_{1,b}| = 8, \]
\[ |E_{1,c}| = 1, \]
\[ |E_{2,a}| = 2, \]
\[ |E_{2,b}| = 12, \]
\[ |E_{2,c}| = 2, \]
\[ |E_{3,a}| = 15, \]
\[ |E_{3,b}| = 1. \]

\[ (13) \]

3. Regression Models

The linear regression model is given by

\[ P = A + b(TI), \]  

where \( P, A, b, TI \) \( \longrightarrow \) physical property of drug, constant, regression coefficient, and topological index.

Using equation (14), the linear models for the respective topological indices considered in the study are obtained as follows.

(1) First Zagreb index \( M_1(G) \):

\[ BP = 402.789 + 1.616[M_1(G)], \]
\[ EV = 71.022 + 0.204[M_1(G)], \]
\[ FP = 198.864 + 0.974[M_1(G)], \]
\[ MR = 2.517 + 0.648[M_1(G)], \]
\[ LogP = -4.399 + 0.036[M_1(G)], \]
\[ MV = -5.607 + 1.816[M_1(G)]. \]  

\[ (15) \]
Table 11: Statistical specifications for the linear model of SS(G).

| Physical properties | N  | A    | b    | r    | r²   | F    | p     | Indicator   | SE  |
|---------------------|----|------|------|------|------|------|-------|-------------|-----|
| BP                  | 16 | 403.887 | 7.542 | 0.878 | 0.771 | 47.211 | 0.000 | Significant | 72.214 |
| EV                  | 16 | 71.803  | 0.934 | 0.814 | 0.663 | 27.497 | 0.000 | Significant | 11.721 |
| FP                  | 16 | 199.664 | 4.541 | 0.881 | 0.776 | 48.582 | 0.000 | Significant | 42.861 |
| MR                  | 21 | 0.734   | 3.071 | 0.986 | 0.972 | 667.793 | 0.000 | Significant | 9.107 |
| LogP                | 21 | −4.620  | 0.175 | 0.818 | 0.669 | 38.403 | 0.000 | Significant | 2.165 |
| MV                  | 21 | −9.715  | 8.58  | 0.962 | 0.925 | 235.493 | 0.000 | Significant | 42.846 |

Table 12: Statistical specifications for the linear model of SO(G).

| Physical properties | N  | A    | b    | r    | r²   | F    | p     | Indicator   | SE  |
|---------------------|----|------|------|------|------|------|-------|-------------|-----|
| BP                  | 16 | 403.876 | 2.211 | 0.898 | 0.807 | 58.391 | 0.000 | Significant | 64.403 |
| EV                  | 16 | 70.907  | 0.281 | 0.854 | 0.729 | 37.7  | 0.000 | Significant | 10.501 |
| FP                  | 16 | 199.511 | 1.332 | 0.902 | 0.813 | 60.973 | 0.000 | Significant | 39.159 |
| MR                  | 21 | 3.071   | 0.888 | 0.976 | 0.952 | 374.281 | 0.000 | Significant | 12.034 |
| LogP                | 21 | −4.342  | 0.050 | 0.792 | 0.628 | 32.017 | 0.000 | Significant | 2.297 |
| MV                  | 21 | −5.060  | 2.495 | 0.957 | 0.916 | 206.671 | 0.000 | Significant | 45.500 |

Table 13: Statistical specifications for the linear model of IS(G).

| Physical properties | N  | A    | b    | r    | r²   | F    | p     | Indicator   | SE  |
|---------------------|----|------|------|------|------|------|-------|-------------|-----|
| BP                  | 16 | 403.935 | 6.883 | 0.885 | 0.783 | 50.557 | 0.000 | Significant | 70.318 |
| EV                  | 16 | 71.717  | 0.855 | 0.822 | 0.676 | 29.263 | 0.000 | Significant | 11.479 |
| FP                  | 16 | 199.559 | 4.148 | 0.889 | 0.789 | 52.503 | 0.000 | Significant | 41.578 |
| MR                  | 21 | 2.259   | 2.771 | 0.980 | 0.960 | 453.933 | 0.000 | Significant | 10.974 |
| LogP                | 21 | −4.456  | 0.156 | 0.804 | 0.646 | 34.657 | 0.000 | Significant | 2.24 |
| MV                  | 21 | −4.813  | 7.726 | 0.954 | 0.910 | 192.077 | 0.000 | Significant | 47.047 |

