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Quantitative Structure Property Relationship Modeling Of Certain Novel Anticancer Drugs Using Molecular Descriptors

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Abstract: *A topological index is a numerical value linked to molecular graphs, capable of predicting the physicochemical and biological properties of various anticancer medications, such as those used for treating blood, breast, and skin cancers. In this paper, intercorrelation between the Balban index B(G), connective eccentric index (CEI), eccentricity connectivity index (ECI), harmonic index (H(G)), hyper Zagreb index $HZ(G)$, first path Zagreb index (FP_1), second path Zagreb index (FP_2), Randic index ($R(G)$), sum connectivity index (SCI(G)), graph energy (E(G)) and Laplacian energy (LE(G)) is studied on the set of molecular graphs of anticancer drugs. Moreover, we also discuss the QSPR analysis and carry the linear regression modeling for the physicochemical properties of anticancer drugs with 9 degree based and 2 eigenvalue based topological indices.*

Keywords: *Anticancer drug, molecular graph, topological index, QSPR-analysis.*

1 INTRODUCTION

Cancer ranks among the leading causes of death globally due to disease. Despite the discovery of numerous chemotherapeutic drugs that target unchecked cell division, their severe side effects pose a significant drawback. Additionally, resistance to multiple drugs presents another critical challenge in cancer treatment. Due to issues such as cytotoxicity and drug resistance, extensive research is underway to find and develop more effective anticancer medications. Symptoms of this disease include the presence of masses, abnormal bleeding, persistent coughing, and unexplained weight loss. Major causes of this malignant illness include tobacco use, obesity, poor dietary habits, sedentary lifestyles, and excessive alcohol consumption. Various treatments such as surgery, radiotherapy, chemotherapy, hormone therapy, and targeted therapy are available to combat this life-threatening disease. Anticancer drugs specifically aim to treat cancer and are categorized into classes such as alkylates and metabolites. Chemical graph theory, a branch of mathematical chemistry, plays a role in characterizing anticancer drugs by defining topological indices, aiding in understanding their physical and chemical properties.B.Basavanagouda.et[1], E.Estrada.et[7],W.Gao.et[8], M.C.Shanmukha.et [15].

A numerical descriptor serves as a mathematical tool to analyze the structure of chemical compounds, offering insights into their physicochemical properties without the necessity of extensive and expensive laboratory experiments. These descriptors, represented by real numbers, provide valuable information about molecules.
Topological indices (TIs) come in various types, such as degree-based, neighborhood degree-based, distance-based, and eigenvalue-based indices. They are utilized in models that link chemical structures to biological activities and other properties, facilitating a deeper understanding of compound behavior and characteristics.B.Basavanagouda et al.[2],E.Estrada et al.[7], Li et al.[13],Shashank kumar et al.[17],Sumiya Nasir et al.[19],R.Todeschini[21].

2 . METHODOLOGY

Definition 2.1 : The Balban index [4,5] is defined as

$$B(G) = \frac{m}{m-n+2}\sum_{uv\in E}\frac{1}{\sqrt{w(u)w(v)}}$$

where the sum is taken over all edges of a connected graph G, n and m are the cardinalities of the vertex and the edge set of G, respectively, and $w(u)$ (resp. $w(v)$) denotes the sum of distances from u (resp. v) to all the other vertices of G.

Definition 2.2: Connective eccentricity index (CEI)[12] of a graph G is defined as

$$\xi^{ce}(G) = \sum_{v\in V(G)}\frac{d_G(v)}{\varepsilon(v)}$$

where $d_G(v)$ and $\varepsilon(v)$ are the degree and eccentricity of a vertex v respectively.

Definition 2.3: Eccentricity connectivity index (ECI)[16] of a graph G is defined as

$$\xi^{c}(G) = \sum_{v\in V(G)}\varepsilon(v)d_G(v)$$

where $d_G(v)$ and $\varepsilon(v)$ are the degree and eccentricity of a vertex v respectively.

Definition2.4: Harmonic Index $H(G)$ of a graph G is defined as[14]

$$H(G) = \sum_{u\sim v}\frac{2}{d_u(G)+d_v(G)}$$

Definition 2.5: Hyper Zagreb Indexv(HZ)[18] of a graph G is defined as

$$HZ(G) = \sum_{uv\in E(G)}[d_G(u)+d_G(v)]^2$$

Definition 2.6: First path Zagreb Index (FP_1)[20] of a graph G is defined as

$$FP_1(G) = \sum_{v\in V(G)}d_2(v/G)^2$$

Definition 2.7: Second path Zagreb Index (FP_2)[20] of a graph G is defined as

$$FP_2(G) = \sum_{uv\in E(G)}d_2(u/G)d_2(v/G)$$

Definition 2.8: Randic′ Index (R)[14] of a graph G is defined as

$$R(G) = \sum_{u\sim v}\frac{1}{\sqrt{d_G(u)d_G(v)}}$$

Definition 2.9: Sum Connectivity Index (SCI)[6] of a graph G is defined as

$$SCI(G) = \sum_{u\sim v}\frac{1}{d_u(G)+d_G(v)}$$

Definition 2.10: Graph Energy (E)[11] of a graph G is defined as

$$E(G) = \sum_{i=1}^{n}|\lambda_i|$$

Definition 2.11: Laplacian Energy (LE)[10]: of a graph G is defined as

$$LE(G) = \sum_{i=1}^{n}|\mu_i - \frac{2m}{n}|$$

Table 1. Various anticancer drugs with physico-chemical Properties.

