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Predicting Physico-Chemical Properties of Anti-Cancer Drugs Using Distance-Based Topological Indices

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Abstract Topological Indices are one of the best molecular descriptors which are widely used in the study of structural properties of various chemicals. Also, they are very much useful in QSPR/QSAR studies. Among several topological indices, distance-based indices are emerging and attracted researchers across the world. In this article, we study the recently introduced sixteen different distance-based topological indices for eleven anti-cancer drugs and also performed QSPR analysis to identify the best predictors for the physico-chemical properties namely, Molar Refractivity, Complexity, Molar Volume, Heavy Atom Count, Monoisotopic Mass and Topological Polar Surface Area with the help of those computed values of the indices.

Index Terms connection number, Zagreb connection indices, distance-based indices, anti-cancer drugs

I. Introduction

The study of the topological indices on the chemical structure of chemical materials and drugs can make up for the lack of chemical experiments and can provide a theoretical basis for the manufacturing of drugs and chemical materials. These results remedy the lack of chemical and medical experiments by providing the theoretical basis for pharmaceutical engineering. Determining the chemical properties of new drugs requires a large number of chemical experiments, thereby greatly increasing the workload of chemical and pharmaceutical researchers. The chemical-based experiments found that there was a strong connection between topological molecular structures and their physical behaviours, chemical characteristics, biological features, and toxicity of drugs.

The human body is made up of trillions of cells that grow and divide as needed throughout a lifetime before dying when they get old or aberrant. Cancer is a disease that occurs when one or more cells lose their ability to control their growth, which can result in haematological malignancies or solid masses of cells known as tumours. If the old or aberrant cells do not die, cancer develops as the cells continue to produce new cells [1]. These cancer cells grow out of control, crowding out healthy cells and causing the body to malfunction. Cancer-causing agents are known as carcinogens. Tobacco smoke contains carcinogens which are chemical substances that cause cancer. It can spread throughout the body.

Global Cancer Observatory (GLOBOCAN) predictions for 2020 state that there were 19.3 million incident cases of cancer worldwide. India placed in third place, after the US and China. According to GLOBOCAN's prediction, the number of cases of cancer in India is projected to grow to 2.08 million by 2040, reflecting a 57.7% increase from 2020.

An anticancer drug, also called an antineoplastic drug, is any drug that is effective in the treatment of malignant, or cancerous, disease. There are several major classes of anti-cancer drugs; these include alkylating agents, antimetabolites, natural products, and hormones. Most anticancer drugs are administered intravenously, but some can be taken orally and others can be injected intramuscularly or intrathecally (within the spinal cord) [2].

An alkylating drug called carmustine is used to treat many cancers, including multiple myeloma and brain tumours. It functions by reducing or halting the proliferation of cancer cells. One class of medication used to prevent breast cancer is referred to as a selective oestrogen receptor modulator (SERM), and it is raloxifene. It can inhibit the hormone oestrogen. Podophyllum peltatum is the source of podophyllotoxin, a well-known naturally occurring aryltetralin lignans that is utilised as a chemotherapeutic treatment for a range of malignancies. An anthracycline antibiotic called daunorubicin is mostly used to treat leukaemias, namely acute myeloid leukaemia (AML).

The specificity of anticancer drugs plays an important role in reducing the severity of side effects associated with the drugs. Indeed, because cancer cells are similar to normal human cells and can cause numerous side effects, some of

which are life-threatening.

Shanmukha et al. [3] computed some degree-based topological indices for anticancer drugs and presented QSAR analysis of their computations. Bokhary et al. [4] performed a QSPR analysis of drugs used for the treatment of breast cancer. Zaman et al. [5] made of some degree-based topological indices and regression models in the QSPR analysis of certain drugs used in the treatment of blood cancer. Miladiyah et al. [6] Investigated anti-cancer properties of xanthone derivatives. Dhanajayamurthy et al. [7] investigated QSPR analysis of anti-cancer drugs using some reduced neighbourhood degree-based topological indices. Havare [8] studied QSPR modelling of some drugs used in the treatment of cancer using recently introduced topological indices. Huang et al. [9] explored QSPR modelling of a set of new antiviral drugs for cancer treatment using topological indices. Zhang et al. [10] applied curve fitting models to analyze the physico-chemical properties of certain anti-cancer drugs using some degree-based indices.

