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Research Article

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

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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 a 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 π-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 refractivity (MR), heat of vaporization (HV), and critical pressure (CP), of which molar refractivity (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

$$M_1(G) = \sum_{vw \in E(G)} (d_v + d_w), \tag{1}$$

$$M_2(G) = \sum_{vw \in E(G)} (d_v d_w). \tag{2}$$

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

$$\mathrm{ABC}(G) = \sum_{vw \in E(G)} \sqrt{\frac{d_v + d_w - 2}{d_v d_w}}. \tag{3}$$

Definition 3. Vukicevic et al. [30] introduced

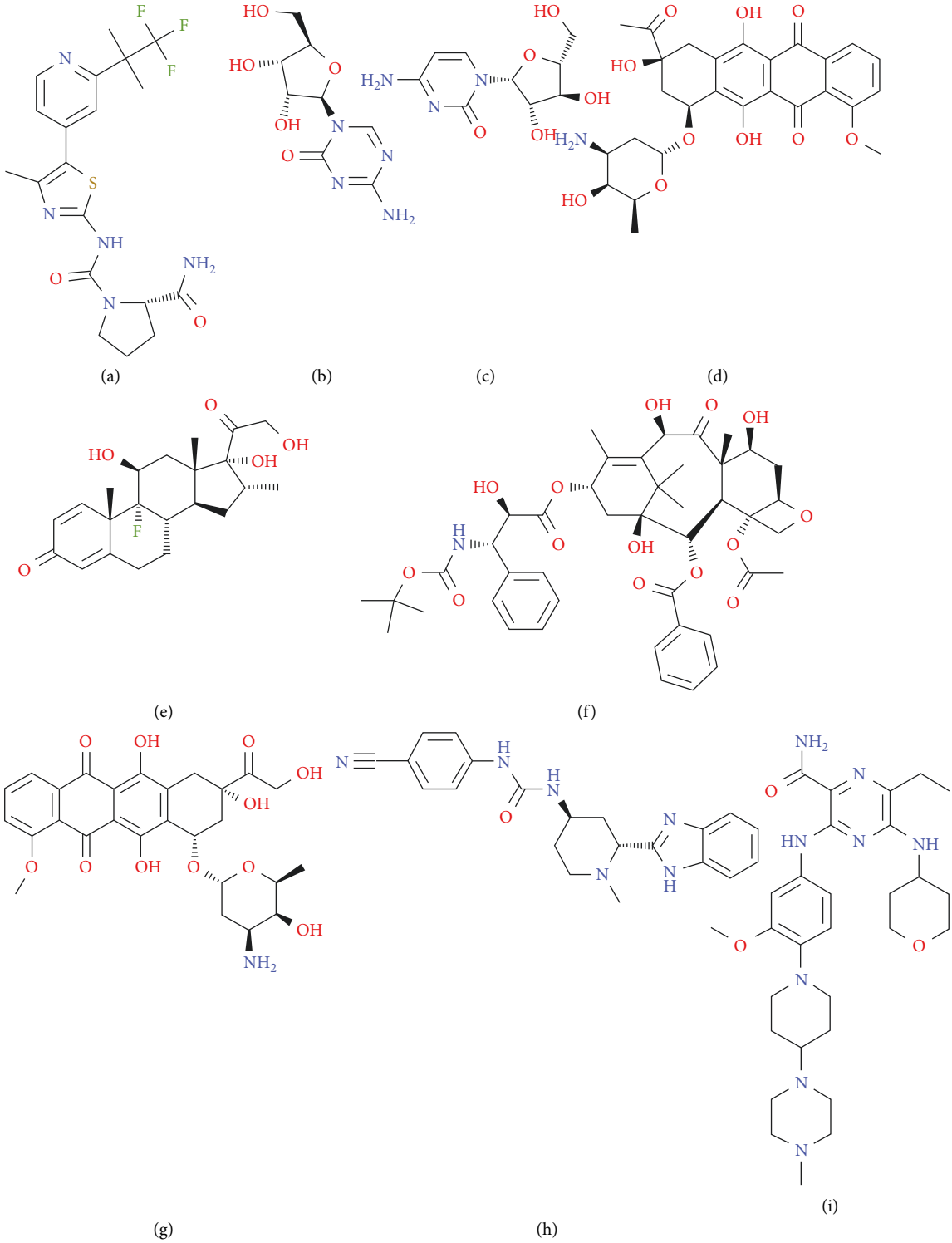
$$\mathrm{IS}(G) = \sum_{vw \in E(G)} \frac{d_v d_w}{d_v + d_w}. \tag{4}$$