Sl. 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		116.2	436	9.116
4	Carmustine	309.6	120.99	63.8	141	46.6
5	Caulibugulone E	373	129.46	62	179.4	52.2
6	Convulutamide A	629.9		97.9	334.7	130.1
7	Convolutamine F	387.7	128.67	63.7	188.3	73.8
8	Convolutamydine 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	78.4	264	67.6
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

3. DATA SETS:

We examined 17 anticancer drugs ranging from Amathaspiramide-E to Tambjamine-K, gathering their physico-chemical properties from Chem Spider, as detailed in Table 1. The structures corresponding to these drugs are conveniently illustrated in Table 2. For our analysis, we have considered the topological indices mentioned in the Definitions 1-11. These indices were used to model five representative physical properties—Boiling point (BP), Melting point (MP), Enthalpy (E), Flash point (FP), and Molar refraction (MR)—of the aforementioned 17 anticancer drugs.

We list in Table 3 the above mentioned topological indices values of molecular graphs of 17 anticancer drugs. The considered topological indices values of anticancer drugs were computed manually by employing definition of each topological index.

4. STATISTICAL PARAMETERS

The effectiveness of the chosen topological indices in correlating with the normal properties (Boiling point, Melting point, Enthalpy, Flash point, and Molar refraction) of the 17 anticancer drugs from Amathaspiramide-E to Tambjamine-K was assessed using linear correlations with the SAS procedure. The quality of each model was evaluated using statistical measures such as the correlation coefficient (r) and the standard error of estimate (s). The models that exhibited the highest correlation coefficients and the lowest standard errors of estimate were selected as the most accurate models for predicting these physical properties based on the structural descriptors derived from the topological indices.

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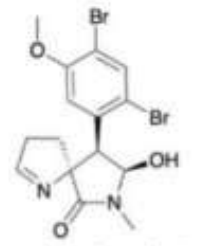
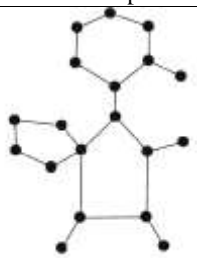
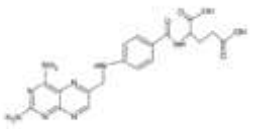
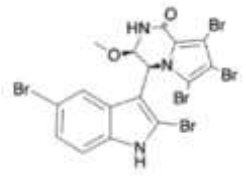
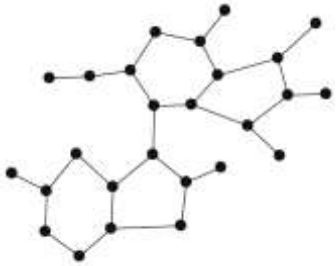
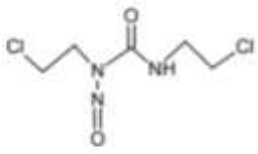
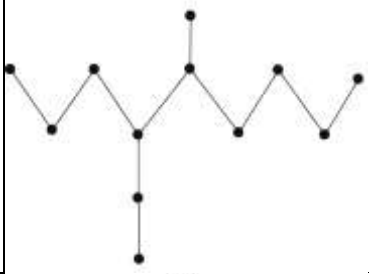
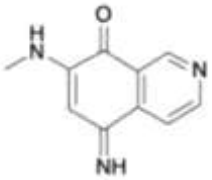
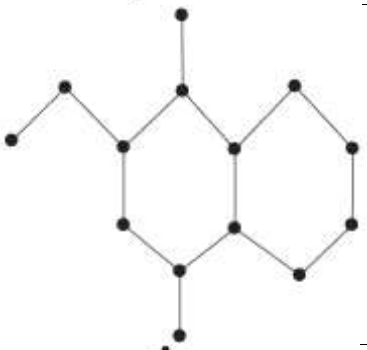
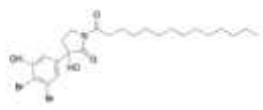
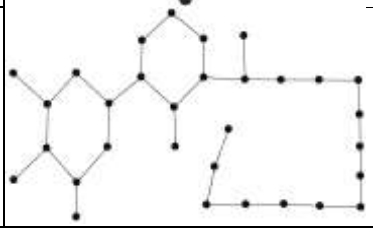
Table 2. Various anticancer drugs with their molecular graphs