The first, second, and third leap Zagreb indices were introduced in 2017 by Gutman et al. [11] and are defined as follows:

$$ZC_1(G) = \sum_{v \in V(G)} \tau(v)^2,$$

$$ZC_2(G) = \sum_{uv \in E(G)} \tau(u)\tau(v),$$

$$ZC_3(G) = \sum_{v \in V(G)} d_v \tau(v),$$

where $\tau(v)$ represents the connection number of the vertex v, (i.e.) the number of vertices that are at a distance two from v in G. Further d_v represents the degree of a vertex v in G. These indices are also known as Zagreb connection indices. Inspired by the F-index, in 2018, Kulli [12] presented the F-leap index as follows:

$$FL(G) = \sum_{v \in V(G)} \tau(v)^3.$$

Reciprocal leap Zagreb indices of a graph are introduced in 2021 by Ammar Alsinai et al. [13].

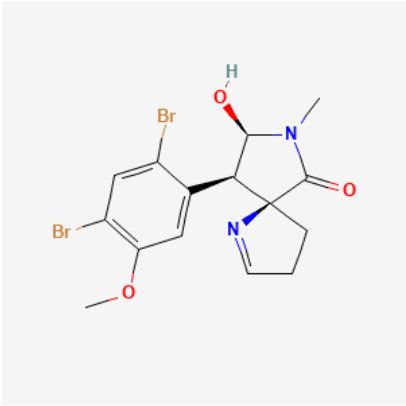
$$RL_1(G) = \sum_{v \in V(G)} \frac{1}{(\tau(v)+1)^2},$$

$$RL_2(G) = \sum_{uv \in E(G)} \frac{1}{(\tau(u)+1)(\tau(v)+1)},$$

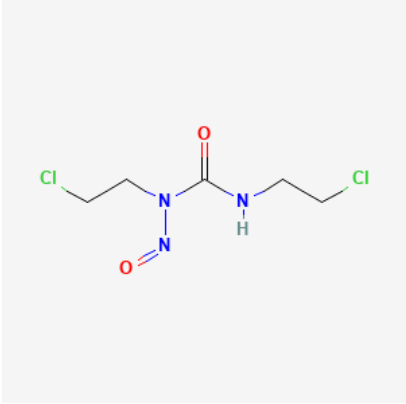
$$RL_3(G) = \sum_{v \in V(G)} \frac{1}{d_v(\tau(v)+1)}.$$

V.R. Kulli [14] introduced the first and second leap-hyper Zagreb indices in 2018 as

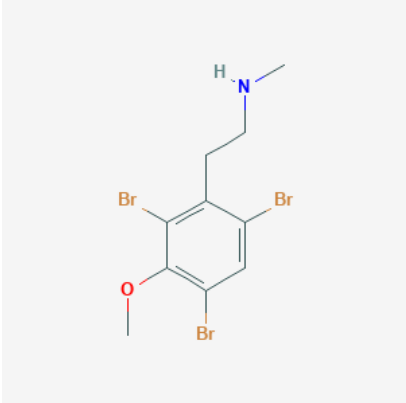
$$HLM_1(G) = \sum_{uv \in E(G)} [\tau(u)+\tau(v)]^2,$$



(a) $\mathcal{D}_1$: Amathaspiramide E



(b) $\mathcal{D}_2$: Carmustine



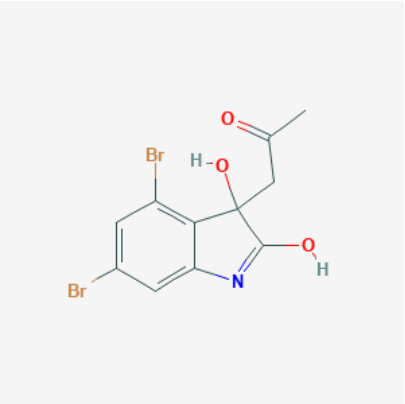
(c) $\mathcal{D}_3$: Convolutamine F

$$HLM_2(G) = \sum_{uv \in E(G)} [\tau(u)\tau(v)]^2.$$

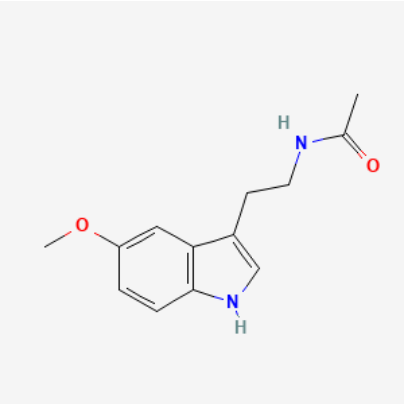
For a few nanostructures, Basavanagoud and Chitra [15] subsequently computed the leap hyper-Zagreb indices. In 2019, Kulli et al. [16] computed the leap hyper-Zagreb indices for particular windmill graphs.