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

$$\mathrm{SS}(G) = \sum_{vw \in E(G)} \sqrt{\frac{d_v d_w}{d_v + d_w}}. \tag{5}$$

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

$$\mathrm{SO}(G) = \sum_{vw \in E(G)} \sqrt{(d_v)^2 + (d_w)^2}. \tag{6}$$



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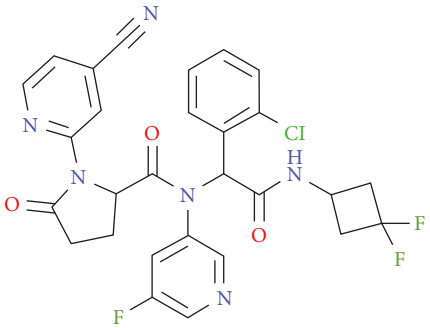

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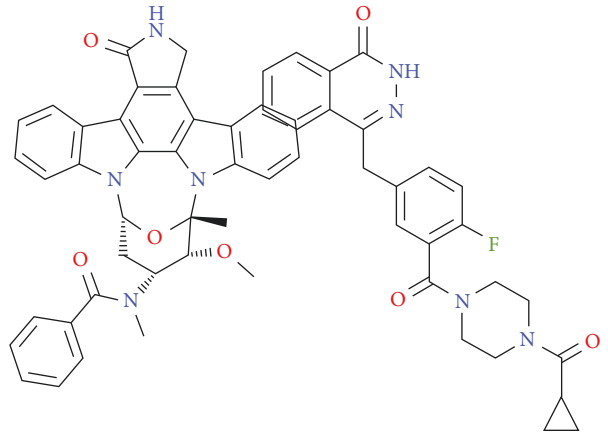

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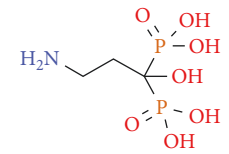

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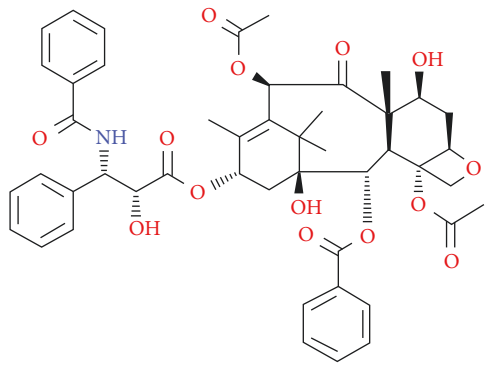

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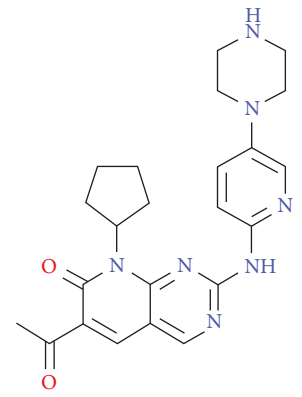

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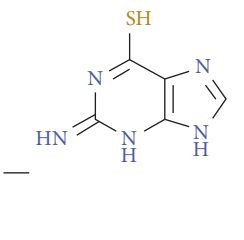

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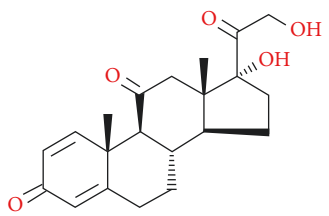