Cancer Drug	Molecular Graphs
 (a) Amathaspiramide E	
 (b) Aminopterin	
 (c) Aspidostomide E	
 (d) Carmustine	
 (e)Caulibugulone E	
 (f) Convolutamide A	

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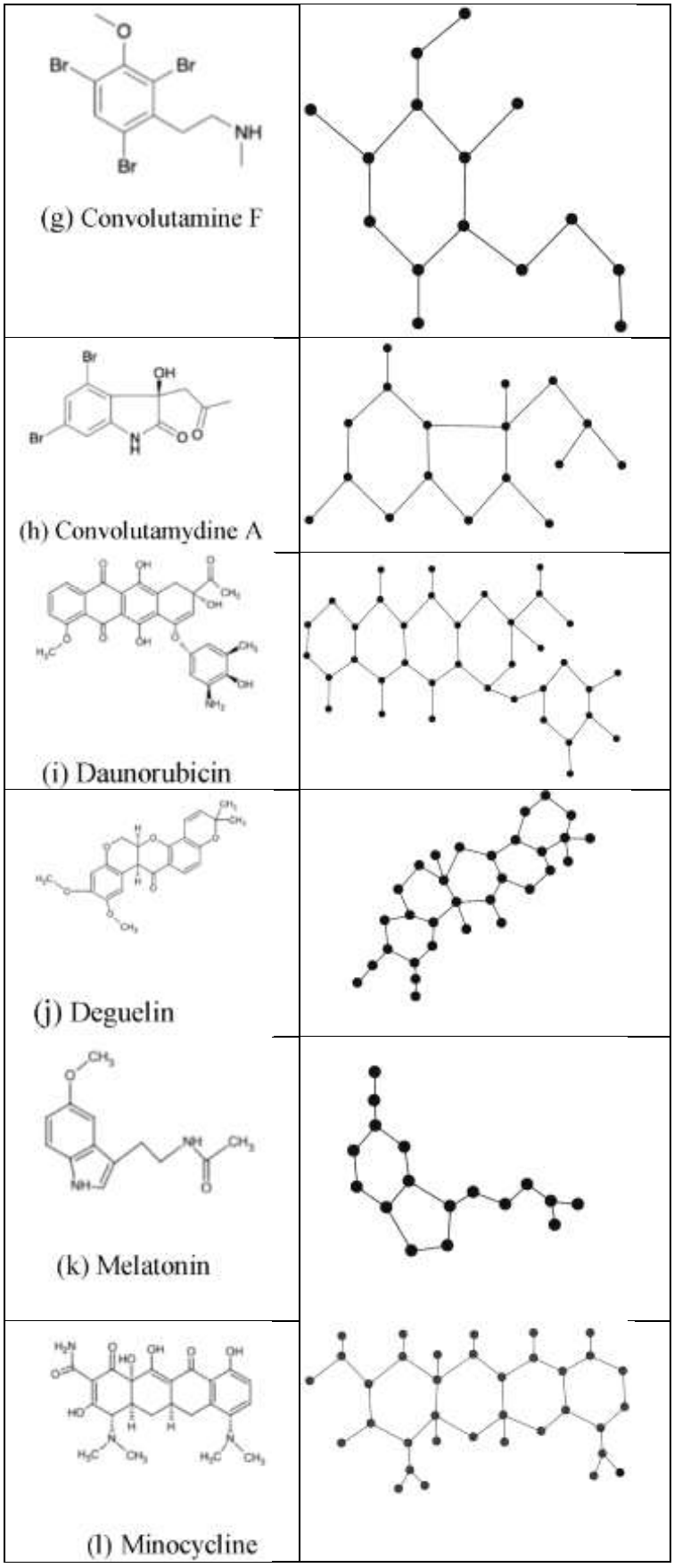