Table 14: Correlation coefficient between physicochemical properties and TI’s of breast cancer drugs.

| Index | BP    | EV    | FP    | MR    | LogP  | MV    |
|-------|-------|-------|-------|-------|-------|-------|
| M1 (G) | 0.895 | 0.845 | 0.898 | 0.977 | 0.797 | 0.956 |
| M2 (G) | 0.887 | 0.849 | 0.892 | 0.958 | 0.781 | 0.933 |
| R (G)  | 0.885 | 0.812 | 0.886 | 0.991 | 0.816 | 0.973 |
| RR (G) | 0.89  | 0.833 | 0.893 | 0.979 | 0.8  | 0.955 |
| H (G)  | 0.873 | 0.793 | 0.874 | 0.993 | 0.827 | 0.972 |
| ABC (G) | 0.823 | 0.729 | 0.824 | 0.902 | 0.656 | 0.871 |
| A (G)  | 0.87  | 0.799 | 0.874 | 0.976 | 0.81 | 0.948 |
| F (G)  | 0.895 | 0.876 | 0.9  | 0.95  | 0.764 | 0.934 |
| SS (G) | 0.878 | 0.814 | 0.881 | 0.986 | 0.818 | 0.962 |
| SO (G) | 0.898 | 0.854 | 0.902 | 0.976 | 0.792 | 0.957 |
| IS (G) | 0.885 | 0.822 | 0.889 | 0.98  | 0.804 | 0.954 |

(II) Second Zagreb index $M_2(G)$:

$$BP = 409.985 + 1.292[M_2(G)],$$

$$EV = 71.424 + 0.165[M_2(G)],$$

$$FP = 202.841 + 0.780[M_2(G)],$$

$$MR = 7.446 + 0.512[M_2(G)],$$

$$\text{LogP} = -4.12 + 0.029[M_2(G)],$$

$$MV = 9.845 + 1.427[M_2(G)].$$

(III) Randic index $R(G)$:

$$BP = 398.262 + 18.974[R(G)],$$

$$EV = 71.492 + 2.325[R(G)],$$

$$FP = 196.716 + 11.395[R(G)],$$

$$MR = -2.012 + 7.809[R(G)],$$

$$\text{LogP} = -4.730 + 0.442[R(G)]$$

$$MV = -19.917 + 21.976[R(G)].$$
(IV) Reciprocal Randic index $RR(G)$:

$$BP = 403.211 + 3.343[RR(G)],$$

$$EV = 71.367 + 0.418[RR(G)],$$

$$FP = 199.12 + 2.014[RR(G)],$$

$$MR = 2.078 + 1.347[RR(G)],$$

$$\log P = -4.439 + 0.076[RR(G)],$$

$$MV = -6.008 + 3.763[RR(G)].$$

(V) Harmonic index $H(G)$:

$$BP = 400.808 + 19.683[H(G)],$$

$$EV = 72.158 + 2.387[H(G)],$$

$$FP = 198.199 + 11.824[H(G)],$$

$$MR = -2.119 + 8.158[H(G)],$$

$$\log P = -4.812 + 0.467[H(G)],$$

$$MV = -19.156 + 22.889[H(G)].$$
VII) Augmented Zagreb index $A(G)$:

\[
BP = 407.355 + 0.979\, [A(G)],
EV = 72.527 + 0.120\, [A(G)],
FP = 201.489 + 0.591\, [A(G)],
MR = 2.965 + 0.397\, [A(G)],
\]

\[
\text{Log}P = -4.491 + 0.023\, [A(G)],
MV = -1.773 + 1.102\, [A(G)].
\]