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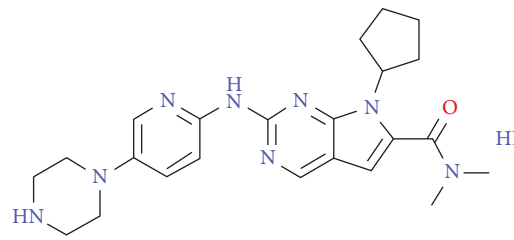

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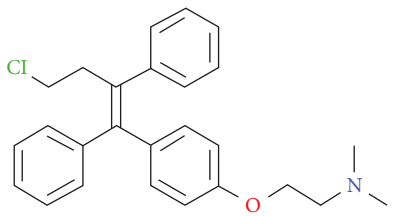

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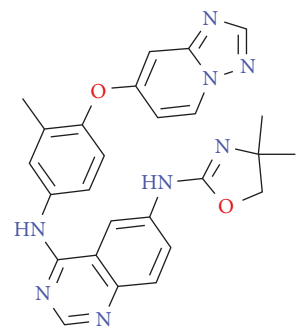

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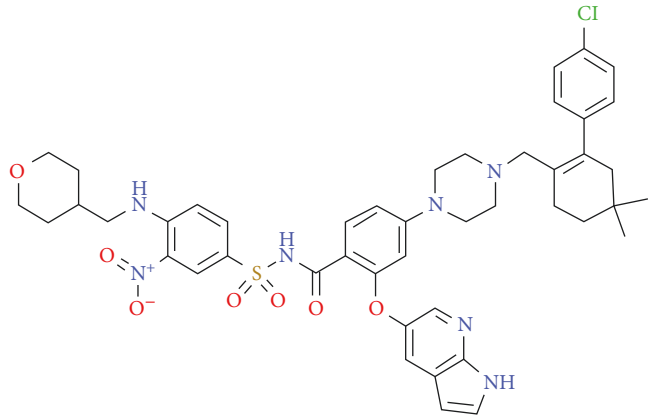

(u)

Figure 1: Molecular structures of breast cancer drugs. (a) Alpelisib. (b) Azacitidine. (c) Cytarabine. (d) Daunorubicin. (e) Dexamethasone. (f) Docetaxel. (g) Doxorubicin. (h) Glasdegib. (i) Gilteritinib. (j) Ivosidenib. (k) Midostaurin. (l) Olaparib. (m) Paclitaxel. (n) Palbociclib. (o) Pamidronic acid. (p) Prednisone. (q) Ribociclib. (r) Tioguanine. (s) Toremifene. (t) Tucatinib. (u) Venetoclax.

Table 1: Computed values of topological indices for breast cancer drugs.

Drug name	$M_1(G)$	$M_2(G)$	$R(G)$	$\mathrm{RR}(G)$	$H(G)$	$\mathrm{ABC}(G)$	$A(G)$	$F(G)$	$\mathrm{SS}(G)$	$\mathrm{SO}(G)$	$\mathrm{IS}(G)$
Alpelisib	162	178	13.914	76.786	13.002	23.501	243.092	460	33.93	119.715	36.614
Azacitidine	92	109	8.541	44.49	8.133	13.67	140.33	242	20.072	66.994	21.567
Cytarabine	88	105	8.041	42.489	7.633	12.963	142.453	234	19.072	64.166	20.567
Daunorubicin	216	270	17.89	104.068	16.919	30.174	345.43	606	45.545	157.722	50.298
Dexamethasone	160	207	12.591	76.37	11.812	21.603	254.87	480	32.767	117.69	36.605
Docetaxel	319	391	26.702	151.612	24.998	45.219	486.765	923	66.36	235.358	72.419
Doxorubicin	220	275	17.971	106.2	17.486	30.771	358.054	614	46.591	160.401	51.414
Glasdegib	145	171	12.911	71.004	12.6	21.311	240.922	369	32.22	104.53	34.8
Gilteritinib	210	247	19.44	102.81	18.93	31.198	358.47	532	46.87	151.404	50.383
Ivosidenib	226	275	19.75	109.509	18.367	32.199	366.3	612	45.652	164.23	53.22
Midostaurin	266	349	20.903	130.503	20.374	35.623	471.18	744	56.8	188.54	64.13
Olaparib	176	212	15.508	86.12	15.067	25.57	296.625	456	38.789	126.906	42.2
Paclitaxel	337	411	29.083	161.874	27.645	48.34	537.83	941	71.713	246.643	78.04
Palbociclib	180	217	16.025	88.221	15.6	26.236	308.016	464	39.823	129.595	43.3
Pamidronic acid	64	74	5.561	28.243	4.8	9.408	78.519	216	12.061	49.712	12.6
Prednisone	151	202	11.252	73.012	10.945	19.762	254.75	451	31.172	109.98	35.388
Ribociclib	174	208	15.597	85.388	15.233	49.996	297.86	444	38.698	125.158	41.95
Tioguanine	58	68	5.271	28.161	5.067	8.623	93.531	150	12.754	40.25	13.7
Toremifene	142	162	14.186	69.823	13.9	21.977	252.312	344	32.497	101.962	34.367
Tucatinib	202	239	17.416	98.18	16.9	29.26	325.68	532	44.154	146.484	47.82
Venetoclax	334	394	29.298	160.574	28.252	48.771	535.931	886	72.763	242.909	78.514