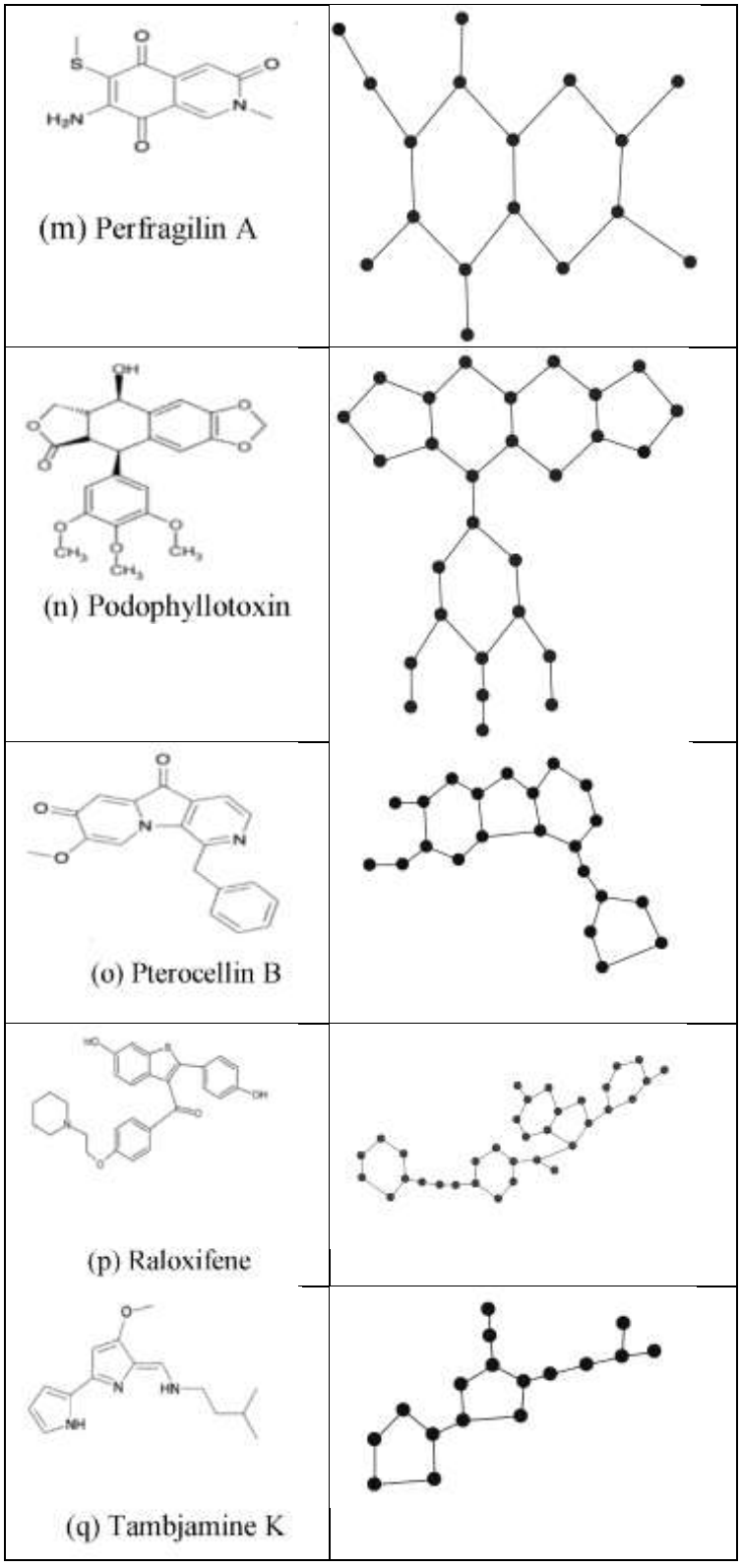
(m) Perfragilin A
(n) Podophyllotoxin
(o) Pterocellin B
(p) Raloxifene
(q) Tambjamine K

Table 3. Various Anticancer drugs with Topological Indices values.

Drugs	B	CEI	ECI	H	HZ	FP_1	FP_2	R	SCI	E	LE
Amathaspiramide E	3.83	7.71	236	8.7	560	64	195	9.08	9.51	24.72	24.72
Aminopterin	2.75	4.9	870	13.7	734	88	215	14.31	14.77	36.14	37.86
Aspidostomide E	3.39	8.44	410	11.77	778	90	278	12.35	13	34.07	33.62
Carmustine	7.2	3.91	129	5.53	202	24	50	5.76	5.48	14.39	14.39
Caulibugulone E	4.17	6.08	153	6.5	358	42	116	6.74	6.95	16.84	18.26
Convolutamide A	3.33	4.2	1072	14.83	726	86	218	15.38	15.58	40.19	40.19
Convolutamine F	5.21	5.23	179	6.77	324	40	103	7.11	7.08	17.84	17.84
Convolutamydine A	4.44	6.48	207	7.27	486	56	155	7.84	8.06	20.11	19.75
Daunorubicin	2.95	8.09	857	16.35	1128	130	385	17.35	18.24	46.46	46.46
Deguelin	2.89	7.26	703	13.89	1128	114	331	14.63	15.5	26.16	39.89
Melatonin	3.57	5.01	269	7.93	402	48	122	8.2	8.42	21.6	21.6
Minocycline	3.71	8.92	666	14.79	1142	128	403	16.04	16.67	40.19	41.49
Perfragilene A	4.4	6.37	210	7.5	466	54	11	7.97	8.17	21.2	21.2
Podophylotoxi n	2.94	8.23	577	14.17	878	102	317	14.57	15.43	39.83	39.91
Pterocellin B	3.06	7.08	396	10.9	648	76	226	11.19	15.43	30.55	30.55
Raloxifene	2.3	5.89	1019	16.2	890	106	291	16.58	1.5	44.97	44.97
Tambjamine K	3.67	5.5	246	7.93	402	48	122	8.2	8.42	21.48	21.48

Note: B: Balban index, CEI: Connective eccentric index, ECI: Eccentric connective index, H: Harmonic index, HZ: Hyper Zagreb index, FP_1: First path Zagreb index, FP_2: Second path Zagreb index, R: Randic′ index, SCI: Sum-connectivity index, E: Graph Energy, LE: Laplacian Energy.