(VIII) Forgotten index $F(G)$:

\[
BP = 413.222 + 0.568\, [F(G)],
EV = 71.046 + 0.074\, [F(G)],
FP = 204.811 + 0.343\, [F(G)],
MR = 8.754 + 0.225\, [F(G)],
\]

\[
\text{Log}P = -3.965 + 0.012\, [F(G)],
MV = 10.357 + 0.634\, [F(G)].
\]

(IX) SS index $SS(G)$:

\[
BP = 403.887 + 7.542\, [SS(G)],
EV = 71.803 + 0.934\, [SS(G)],
FP = 202.841 + 0.780\, [SS(G)],
MR = 0.0734 + 3.071\, [SS(G)],
\]

\[
\text{Log}P = -4.620 + 0175\, [SS(G)],
MV = -9.715 + 8.58\, [SS(G)].
\]

(X) Somber index $SO(G)$:

\[
BP = 403.876 + 2.211\, [SO(G)],
EV = 70.907 + 0.281\, [SO(G)],
FP = 199.511 + 1.332\, [SO(G)],
MR = 3.071 + 0.888\, [SO(G)],
\]

\[
\text{Log}P = -4.342 + 0.050\, [SO(G)],
MV = -5.060 + 2.495\, [SO(G)].
\]

(XI) Inverse indeg index $IS(G)$:

\[
BP = 439.633 + 9.227\, [ABC(G)],
EV = 77.576 + 1.092\, [ABC(G)],
FP = 221.533 + 5.543\, [ABC(G)],
MR = 15.643 + 3.868\, [ABC(G)],
\]

\[
\text{Log}P = -3.013 + 0.193\, [ABC(G)],
MV = 34.986 + 10.699\, [ABC(G)].
\]

4. Conclusion

In the present work, drugs used in the treatment of breast cancer are studied for which various numerical descriptors are computed. To develop any novel drug, the properties of its structure are required and these properties can be obtained from QSPR modelling using TIs. The aim of this work is to obtain data regarding the topology of structure using topological indices with less cost and less time. The correlation coefficient between topological indices against the six physicochemical properties of the drugs is represented in Table 14. By inspection, it is observed that BP has the highest correlation with SO (G) with $r = 0.898$. Also, EV has the highest correlation with F (G) having $r = 0.896$, and FP has a good correlation with SO (G) with $r = 0.902$, while MR with $H\, (G)$ has high correlation with $r = 0.993$, LogP with $H\, (G)$ has $r = 0.827$, and MV with $R\, (G)$ has $r = 0.973$. The obtained results have good correlation coefficients between physical properties and their respective topological indices. It is obvious from the study that MR is supposed to have good correlation with all topological indices considered in the study. It is observed that the correlation coefficient is more than 0.7 except a value (0.656) for ABC (G) index, and in all models, the value of $p$ is less than or equal to 0.001 ($p \leq 0.05$), indicating the significance of the results.

4.1. Study Implications. The capacity of a molecular entity to reach a target implies the biological activity measured in terms of potency or concentration needed for the entity to
produce the effect. The physicochemical properties include solubility, hydrogen bonding, ionization, isosterism, etc. The QSPR analysis carried out in this work assists the readers to know the properties of drugs required to include in the treatment or inclusion of this compound in the discovery of new drug.

The work provides right direction to the chemists and pharmacists to develop new drugs required for the treatment of different ailments. The anticipation of physicochemical properties is extensively done using TI’s. The indices are used in prediction studies for models developed for soil absorption, boiling point, viscosity, densities of organic solvents, and chromatographic retention of data.

Biological studies performed using TI’s help in providing good predictions. Some examples are enzyme inhibition, carcinogenicity, and hallucinogenic activity. The biological predictions include studies that are related to environmental pollution and toxicity.

The TI’s obtained here may be considered as reference in composing new compounds for further research. It is observed from the study that the physicochemical properties of the drugs show high positive correlation, indicating that these components or the drugs may be utilized in the discovery of novel drugs for various ailments.