The geometric-arithmetic leap indices and sum connectivity indices of a graph are defined by Kulli [17] in 2019. They are described as

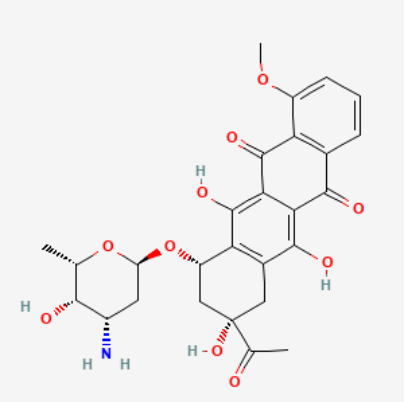
$$SL(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\tau(u)+\tau(v)}},$$



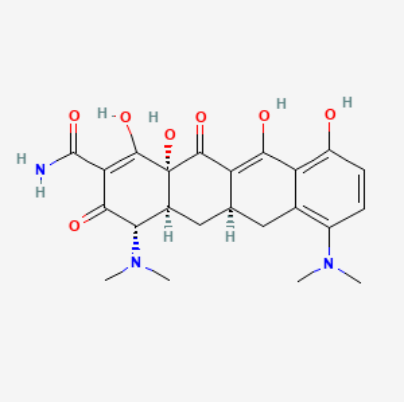
(d) $\mathcal{D}_4$:Convolutamydine A



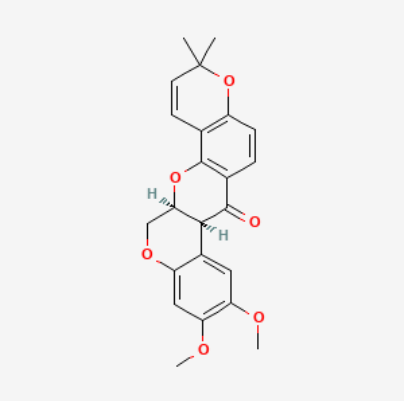
(g) $\mathcal{D}_7$:Melatonin



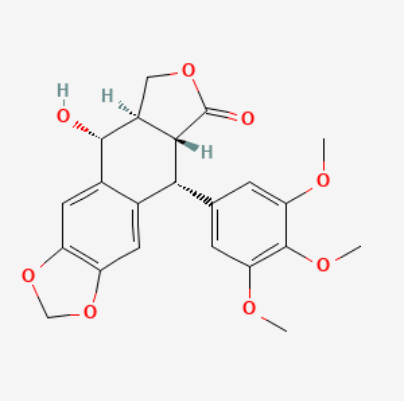
(e) $\mathcal{D}_5$:Daunorubicin



(h) $\mathcal{D}_8$:Minocycline



(f) $\mathcal{D}_6$:Deguelin



(i) $\mathcal{D}_9$:Podophyllotoxin

$$GAL(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\tau(u)\tau(v)}}{\tau(u) + \tau(v)}.$$

In 2018, Kulli [18] introduced the Product connectivity leap index and atom bond connectivity (ABC) leap index, which are presented below.

$$PL(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\tau(u)\tau(v)}},$$

$$ABCL(G) = \sum_{uv \in E(G)} \frac{\sqrt{\tau(u) + \tau(v) - 2}}{\tau(u)\tau(v)}.$$

Dayan et al. [20] formulated the first and second leap Gourava indices of graphs, which are influenced by Kulli's [19] Gourava indices. Additionally, for a few wheel-related graphs, they calculated jump Gourava indexes in 2018. The aforementioned indices have the following definitions:

$$LG_1(G) = \sum_{uv \in E(G)} [\tau(u) + \tau(v)] + [\tau(u)\tau(v)],$$

$$LG_2(G) = \sum_{uv \in E(G)} [\tau(u) + \tau(v)][\tau(u)\tau(v)].$$

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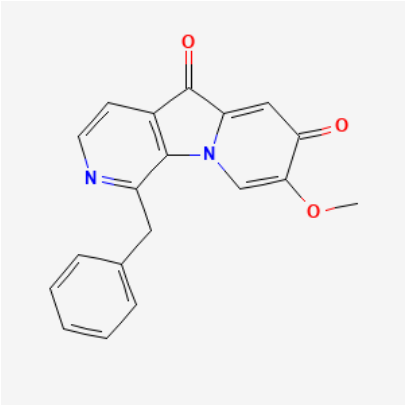
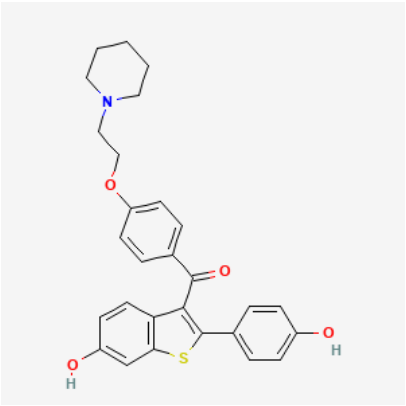


(j) $\mathcal{D}_{10}$:Pterocellin B



(k) $\mathcal{D}_{11}$:Raloxifene

Figure 1: Molecular graphs of anti-cancer drugs

The Sombor leap index was established in 2022 by Kulli [21] and is provided below:

$$SOL(G) = \sum_{uv \in E(G)} \sqrt{\tau(u)^2 + \tau(v)^2}.$$

In this article, we compute the aforementioned 16 distance-based topological indices for the 11 anti-cancer drugs listed in Table 1 using vertex and edge partitions. Further, we conduct a thorough QSPR analysis to identify the best predictors for the physico-chemical properties: Molar Refractivity, Complexity, Molar Volume, Heavy Atom Count, Monoisotopic Mass and Topological Polar Surface Area of the chosen anti-cancer drugs.

Drugs/Connection no.	1	2	3	4	5	6	7
Amathaspiramide ($\mathcal{D}_1$)	1	8	2	7	2	1	1
Carmustine ($\mathcal{D}_2$)	5	3	3	1	-	-	-
Convolutamine F ($\mathcal{D}_3$)	3	5	3	2	2	-	-
Convolutamydine A ($\mathcal{D}_4$)	1	6	2	5	2	-	1
Daunorubicin ($\mathcal{D}_5$)	1	11	7	11	4	4	-
Deguelin ($\mathcal{D}_6$)	2	4	7	10	5	1	-
Melatonin ($\mathcal{D}_7$)	2	4	6	4	1	-	-
Minocycline ($\mathcal{D}_8$)	-	14	4	5	4	6	-
Podophyllotoxin ($\mathcal{D}_9$)	3	6	5	10	4	2	-
Pterocellin B ($\mathcal{D}_{10}$)	1	8	5	6	3	1	-
Raloxifene ($\mathcal{D}_{11}$)	-	9	16	6	2	1	-

Table 1: Connection number based vertex partition

$(\tau(u), \tau(v))$	$\mathcal{D}_1$	$\mathcal{D}_2$	$\mathcal{D}_3$	$\mathcal{D}_4$	$\mathcal{D}_5$	$\mathcal{D}_6$	$\mathcal{D}_7$	$\mathcal{D}_8$	$\mathcal{D}_9$	$\mathcal{D}_{10}$	$\mathcal{D}_{11}$
(1,1)	-	2	1	-	-	-	-	-	-	-	-
(1,2)	1	2	2	2	1	2	3	-	3	1	-
(1,3)	-	1	-	-	-	-	1	-	-	-	-
(1,5)	-	-	-	1	-	-	-	-	-	-	-
(2,2)	1	-	-	1	-	-	2	6	-	2	4
(2,3)	2	2	3	1	6	2	-	1	3	5	7
(2,4)	5	1	1	3	6	4	1	2	3	2	2
(2,5)	1	-	1	-	-	1	-	3	1	-	-
(2,6)	-	-	-	-	-	-	-	2	-	-	-