5. RESULTS AND DISCUSSION

In this section, first we consider the intercorrelation between the topological indices. This test will help to select the useful topological indices for the study.

5.1. Intercorrelation between considered topological indices

The dataset presented in Table 3 was used to analyze the correlations among the topological indices mentioned in the Definitions 1-11. The strength of these correlations was evaluated using correlation coefficient r. Pairs of indices with $r \geq 0.993$ were considered highly correlated, those with $r > 0.9$ were categorized as appreciably correlated, indices with $r < 0.9$ were considered weakly correlated, and indices with $r < 0.5$ were deemed not correlated.

Table 4. Correlation matrix of selected topological indices.

	B	CEI	ECI	H	HZ	FP_1	FP_2	R	SCI	E	LE
B	1	-0.415	-0.680	-0.759	-0.700	-0.725	-0.663	-0.746	-0.443	-0.725	-0.769
CEI		1	0.077	0.401	0.651	0.637	0.680	0.423	0.495	0.417	0.444
ECI			1	**0.937**	0.764	0.799	0.700	0.930	0.456	0.883	**0.920**
H				1	**0.918**	**0.946**	0.880	**0.999**	0.593	**0.957**	**0.998**
HZ					1	**0.993**	**0.944**	**0.932**	0.673	0.829	**0.934**
FP_1						1	**0.949**	**0.958**	0.665	0.887	**0.959**
FP_2							1	0.890	0.656	0.827	0.892
R								1	0.611	**0.954**	**0.998**
SCI									1	0.539	0.606
E										1	**0.952**
LE											1

The data in Table 4 shows the correlation coefficients among various graph indices, highlighting the strength of

intercorrelations. Here are the key points:

1. Eccentric Connective Index: Intercorrelated with Laplacian energy (r=0.937) and (r=0.920) respectively).

2. Harmonic Index: Highly intercorrelated with Randic index and Laplacian energy (r=0.999) and r=0.998) respectively). Appreciably intercorrelated with hyper Zagreb and first path Zagreb indices (r=0.918) and (r=0.946) respectively).

3. Hyper Zagreb Index: Highly intercorrelated with first path Zagreb index (r > 0.98). Appreciably intercorrelated with second path Zagreb index and Randic index (r=0.944) and (r=0.932) respectively.

4. First Path Zagreb Index: Appreciably intercorrelated with second path Zagreb index, Randic index, and Laplacian energy (r=0.949), (r=0.958), and (r=0.959) respectively.

5. Randic Index: Highly intercorrelated with Laplacian energy (r=0.998). Appreciably intercorrelated with graph energy (r=0.954).

6. Graph Energy: Appreciably intercorrelated with Laplacian energy (r=0.952).

These correlations indicate strong relationships between these indices, suggesting they may provide overlapping or related information about the graph properties.

6. REGRESSION MODELS

Balban Index

$$BP = -0.689(BI) - 97.493(\pm 26.469) \quad (1)$$
$$MP = -0.666(BI) - 36.146(\pm 11.689) \quad (2)$$
$$E = -0.580(BI) - 10.435(\pm 3.920) \quad (3)$$
$$FP = -0.110(BI) - 69.978(\pm 168.346) \quad (4)$$
$$MR = -0.744(BI) - 18.51(\pm 4.289) \quad (5)$$

Table 5. Statistical parameters for the Balban index

Physical Properties	R	S	F	p	Indicator
BP	0.689	121.54	13.56	0.002	Significant
MP	0.666	53.19	9.56	0.009	Significant
E	0.580	17.54	7.08	0.019	Significant
FP	0.110	753.28	0.17	0.684	Not-significant
MR	**0.744**	19.69	18.62	0.001	Significant

The best mono-parametric correlation is obtained for BP, MP, E and MR whereas there is no good model to predict the flash point of selected anticancer drugs. The statistical parameters shows that the models (1)-(3) and (5) are significant with $p < 0.05$. The highest correlation coefficient value of Balban index is 0.744 for molar refraction of anticancer drugs.

Connective Eccentric Index

$$BP = 0.513(CEI) + 54.489(\pm 23.542) \quad (6)$$
$$MP = 0.361(CEI) + 17.039(\pm 12.698) \quad (7)$$
$$E = 0.629(CEI) + 8.578(\pm 2.832) \quad (8)$$
$$FP = -0.110(CEI) - 52.896(\pm 127.499) \quad (9)$$
$$MR = 0.365(CEI) + 6.807(\pm 4.490) \quad (10)$$

Table 6. Statistical parameters for connective eccentric index

Physical Properties	R	S	F	p	Indicator
BP	0.513	143.97	5.35	0.035	Significant
MP	0.361	66.49	1.80	0.204	Not-significant
E	0.629	16.73	9.17	0.009	Significant
FP	0.110	753.3	0.172	0.685	Not-significant
MR	0.365	27.45	2.29	0.150	Not-significant

For connective eccentric index the statistical test revealed that the models (6) and (8) are significant with $p < 0.05$. The highest correlation coefficient value of connective eccentric index is 0.629 for enthalpy of anticancer drugs.