To analyse the chemical information of chemical compound obtained by optimal procedures and experiments, the chemical discipline known as chemometrics is used. This discipline uses the statistical methods to obtain maximum chemical information of the compound.

4.2. Future Scope. A similar study may be carried out for different chemical compounds useful for chemists in their further research. Also, various drugs used in the treatment of COVID-19 may also be considered for a similar study which helps the researchers.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors’ Contributions

Dr. M.C. Shanmukha was responsible for conceptualization, methodology, article writing, formal analysis, resources, data curation, and investigation. Dr. A. Usha was responsible for review of the manuscript and conceptualization and gave suggestions for correction of the manuscript. Dr. B.M. Praveen was responsible for review of the manuscript, supervision, and validation and gave suggestions for correction of the manuscript. Dr. Abalo Douhadjii was responsible for formal analysis, resources, and software.

References

[1] B. Figuerola and C. Avila, “The phylum bryozoa as a promising source of anticancer drugs,” Marine Drugs, vol. 17, no. 8, p. 477, 2019.
[2] L. J. Kristjanson and T. Ashcroft, “The family’s cancer journey,” Cancer Nursing, vol. 17, no. 1, pp. 1–17, 1994.
[3] S. Kumar, M. K. Ahmad, M. Waseem, and A. K. Pandey, “Drug targets for cancer treatment: an overview,” Medicinal Chemistry, vol. 5, pp. 115–123, 2015.
[4] R. C. Richie and J. O. Swanson, “Breast cancer: a review of the literature,” Journal of Insurance Medicine, vol. 35, pp. 85–101, 2003.
[5] A. G. Waks and E. P. Winer, “Breast cancer treatment,” JAMA, vol. 321, no. 3, pp. 288–300, 2019.
[6] H. Ali, A. Q. Baig, and M. K. Shafiq, “On topological properties of hierarchical interconnection networks,” Journal of Applied Mathematics and Computing, vol. 55, pp. 313–334, 2017.
[7] E. Estrada, L. Torres, L. Rodriguez, and I. Gutman, “An atom-bond connectivity index: modeling the enthalpy of formation of alkanes,” Indian Journal of Chemistry, vol. 37, pp. 849–855, 1998.
[8] S. Fajtlowicz, “On conjectures of graﬃti II,” Congressus Numerantium, vol. 60, pp. 189–197, 1987.
[9] J. Fang, M. Rafullah, and H. M. Siddiqui, “Topological properties of sierpinski network and its application,” Combinatorial Chemistry & High Throughput Screening, vol. 25, pp. 568–578, 2022.
[10] W. Gao, S. Akhter, Z. Qasim, and A. Aslam, “The topological aspects of phthalocyanines and porphyrins dendrimers,” IEEE Access, vol. 8, pp. 168631–168649, 2020.
[11] R. Gozalbes, J. Doucet, and F. Derouin, “Application of topological descriptors in QSAR and drug design: history and new trends,” Current Drug Targets - Infectious Disorders, vol. 2, no. 1, pp. 93–102, 2002.
[12] J.-F. Zhong, A. Rauf, M. Naeem, J. Rahman, and A. Aslam, “Quantitative structure-property relationships (QSPR) of valency based topological indices with Covid-19 drugs and application,” Arabian Journal of Chemistry, vol. 14, pp. 1–16, 2021.
[13] J.-B. Liu, H. Ali, M. K. Shafiq, G. Dustigeer, and P. Ali, “On topological properties of planar octahedron networks,” Poly cyclic Aromatic Compounds, vol. 2022, pp. 1–17, 2022.
[14] M. Imran, M. Naeem, and A. Q. Baig, “Topological indices of polyhydroxybutyrate and polycaprolactone,” Journal of Information and Optimization Sciences, vol. 41, no. 4, pp. 1025–1041, 2020.
[15] M. Azeeem, A. Aslam, Z. Iqbal, M. Ahsan Binyamin, and W. Gao, “Topological aspects of 2D structures of trans-Pd(NH2)Slattice and a metal-organic superlattice,” Arabian Journal of Chemistry, vol. 14, Article ID 102963, 2021.
[16] S. A. K. Kirmani, P. Ali, and F. Azam, “Topological indices and QSPR/QSAR analysis of some antiviral drugs being investigated for the treatment of COVID-19 patients,” International Journal of Quantum Chemistry, vol. 121, no. 9, pp. 1–22, 2021.
[17] A. Yurtas, M. Togan, V. Lokesh, I. N. Cangul, and I. Gutman, “Inverse problem for Zagreb indices,” Journal of Mathematical Chemistry, vol. 57, no. 2, pp. 609–615, 2019.
[18] K. Roy, “Topological descriptors in drug design and modeling studies,” Molecular Diversity, vol. 8, no. 4, pp. 321–323, 2004.
[19] W. Gao, W. Wang, and M. R. Farahani, “Topological indices study of molecular structure in anticancer drugs,” Journal of Chemistry, vol. 2016, Article ID 3216327, 8 pages, 2016.
[20] O. C. Havare, “Topological indices and QSPR modeling of some novel drugs used in the cancer treatment,” *International Journal of Quantum Chemistry*, vol. 121, pp. 1–23, 2021.