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

$$A(G) = \sum_{vw \in E(G)} \left\{ \frac{d_v d_w}{d_v + d_w - 2} \right\}^3. \tag{7}$$

Definition 7. Randic [23] introduced

$$R(G) = \sum_{vw \in E(G)} \frac{1}{\sqrt{d_v d_w}}. \tag{8}$$

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

$$\mathrm{RR}(G) = \sum_{vw \in E(G)} \sqrt{d_v d_w}. \tag{9}$$

Definition 9. Harmonic index [8] is given by

$$H(G) = \sum_{vw \in E(G)} \frac{2}{d_v + d_w}. \tag{10}$$

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

$$F(G) = \sum_{vw \in E(G)} (d_v)^2 + (d_w)^2. \tag{11}$$

Table 2: Physicochemical properties of breast cancer drugs.

SI no	Drug name	BP	EV	FP	MR	LogP	MV
1	Alpelisib	—	—	—	106.7	−0.02	317.4
2	Azacitidine	534.5	93.2	277	51.1	−1.99	117.1
3	Cytarabine	545.7	94.8	283.8	52.6	−1.93	128.4
4	Daunorubicin	770	117.6	419.5	130	2.92	339.4
5	Dexamethasone	568.2	98	297.5	100.2	1.87	296.2
6	Docetaxel	900.5	137.1	498.4	205.2	6.55	585.7
7	Doxorubicin	810.3	123.5	443.8	131.5	2.82	336.6
8	Glasdegib	633.4	93.6	336.9	106.9	2.77	281
9	Gilteritinib	696.9	102.1	375.3	157.8	4.35	444.9
10	Ivosidenib	854.3	124.1	470	140.1	0.38	383.6
11	Midostaurin	—	—	—	160.3	5.27	385.7
12	Olaparib	—	—	—	116.9	0	301.8
13	Paclitaxel	957.1	146	532.6	219.3	7.38	610.6
14	Palbociclib	711.5	104	384.1	123.9	0.99	340.7
15	Pamidronic acid	658.7	111	352.2	40.9	−3.4	117.6
16	Prednisone	573.7	98.7	314.8	94.1	1.57	273.6
17	Ribociclib	730.8	106.7	395.8	123.4	−0.74	311.4
18	Tioguanine	460.7	72.1	232.4	41.9	−0.99	80.2
19	Toremifene	535.1	81.2	277.4	123.7	7.82	367.6
20	Tucatinib	—	—	—	135.2	3.62	339
21	Venetoclax	—	—	—	234.4	10.88	647.7

2. Results and Discussion

In this work, topological indices are computed for chemical structures of drugs used in the treatment of breast cancer. The QSPR 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, dexamethasone, docetaxel, doxorubicin, glasdegib, gilteritinib, ivosidenib, midostaurin, olaparib, paclitaxel, palbociclib, pamidronic acid, prednisone, ribociclib, tioguanine, toremifene, tucatinib, and venetoclax. The molecular structure of these drugs is represented in Figure 1.