Eccentric Connective Index

$$BP = 0.751(ECI) + 0.378(\pm 0.086) \quad (11)$$
$$MP = 0.789(ECI) + 0.174(\pm 0.39) \quad (12)$$
$$E = 0.726(ECI) + 0.048(\pm 0.012) \quad (13)$$
$$FP = -0.096(ECI) - 0.221(\pm 0.614) \quad (14)$$
$$MR = 0.914(ECI) + 0.081(\pm 0.009) \quad (15)$$

Table 7. Statistical parameters for eccentric connective index

Physical Properties	R	S	F	p	Indicator
BP	0.751	110.78	19.38	0.001	Significant
MP	0.789	43.85	19.72	0.001	Significant
E	0.726	14.79	15.62	0.001	Significant
FP	0.096	754.45	0.12	0.725	Not-significant
MR	**0.914**	11.99	75.65	0.000	Significant

The eccentric connective index is highly significant for the models (11)-(13) and (15) with $p < 0.05$. The highest correlation coefficient value of eccentric connective index is 0.914 for molar refraction of anticancer drugs.

Harmonic Index

$$BP = 0.849(H) + 36.436(\pm 5.860) \quad (16)$$
$$MP = 0.769(H) + 13.307(\pm 3.197) \quad (17)$$
$$E = 0.843(H) + 4.574(\pm 0.779) \quad (18)$$
$$FP = -0.098(H) - 18.737(\pm 50.797) \quad (19)$$
$$MR = 0.955(H) + 7.204(\pm 0.589) \quad (20)$$

Table 8. Statistical parameters for harmonic index

Physical Properties	R	S	F	p	Indicator
BP	0.849	88.68	38.65	0.000	Significant
MP	0.769	45.61	17.32	0.001	Significant
E	0.843	11.57	34.43	0.000	Significant
FP	0.098	754.26	0.13	0.718	Not-significant
MR	**0.955**	8.78	153.84	0.000	Significant

The harmonic index is highly significant for the models (16)-(18) and (20) with $p < 0.05$. The highest correlation coefficient value of harmonic index is 0.955 for molar refraction of anticancer drugs.

Hyper Zagreb Index

$$BP = 0.814(HZ) + 0.444(\pm 0.082) \quad (21)$$

$$MP = 0.688(HZ) + 0.147(\pm 0.045) \quad (22)$$
$$E = 0.830(HZ) + 0.056(\pm 0.010) \quad (23)$$
$$FP = -0.131(HZ) - 0.312(\pm 0.632) \quad (24)$$
$$MR = 0.842(HZ) + 0.081(\pm 0.013) \quad (25)$$

Table 9. Statistical parameters for hyper Zagreb Index

Physical Properties	R	S	F	p	Indicator
BP	0.814	97.48	29.40	0.000	Significant
MP	0.688	51.71	10.81	0.006	Significant
E	0.830	12.01	30.93	0.000	Significant
FP	0.131	751.41	0.24	0.629	Not-significant
MR	**0.842**	15.92	36.46	0.000	Significant

The hyper Zagreb index is highly significant for the models (21)-(23) and (25) with $p < 0.05$. The highest correlation coefficient value of hyper Zagreb index is 0.842 for molar refraction of anticancer drugs.

First Path Zagreb Index

$$BP = 0.855(FP_1) + 4.283(\pm 0.082) \quad (26)$$
$$MP = 0.727(FP_1) + 1.430(\pm 0.390) \quad (27)$$
$$E = 0.868(FP_1) + 0.541(\pm 0.083) \quad (28)$$
$$FP = 0.123(FP_1) - 2.706(\pm 5.823) \quad (29)$$
$$MR = 0.881(FP_1) + 0.775(\pm 0.108) \quad (30)$$

Table 10. Statistical parameters for first path Zagreb index

Physical Properties	R	S	F	p	Indicator
BP	0.855	86.87	40.91	0.000	Significant
MP	0.727	49.99	13.42	0.003	Significant
E	0.868	10.70	42.65	0.000	Significant
FP	0.123	752.14	0.21	0.649	Not-significant
MR	**0.881**	13.96	51.86	0.000	Significant

The first path Zagreb index is highly significant for the models (26)-(28) and (30) with $p < 0.05$. The highest correlation coefficient value of first path Zagreb index is 0.881 for molar refraction of anticancer drugs.