Table 2: Connection number-based edge partition

$(\tau(u), \tau(v))$	$\mathcal{D}_1$	$\mathcal{D}_2$	$\mathcal{D}_3$	$\mathcal{D}_4$	$\mathcal{D}_5$	$\mathcal{D}_6$	$\mathcal{D}_7$	$\mathcal{D}_8$	$\mathcal{D}_9$	$\mathcal{D}_{10}$	$\mathcal{D}_{11}$
(3,3)	-	1	-	-	-	2	2	2	2	2	11
(3,4)	3	2	2	1	10	4	5	-	2	4	4
(3,5)	1	-	3	1	1	2	-	1	1	1	1
(3,6)	-	-	-	-	-	-	-	2	1	-	-
(3,7)	-	-	-	1	-	-	-	-	-	-	-
(4,4)	2	-	-	3	1	5	1	2	7	2	3
(4,5)	2	-	2	1	5	6	3	1	6	4	3
(4,6)	2	-	-	-	8	2	-	6	1	1	1
(4,7)	1	-	-	1	-	-	-	-	-	-	-
(5,5)	-	-	-	1	1	2	-	1	1	1	-
(5,6)	1	-	-	-	2	1	-	5	2	2	2
(5,7)	1	-	-	1	-	-	-	-	-	-	-
(6,6)	-	-	-	-	1	-	-	2	1	-	-
(6,7)	1	-	-	-	-	-	-	-	-	-	-

Table 3: Connection number-based edge partition contd

$(deg(v), \tau(v))$	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9	D_{10}	D_{11}
(1,1)	1	3	2	-	1	2	1	-	3	1	-
(1,2)	5	1	3	5	9	1	2	11	2	2	3
(1,3)	-	-	-	1	1	2	-	1	-	-	-
(2,1)	-	2	1	-	-	-	-	-	-	-	-
(2,2)	3	2	2	-	2	2	2	-	4	5	4
(2,3)	-	2	1	-	2	5	6	2	4	4	14
(2,4)	4	-	1	3	3	4	1	2	4	3	2
(2,5)	-	-	-	1	2	1	-	-	-	-	-
(3,1)	-	-	-	1	-	-	1	-	-	-	-
(3,2)	-	-	-	1	-	-	-	3	-	-	2
(3,3)	2	1	2	1	4	-	-	1	1	2	2
(3,4)	3	1	1	2	7	6	3	3	6	3	4
(3,5)	2	-	2	-	2	4	1	4	4	3	2
(3,6)	-	-	-	-	4	1	-	5	2	1	1
(3,7)	1	-	-	1	-	-	-	-	-	-	-
(4,2)	-	-	-	-	-	1	-	-	-	-	-
(4,4)	-	-	-	-	1	-	-	-	-	-	-
(4,5)	-	-	-	1	-	-	-	-	-	-	-
(4,6)	1	-	-	-	-	-	-	1	-	-	-

Table 4: Degree and connection number-based vertex partition

II. QSPR Analysis of Anti-Cancer Drugs

A. Linear Regression Model

This section deals with a QSPR analysis of the 11 anti-cancer drugs using linear regression model to predict the chosen physico-chemical properties via distance-based topological indices.

The experimental values of the physico-chemical properties for the 11 anti-cancer drugs are given in Table 5.

The following table provides the values of the sixteen distance-based topological indices that are computed using the connection number-based vertex and edge partitions given in Tables 1 to 4.

The following table gives the calculated coefficient of determination (R^2) between distance-based indices and chosen physico-chemical properties of anti-cancer drugs using the linear regression model. The highest R^2 values are highlighted in Table 7.

The model Equations (1) to (5) are helpful in identifying the best predictors among the sixteen molecular descriptors

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Drugs	MR	C	MV	HAC	MM	$TPSA$
Amathaspiramide E	89.4	489	233.9	22	429.953	62.1
Carmustine	46.6	156	146.4	12	213.007	61.8
Convolutamine F	73.8	194	220.1	15	398.847	21.3
Convolutamydine A	68.2	363	190	17	360.895	66.4
Daunorubicin	130	960	339.4	38	527.179	186
Deguelin	105.1	674	314.2	29	394.142	63.2
Melatonin	67.6	270	197.6	17	232.121	54.1
Minocycline	116	971	294.6	33	457.185	165
Podophyllotoxin	104.3	629	302.4	30	414.131	92.7
Pterocellin B	87.4	604	302.4	24	318.1	59.5
Raloxifene	136.6	655	367.3	34	473.166	98.2

Table 5: Physico-chemical properties of anti-cancer drugs

considered for this study.

$$MR = 7.599208(SL) + 13.41353, \quad (1)$$

$$C = 0.345844(HLM_1) + 14.04273, \quad (2)$$

$$MV = 18.61086(SL) + 68.37292, \quad (3)$$

$$HAC = 1.286284(ABCL) + 2.505058, \quad (4)$$

$$TPSA = 42.74069(RL_3) - 83.6563. \quad (5)$$

Figures 2–4 represent the graphics of the best predictive fits given in Table 8.