The analysis includes computing 11 indices such as $M_1(G)$, $M_2(G)$, $R(G)$, $\mathrm{RR}(G)$, $H(G)$, $\mathrm{ABC}(G)$, $A(G)$, $F(G)$, $\mathrm{SS}(G)$, $\mathrm{SO}(G)$, and $\mathrm{IS}(G)$. 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.

$$\begin{aligned}
E_{1,2} &= \{e = vw \in E(a) | d_v = 1, d_w = 2\},\\
E_{1,3} &= \{e = vw \in E(a) | d_v = 1, d_w = 3\},\\
E_{1,4} &= \{e = vw \in E(a) | d_v = 1, d_w = 4\},\\
E_{2,2} &= \{e = vw \in E(a) | d_v = 2, d_w = 2\},\\
E_{2,3} &= \{e = vw \in E(a) | d_v = 2, d_w = 3\},\\
E_{2,4} &= \{e = vw \in E(a) | d_v = 2, d_w = 4\},\\
E_{3,3} &= \{e = vw \in E(a) | d_v = 3, d_w = 3\},\\
E_{3,4} &= \{e = vw \in E(a) | d_v = 3, d_w = 4\},
\end{aligned} \tag{12}$$

such that

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
Log$P$	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
Log$P$	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
Log$P$	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
Log$P$	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
Log$P$	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

Table 8: Statistical specifications for the linear model of ABC(G).

Physical properties	N	A	b	r	r^2	F	p	Indicator	SE
BP	16	439.633	9.227	0.823	0.678	29.487	0.000	Significant	85.675
EV	16	77.576	1.092	0.729	0.532	15.908	0.001	Significant	13.807
FP	16	221.533	5.543	0.824	0.679	29.649	0.000	Significant	51.321
MR	21	15.643	3.868	0.902	0.814	82.965	0.000	Significant	23.63
Log$P$	21	−3.013	0.193	0.656	0.431	14.376	0.001	Significant	2.839
MV	21	34.986	10.699	0.871	0.759	59.765	0.000	Significant	77.017

Table 9: Statistical specifications for the linear model of $A(G)$.

Physical properties	N	A	b	r	r^2	F	p	Indicator	SE
BP	16	407.355	0.979	0.870	0.756	43.408	0.000	Significant	74.567
EV	16	72.527	0.120	0.799	0.638	24.727	0.000	Significant	12.133
FP	16	201.489	0.591	0.874	0.763	45.187	0.000	Significant	44.073
MR	21	2.965	0.397	0.976	0.953	385.282	0.000	Significant	11.87
Log$P$	21	−4.491	0.023	0.81	0.656	36.154	0.000	Significant	2.209
MV	21	−1.773	1.102	0.948	0.898	166.851	0.000	Significant	50.138

Table 10: Statistical specifications for the linear model of $F(G)$.

Physical properties	N	A	b	r	r^2	F	p	Indicator	SE
BP	16	413.222	0.568	0.895	0.8	56.059	0.000	Significant	67.500
EV	16	71.046	0.074	0.876	0.768	46.383	0.000	Significant	9.717
FP	16	204.811	0.343	0.9	0.81	59.708	0.000	Significant	39.494
MR	21	8.754	0.225	0.95	0.903	176.218	0.000	Significant	17.081
Log$P$	21	−3.965	0.012	0.764	0.584	26.695	0.000	Significant	2.427
MV	21	10.357	0.634	0.934	0.872	128.961	0.000	Significant	56.192

$$\begin{aligned}
|E_{1,2}| &= 2,\\
|E_{1,3}| &= 8,\\
|E_{1,4}| &= 1,\\
|E_{2,2}| &= 2,\\
|E_{2,3}| &= 12,\\
|E_{2,4}| &= 2,\\
|E_{3,3}| &= 15,\\
|E_{3,4}| &= 1.
\end{aligned} \tag{13}$$

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. The 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. □

3. Regression Models

The linear regression model is given by

$$P = A + b(\mathrm{TI}), \tag{14}$$

where P, A, b, TI ⟶ 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.