Second Path Zagreb Index

$$BP = 0.815(FP_2) + 1.156(\pm 0.212) \quad (31)$$
$$MP = 0.641(FP_2) + 0.357(\pm 0.123) \quad (32)$$
$$E = 0.858(FP_2) + 0.151(\pm 0.024) \quad (33)$$
$$FP = -0.099(FP_2) - 0.614(\pm 1.647) \quad (34)$$
$$MR = 0.827(FP_2) + 0.206(\pm 0.036) \quad (35)$$

Table 11. Statistical parameters for second path Zagreb index

Physical Properties	R	S	F	p	Indicator
BP	0.815	97.17	29.68	0.000	Significant
MP	0.641	54.72	8.38	0.013	Significant
E	**0.858**	11.06	38.98	0.000	Significant
FP	0.099	754.18	0.13	0.715	Not-significant
MR	0.827	16.57	32.47	0.000	Significant

The second path Zagreb index is highly significant for the models (31)-(33) and (35) with $p < 0.05$. The highest correlation coefficient value of second path Zagreb index is 0.858 for enthalpy of anticancer drugs.

Randic Index

$BP = 0.859(R) + 35.17(\pm 5.410)$ (36)
$MP = 0.774(R) + 12.767(\pm 3.012)$ (37)
$E = 0.856(R) + 4.429(\pm 0.714)$ (38)
$FP = -0.102(R) - 18.630(\pm 48.408)$ (39)
$MR = 0.952(R) + 6.851(\pm 0.570)$ (40)

Table 12. Statistical parameters for Randic index

Physical Properties	R	S	F	p	Indicator
BP	0.859	85.84	42.26	0.000	Significant
MP	0.774	45.12	17.96	0.001	Significant
E	0.856	11.11	38.49	0.000	Significant
FP	0.102	753.99	0.14	0.706	Not-significant
MR	**0.952**	9.03	144.71	0.000	Significant

The Randic index is highly significant for the models (36)-(38) and (40) with $p < 0.05$. The highest correlation coefficient value of Randic index is 0.952 for molar refraction of anticancer drugs.

Sum Connectivity Index

$BP = 0.546(SCI) + 18.492(\pm 7.325)$ (41)
$MP = 0.397(SCI) + 5.346(\pm 3.572)$ (42)
$E = 0.502(SCI) + 2.153(\pm 0.990)$ (43)
$FP = -0.082(SCI) - 12.339(\pm 40.182)$ (44)
$MR = 0.514(SCI) + 3.058(\pm 1.319)$ (45)

Table 13. Statistical parameters for sum connectivity index

Physical Properties	R	S	F	p	Indicator
BP	**0.546**	140.51	6.37	0.023	Significant
MP	0.397	65.46	2.24	0.160	Not-significant
E	0.502	18.61	4.72	0.047	Significant
FP	0.082	755.37	0.09	0.763	Not-significant
MR	0.514	25.29	5.37	0.035	Significant

The sum connectivity index is significant for the models (41), (43) and (45) with $p < 0.05$. The highest correlation coefficient value of sum connectivity index is 0.546 for boiling points of anticancer drugs.

Graph Energy

$BP = 0.874(E) + 13.498(\pm 1.938)$ (46)
$MP = 0.762(E) + 4.765(\pm 1.169)$ (47)
$E = 0.885(E) + 1.719(\pm 0.242)$ (48)
$FP = -0.081(E) - 5.508(\pm 18.225)$ (49)
$MR = 0.942(E) + 2.558(\pm 0.235)$ (50)

Table 14. Statistical parameters for graph energy

Physical Properties	R	S	F	p	Indicator
BP	0.874	81.51	48.5	0.000	Significant
MP	0.762	46.17	16.61	0.002	Not-significant
E	0.885	10.03	50.43	0.000	Significant
FP	0.081	755.45	0.09	0.767	Not-significant
MR	**0.942**	9.87	118.74	0.000	Significant

The graph energy is highly significant for the models (46), (48) and (50) with $p < 0.05$. The highest correlation coefficient value of graph energy is 0.942 for molar refraction of anticancer drugs.

Laplacian Energy

$$BP = 0.854(LE) + 12.775(\pm 2.011) \quad (51)$$
$$MP = 0.758(LE) + 4.548(\pm 1.129) \quad (52)$$
$$LE = 0.848(LE) + 1.599(\pm 0.268) \quad (53)$$
$$FP = -0.107(LE) - 7.082(\pm 17.652) \quad (54)$$
$$MR = 0.949(LE) + 2.496(\pm 0.214) \quad (55)$$

Table 15. Statistical parameters for Laplacian energy

Physical Properties	R	S	F	p	Indicator
BP	0.854	87.36	40.29	0.000	Significant
MP	0.758	46.50	16.22	0.002	Significant
E	0.848	11.42	35.72	0.000	Significant
FP	0.107	753.59	0.16	0.694	Not-significant
MR	**0.949**	9.30	135.51	0.000	Significant

The Laplacian index is highly significant for the models (51)-(53) and (55) with $p < 0.05$. The highest correlation coefficient value of Laplacian index is 0.949 for molar refraction of anticancer drugs.