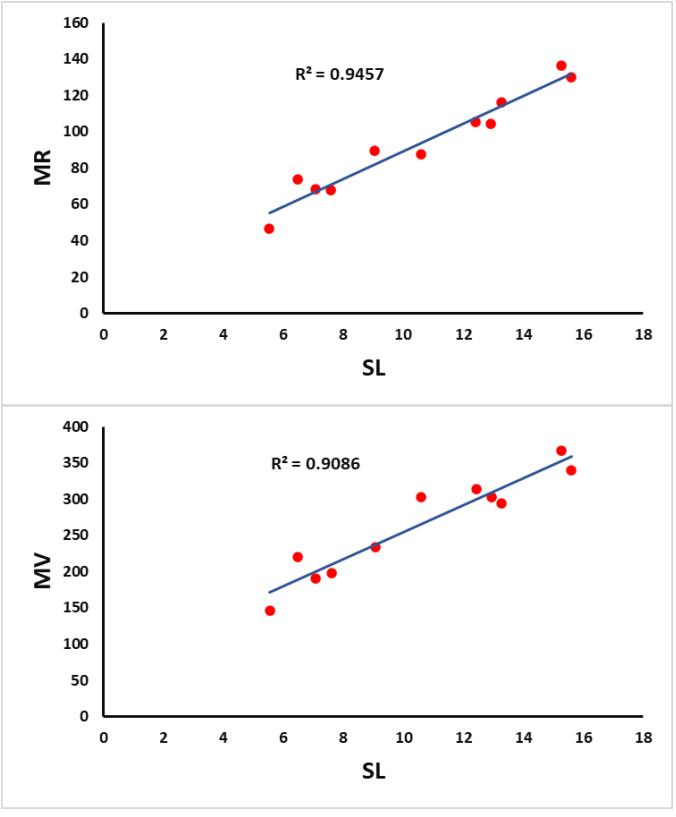
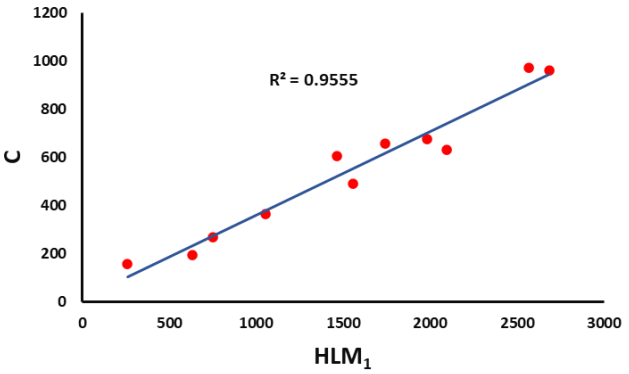


Figure 2: SL against MR and MV

With the help of the summary given in Table 8, we observe that the index SL plays a major role in the better prediction of the properties MR and MV with ($R^2 = 0.9457,\ RMSE = 6.905676$) and ($R^2 = 0.9086,\ RMSE = 22.37583$) respectively at 5% level of significance. It is noted further that the index HLM_1 is the best predictor for the property C with $R^2 = 0.9555$ and $RMSE = 62.09998$. Furthermore, the index $ABCL$ gives a better prediction of the property HAC with the highest $R^2 = 0.9891$ and least $RMSE = 0.961289$ when compared to the other predictors. The index RL_3 acts as the best predictor for the property $TPSA$ with $R^2 = 0.8472$ and $RMSE = 20.34631$.