(I) First Zagreb index $M_1(G)$:

$$\begin{aligned}
\mathrm{BP} &= 402.789 + 1.616[M_1(G)],\\
\mathrm{EV} &= 71.022 + 0.204[M_1(G)],\\
\mathrm{FP} &= 198.864 + 0.974[M_1(G)],\\
\mathrm{MR} &= 2.517 + 0.648[M_1(G)],\\
\mathrm{Log}P &= -4.399 + 0.036[M_1(G)],\\
\mathrm{MV} &= -5.607 + 1.816[M_1(G)].
\end{aligned} \tag{15}$$

Table 11: Statistical specifications for the linear model of SS(G).

Physical properties	N	A	b	r	r^2	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
Log$P$	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	r^2	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
Log$P$	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	r^2	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
Log$P$	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 $M_2(G)$:

$$\begin{aligned} \mathrm{BP} &= 409.985 + 1.292\left[M_2(G)\right], \\ \mathrm{EV} &= 71.424 + 0.165\left[M_2(G)\right], \\ \mathrm{FP} &= 202.841 + 0.780\left[M_2(G)\right], \\ \mathrm{MR} &= 7.446 + 0.512\left[M_2(G)\right], \\ \mathrm{Log}P &= -4.12 + 0.029\left[M_2(G)\right], \\ \mathrm{MV} &= 9.845 + 1.427\left[M_2(G)\right]. \end{aligned} \tag{16}$$

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

$$\begin{aligned} \mathrm{BP} &= 398.262 + 18.974\left[R(G)\right], \\ \mathrm{EV} &= 71.492 + 2.325\left[R(G)\right], \\ \mathrm{FP} &= 196.716 + 11.395\left[R(G)\right], \\ \mathrm{MR} &= -2.012 + 7.809\left[R(G)\right], \\ \mathrm{Log}P &= -4.730 + 0.442\left[R(G)\right] \\ \mathrm{MV} &= -19.917 + 21.976\left[R(G)\right]. \end{aligned} \tag{17}$$