[21] M. C. Shanmukha, A. Usha, N. S. Basavarajappa, and K. C. Shilpa, “M-polynomials and topological indices of styrene-butadiene rubber (SBR),” *Polycyclic Aromatic Compounds*, vol. 6, pp. 1–16, Article ID e04235, 2020.

[22] I. Gutman, B. Ruscic, N. Trinajstic, and C. F. Wilcox Jr., “Graph theory and molecular orbitals. XII. Acyclic polyenes,” *The Journal of Chemical Physics*, vol. 62, no. 9, pp. 3399–3405, 1975.

[23] M. Randic, “Characterization of molecular branching,” *Journal of the American Chemical Society*, vol. 97, no. 23, pp. 6609–6615, 1975.

[24] I. Gutman, B. Furtula, and C. Elphick, “Three new/old vertex–degree–based topological indices,” *MATCH Communications Mathematical and in Computer Chemistry*, vol. 72, pp. 617–632, 2014.

[25] B. Furtula, A. Graovac, and D. Vukičević, “Augmented Zagreb index,” *Journal of Mathematical Chemistry*, vol. 48, no. 2, pp. 370–380, 2010.

[26] B. Furtula and I. Gutman, “A forgotten topological index,” *Journal of Mathematical Chemistry*, vol. 53, pp. 213–220, 2015.

[27] W. Zhao, M. C. Shanmukha, A. Usha, M. R. Farahani, and K. C. Shilpa, “computing SS index of certain dendrimers,” *Journal of Mathematics*, vol. 2021, Article ID 7483508, 14 pages, 2021.

[28] I. Gutman, “Geometric approach to degree-based topological indices: Sombor indices,” *MATCH Communications Mathematical and in Computer Chemistry*, vol. 86, pp. 11–16, 2021.

[29] I. Redzepovic, “Chemical applicability of Sombor indices,” *Journal of the Serbian Chemical Society*, vol. 86, no. 5, pp. 445–457, 2021.

[30] D. Vukicevic and M. Gasperov, “Bond aditive mdelling 1. Ariatic indices,” *Croatica Chemica Acta*, vol. 83, pp. 243–260, 2010.

[31] V. Gayathri, R. Muthucumaraswamy, S. Prabhu, and M. R. Farahani, “Omega, Theta, PI, Sadhana polynomials, and subsequent indices of convex benzenoid system,” *Computational and Theoretical Chemistry*, vol. 1203, Article ID 113310, 2021.

[32] F. Harary, *Graph Theory*, Addison-Wesely, Boston, MA, USA, 1969.

[33] V. R. Kulli, *College Graph Theory*, Vishwa International Publications, Gulbarga, India, 2012.

[34] N. Trinajstic, *Chemical Graph Theory*, CRC Press, Boca Raton, FL, USA, 1992.