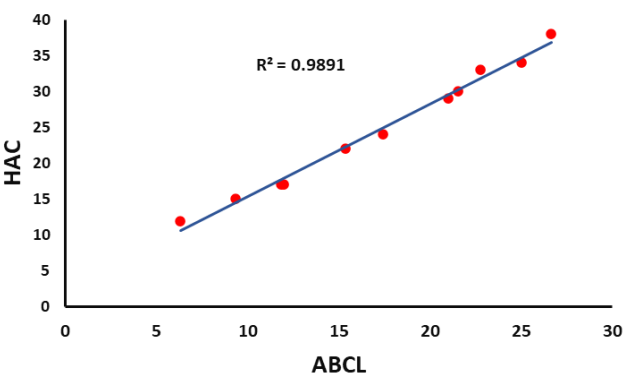


Figure 3: HLM_1 against C and $ABCL$ against HAC

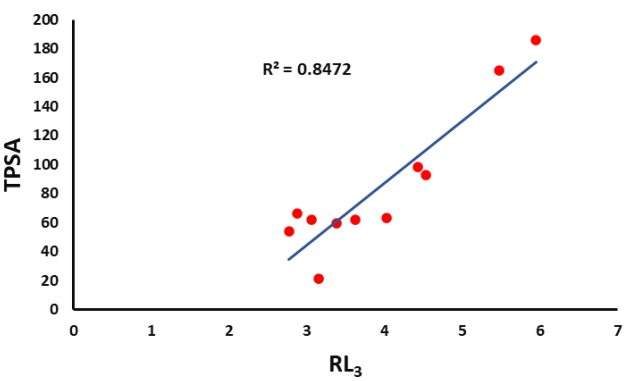


Figure 4: RL_3 against $TPSA$

Although the linear regression model helps to identify the best predictive fits for these five properties, it won't address the property MM. Therefore, we proceed with the Multiple

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Drugs	ZC_1	ZC_2	ZC_3	FL	RL_1	RL_2	RL_3	HLM_1	HLM_2	PL	$ABCL$	SL	GAL	LG_1	LG_2	SOL
Amathaspiramide E	298	374	184	1376	1.635478	1.31631	3.621825	1560	8306	2.554762	15.363634	9.053707	87.688739	558	3464	133.088933
Carmustine	60	62	50	174	1.810833	1.354167	3.066667	262	524	4.069444	6.309692	5.535767	23.490476	112	358	36.38872
Convolutamine F	132	150	92	502	1.628611	1.247222	3.152778	634	2044	3.191667	9.321324	6.472917	43.386508	242	1110	66.859408
Convolutamydine A	222	247	130	1016	1.312847	1.160972	2.877778	1054	4889	2.531071	11.835221	7.083061	60.480592	377	2188	94.977605
Daunorubicin	528	650	324	2346	2.542466	2.139376	5.951587	2684	12854	3.930278	26.657207	15.601287	156.300361	974	5724	233.071288
Deguelin	402	482	248	1704	1.941241	1.767063	4.028175	1984	8606	3.431389	20.989498	12.429736	119.925974	730	4048	178.181739
Melatonin	161	183	111	577	1.507222	1.373333	2.772222	753	2495	3.143056	12.007153	7.594599	53.442857	294	1334	79.905228
Minocycline	488	612	290	2336	2.239116	1.855737	5.479365	2568	13968	3.470556	22.751348	13.280368	137.571934	902	5816	210.133959
Podophyllotoxin	404	510	256	1758	2.281094	1.912313	4.534127	2094	9900	3.899722	21.553243	12.93474	124.040043	766	4438	183.755544
Pterocellin B	285	358	190	1175	1.79513	1.622857	3.380952	1464	6420	3.178889	17.448503	10.587741	92.617821	548	2974	136.010059
Raloxifene	362	428	248	1354	2.315964	2.386468	4.430952	1744	6480	4.484722	25.024903	15.283045	121.640043	676	3244	177.008376

Table 6: Distance-based indices values

Index/Property	MR	C	MV	HAC	MM	$TPSA$
ZC_1	0.8079	0.9526	0.7106	0.9223	0.6652	0.6585
ZC_2	0.7892	0.9545	0.6992	0.9111	0.6512	0.6555
ZC_3	0.8675	0.9437	0.7926	0.9652	0.6632	0.6346
FL	0.7073	0.9413	0.5877	0.8379	0.6486	0.6800
RL_1	0.6787	0.6117	0.6176	0.7602	0.4221	0.6180
RL_2	0.8201	0.5817	0.8082	0.8203	0.3992	0.4619
RL_3	0.7278	0.8404	0.5591	0.8357	0.6382	**0.8472**
HLM_1	0.7782	**0.9555**	0.6809	0.9007	0.6548	0.6630
HLM_2	0.6325	0.9160	0.5079	0.7700	0.6051	0.6768
PL	0.2138	0.0826	0.2229	0.2210	0.0345	0.1666
$ABCL$	0.9433	0.8672	0.8960	**0.9891**	0.6268	0.5657
SL	**0.9457**	0.8276	**0.9086**	0.9849	0.5933	0.5639
GAL	0.8769	0.9362	0.8117	0.9716	0.6559	0.6217
LG_1	0.8162	0.9543	0.7305	0.9312	0.6572	0.6510
LG_2	0.7020	0.9425	0.5909	0.8366	0.6310	0.6739
SOL	0.8627	0.9466	0.7835	0.9617	0.6663	0.6402