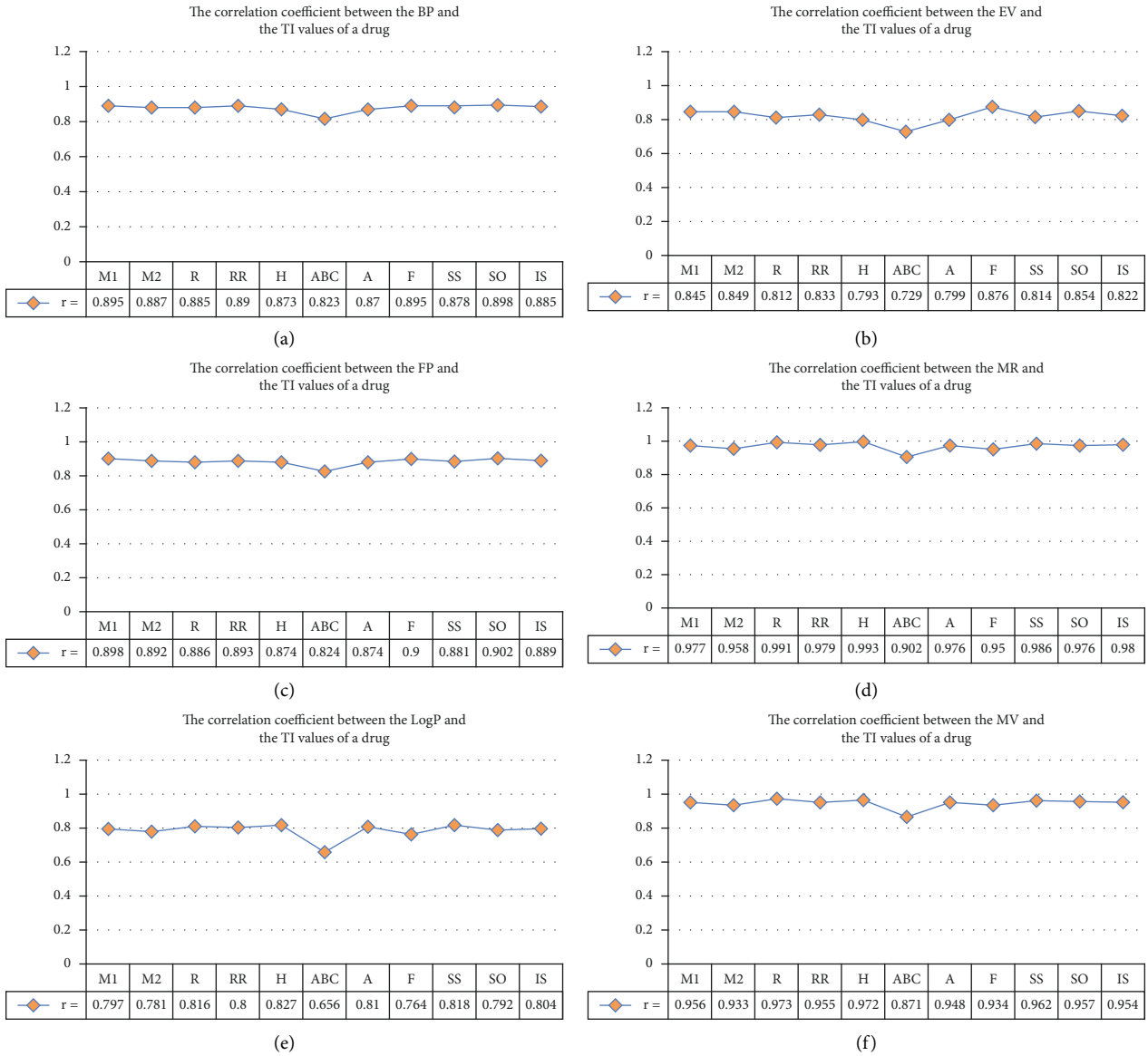

Figure 2: Topological indices and physicochemical properties of breast cancer drugs.

(IV) Reciprocal Randic index $RR(G)$:

$$\begin{aligned} BP &= 403.211 + 3.343[RR(G)],\\ EV &= 71.367 + 0.418[RR(G)],\\ FP &= 199.12 + 2.014[RR(G)],\\ MR &= 2.078 + 1.347[RR(G)],\\ LogP &= -4.439 + 0.076[RR(G)],\\ MV &= -6.008 + 3.763[RR(G)]. \end{aligned} \tag{18}$$

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

$$\begin{aligned} BP &= 400.808 + 19.683[H(G)],\\ EV &= 72.158 + 2.387[H(G)],\\ FP &= 198.199 + 11.824[H(G)],\\ MR &= -2.119 + 8.158[H(G)],\\ LogP &= -4.812 + 0.467[H(G)],\\ MV &= -19.156 + 22.889[H(G)]. \end{aligned} \tag{19}$$

(VI) Atom bond connectivity index $ABC(G)$:

$$\begin{aligned}
\mathrm{BP} &= 439.633 + 9.227[\mathrm{ABC}(G)],\\
\mathrm{EV} &= 77.576 + 1.092[\mathrm{ABC}(G)],\\
\mathrm{FP} &= 221.533 + 5.543[\mathrm{ABC}(G)],\\
\mathrm{MR} &= 15.643 + 3.868[\mathrm{ABC}(G)],\\
\mathrm{Log}P &= -3.013 + 0.193[\mathrm{ABC}(G)],\\
\mathrm{MV} &= 34.986 + 10.699[\mathrm{ABC}(G)].
\end{aligned} \tag{20}$$

(VII) Augmented Zagreb index $A(G)$:

$$\begin{aligned}
\mathrm{BP} &= 407.355 + 0.979[A(G)],\\
\mathrm{EV} &= 72.527 + 0.120[A(G)],\\
\mathrm{FP} &= 201.489 + 0.591[A(G)],\\
\mathrm{MR} &= 2.965 + 0.397[A(G)],\\
\mathrm{Log}P &= -4.491 + 0.023[A(G)],\\
\mathrm{MV} &= -1.773 + 1.102[A(G)].
\end{aligned} \tag{21}$$