7 . CONCLUSION

The following results are obtained:

• We established that the pairs consisting of (harmonic index and Randic index), (harmonic index and Laplacian energy), (hyper Zagreb index and first path Zagreb index), (Randic index and Laplacian energy) are highly intercorrelated for the studied molecules; the correlation coefficients being greater than 0.97.
• The best mono-parametric structure-boiling point correlations in all topological index is graph energy though the standard error of estimate was 81.54.
• The selected topological indices shown good prediction power for molar refraction of anticancer drugs.
• It appears that the selected topological indices are not particularly useful in the linear structure-flash point modeling of anticancer drugs.

8. REFERENCES

[1] S. P. B Basavanagouda, "Topological indices of some anticancer drugs," Ratio Mathematica, vol. 42, no. 22, pp. 29-59, 2022.
[2] S. P. B. Basavanagoud, "Chemical applicability of Gourava and hyper-Gourava indices," NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, vol. 12, no. 2, p. 142–150, 2021.
[3] A. T. B. James Devillers, "Historical Development of Topological Indices," in Topological Indices and Related Descriptors in QSAR and QSPR, United kingdom, Taylor's Francis group, 1999, pp. 21-57.
[4] A. T. Balaban, "Highly discriminating distance-based topological index," Chemical Physics Letters, vol. 89, no. 5, pp. 399-404, 1982.
[5] A. T. Balaban, "Topological indices based on topological distances in molecular graphs," Pure and Applied Chemistry, vol. 55, no. 2, pp. 199-206, 1983.
[6] S. D. B. Z. Kinkar Ch. Das, " Sum–connectivity index of a graph," Frontiers of Mathematics in China , vol. 11, no. 1, pp. 47-54, 2016.
[7] U. E. Estrada E, "Recent advances on the role of topological indices in drug discovery research," Current medicinal chemistry, vol. 8, no. 13, pp. 1573-88, 2001.
[8] W. W. M. R. F. Wei Gao, "Topological Indices Study of Molecular Structure in Anticancer Drugs," Journal of chemistry, vol. 2016, no. 1, p. 8, 2016.
[9] H. W. ,. M. K. S. ,. A. Q. B. Wei Gao, "Study of biological networks using graph theory," Saudi Journal of Biological sciences, vol. 25, no. 6, pp. 1212-1219, 2018.
[10] B. Z. Ivan Gutman, "Laplacian energy of a graph," Linear Algebra and its Applications, vol. 414, no. 1, pp. 29-37, 2006.
[11] G. I. Ivan Gutman, "The Energy of a Graph: Old and New Results," in Algebraic Combinatorics and Applications, Berlin, Heidelberg, , Springer , 2001, p. 196–211.
[12] L. F. Guilhai Yu, "On the Connective Eccentricity Index of Graphs," MATCH Communications in Mathematical and in Computer Chemistry, vol. 69, no. 3, pp. 611-628, 2013.

[13] Y. A. S. G. S. Li, "Targeting highly resisted anticancer drugs through topological descriptors using VIKOR multi-criteria decision analysis," The European Physical Journal Plus, vol. 137, no. 11, p. 1245, 2022.
[14] M. Randic, "Characterization of molecular branching," Journal of the American Chemical Society, vol. 97, no. 23, p. 6609–6615, 1975.
[15] N. S. B. K. C. S. A. U. M. C. Shanmukha, "Degree-based topological indices on anticancer drugs with QSPR analysis," Heliyon, vol. 6, no. 6, p. e04235, 2020.
[16] R. G. a. A. K. M. Vikas Sharma, "Eccentric Connectivity Index: A Novel Highly Discriminating Topological Descriptor for Structure−Property and Structure−Activity Studies," Journal of Chemical Information and Computer Sciences, vol. 37, no. 2, p. 273–282, 1997.
[17] M. K. A. W. K. P. Shashank Kumar, "Drug Targets for Cancer Treatment: An Overview," Medicinal chemistry, vol. 5, no. 3, pp. 115-123, 2015.
[18] H. R. a. A. M. S. G. H. Shirdel, "The Hyper-Zagreb Index of Graph Operations," Iranian Journal of Mathematical chemistry, vol. 4, no. 2, pp. 213-220, 2013.
[19] N. u. H. A. F. B. F. S. P. Sumiya Nasir, "Topological indices of novel drugs used in blood cancer treatment and its QSPR modeling," AIMS Mathematics, vol. 7, no. 7, pp. 11829-11850, 2022.
[20] D. S. N. Vukicevic, "On the path-Zagreb matrix," Journal of Mathematical chemistry, vol. 45, no. 2, pp. 538-543, 2009.
[21] D. V. C. Prof. Dr. Roberto Todeschini, Handbook of Molecular Descriptorsy, Hoboken, New Jersey, United States: Willey -Methods and Principles in Medicinal Chemistr, 2000.