Table 7: R^2 obtained by Linear regression model

Property	Curve equation	Predictor	R^2	$RMSE$	p-value	F-Stat
MR	(1)	SL	0.9457	6.905676	0.000001	156.634
C	(2)	HLM_1	0.9555	62.09998	0.000001	193.0803
MV	(3)	SL	0.9086	22.37583	0.000001	89.4822
HAC	(4)	$ABCL$	0.9891	0.961289	0.000001	816.0337
$TPSA$	(5)	RL_3	0.8472	20.34631	0.000059	49.89068

Table 8: Summary of best predictive fits from Linear regression model

linear regression model to search for the enhanced predictive ability of the selected indices against all six properties.

B. Multiple Linear Regression Model

In this subsection, we carry out a QSPR study using a multiple linear regression model to cover the property MM that is not addressed by the linear regression model analyzed in the previous section.

The following are the model equations that provide the best predictors for all six properties. The summary of the best predictive fits resulting from this study is given in Table 9.

$$\begin{aligned} MR =& 6.150771(ZC_2) + 2.266407(HLM_1) \\ &+ 0.193652(HLM_2) - 4.98034(LG_1) \\ &- 1.26859(LG_2) - 0.7021(ZC_1) \\ &+ 6.509433(RL_3) + 3.971167, \end{aligned} \tag{6}$$

$$C = 0.976849(LG_1) - 6.4501, \tag{7}$$

$$\begin{aligned} MV =& -4.10859(ZC_1) - 45.2008(ZC_2) \\ &- 56.6554(RL_3) - 0.24317(HLM_2) \\ &- 58.316(ABCL) + 28.43776(LG_1) \\ &+ 1.58751(LG_2) - 56.6554(RL_3) \\ &+ 114.7895, \end{aligned} \tag{8}$$

$$\begin{aligned} HAC =& 0.256135(PCLI) + 1.054287(ABC) \\ &+ 1.620144(RL_3) - 0.76241, \end{aligned} \tag{9}$$

$$\begin{aligned} MM =& 144.0558(ZC_2) + 20.34892(HLM_1) \\ &+ 20.34892(HLM_2) - 65.7588(LG_1) \\ &- 15.9421(LG_2) - 22.2702(ZC_1), \\ &+ 3.77016(FL) + 86.23568(RL_3) - 102.2737, \end{aligned} \tag{10}$$

$$\begin{aligned} TPSA =& -3.75515(HLM_1) - 0.35429(HLM_2) \\ &+ 53.90495(ABCL) + 2.127128(LG_2) \\ &+ 0.4162(FL) + 57.41319(RL_3) - 121.426. \end{aligned} \tag{11}$$

Property	Curve equation	R^2	Adj-R^2	$RMSE$	p-value	F-Stat
MR	(6)	0.9999	0.9997	0.407216	0.000001	6804.363
C	(7)	0.9543	0.9492	62.92061	0.000001	187.8435
MV	(8)	0.9964	0.9878	7.74186	0.00119	117.0956
HAC	(9)	0.9997	0.9996	0.170596	0.000001	8708.619
MM	(10)	0.9982	0.9912	9.109898	0.00702	141.8294
$TPSA$	(11)	0.9860	0.9651	9.222352	0.001147	47.10643

Table 9: Summary of best predictive fits from multiple linear regression model

From the summary given in Table 9, it is evident that all six physico-chemical properties of the selected anti-cancer drugs are better predicted using the multiple linear regression model with greater R^2 and least $RMSE$ when compared to the linear regression model.

III. Conclusion

QSPR analysis is one of the essential tools in predicting the physico-chemical properties of new drugs or a combination of drugs well before the wet lab experiments. This kind of study helps the pharmaceutical industry to minimize the cost while dealing with the design of new drugs to treat various diseases. In this study on anti-cancer drugs, we calculated sixteen recently introduced distance-based topological indices for eleven different drugs used in the treatment of various

types of cancer. Also, we performed a QSPR analysis to identify the best predictors for six physico-chemical properties of these drugs using linear and multiple linear regression models. Our study revealed that the multiple linear regression model would give a better predictive ability than the linear regression model.

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