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

$$\begin{aligned}
\mathrm{BP} &= 413.222 + 0.568[F(G)],\\
\mathrm{EV} &= 71.046 + 0.074[F(G)],\\
\mathrm{FP} &= 204.811 + 0.343[F(G)],\\
\mathrm{MR} &= 8.754 + 0.225[F(G)],\\
\mathrm{Log}P &= -3.965 + 0.012[F(G)],\\
\mathrm{MV} &= 10.357 + 0.634[F(G)].
\end{aligned} \tag{22}$$

(IX) SS index $\mathrm{SS}(G)$:

$$\begin{aligned}
\mathrm{BP} &= 403.887 + 7.542[\mathrm{SS}(G)],\\
\mathrm{EV} &= 71.803 + 0.934[\mathrm{SS}(G)],\\
\mathrm{FP} &= 202.841 + 0.780[\mathrm{SS}(G)],\\
\mathrm{MR} &= 0734 + 3.071[\mathrm{SS}(G)],\\
\mathrm{Log}P &= -4.620 + 0175[\mathrm{SS}(G)],\\
\mathrm{MV} &= -9.715 + 8.58[\mathrm{SS}(G)].
\end{aligned} \tag{23}$$

(X) Somber index $\mathrm{SO}(G)$:

$$\begin{aligned}
\mathrm{BP} &= 403.876 + 2.211[\mathrm{SO}(G)],\\
\mathrm{EV} &= 70.907 + 0.281[\mathrm{SO}(G)],\\
\mathrm{FP} &= 199.511 + 1.332[\mathrm{SO}(G)],\\
\mathrm{MR} &= 3.071 + 0.888[\mathrm{SO}(G)],\\
\mathrm{Log}P &= -4.342 + 0.050[\mathrm{SO}(G)],\\
\mathrm{MV} &= -5.060 + 2.495[\mathrm{SO}(G)].
\end{aligned} \tag{24}$$

(XI) Inverse indeg index $\mathrm{IS}(G)$:

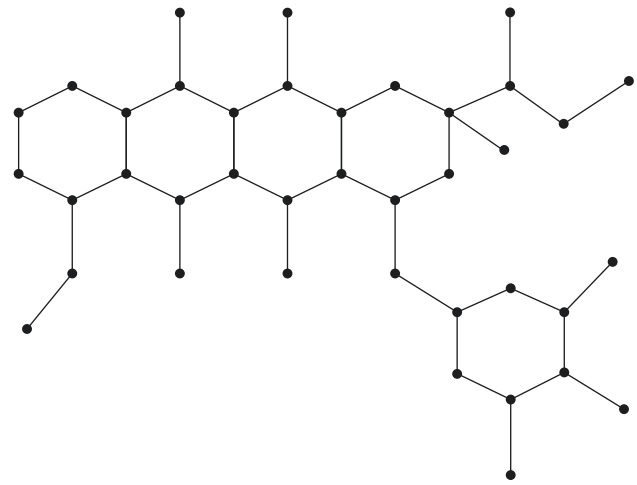

Figure 3: Molecular graph of Figure 1(g): doxorubicin.

$$\begin{aligned}
\mathrm{BP} &= 403.935 + 6.883[\mathrm{IS}(G)],\\
\mathrm{EV} &= 71.717 + 0.855[\mathrm{IS}(G)],\\
\mathrm{FP} &= 199.559 + 4.148[\mathrm{IS}(G)],\\
\mathrm{MR} &= 2.259 + 2.771[\mathrm{IS}(G)],\\
\mathrm{Log}P &= -4.456 + 0.156[\mathrm{IS}(G)],\\
\mathrm{MV} &= -4.813 + 7.726[\mathrm{IS}(G)].
\end{aligned} \tag{25}$$

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 TI's. 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 $\mathrm{SO}(G)$ with $r = 0.902$, while MR with $H(G)$ has high correlation with $r = 0.993$, Log$P$ 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 $\mathrm{ABC}(G)$ 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 Douhadji was responsible for formal analysis, resources, and software.

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