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(RESEARCH ARTICLE)

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Degree-based topological indices and QSPR analysis of lung cancer Drugs

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Abstract

A numerical value that characterizes the topology of a graph G is called topological index. It represents the theoretical characteristics of the chemical com- pounds when applied to their molecular structure. In this study, the chemical structures of lung cancer drugs are analyzed using well-known Degree-Based topological indices. The elements of a chemical structure are viewed as vertices, and the boundaries that separate them are represented as edges, in a graph. Furthermore, QSPR analysis of the said topological indices are discussed, and it is shown that these topological indices are highly correlated with the Physical properties of Lung cancer drugs. This theocratic approach may assist chemists and those working in the pharmaceutical industry in predicting the qualities of lung cancer drugs without experimenting.

Keywords: Topological indices; Lung cancer; QSPR; Physical properties; Molecular structure

1. Introduction

Human body is concocted with trillions of cells which normally grows over the life time and gets divided as needed and they die when the cells got old or become abnormal. But as the cells keep producing the new cells, if the old or abnormal cells don't die, the cancer starts. These cancer cells grow uncontrollably and they crowd the normal cells and hence the body does not function the way it is supposed to. When cancer starts in the lungs, it is called Lung cancer. It is also known as Lung carcinoma and is the leading cause of cancer deaths world wide. People who have the greatest risk of Lung cancer, through Lung cancer can also occur in people who have never smoked. This risk of Lung cancer increases with the length of time and number of cigarettes you've smoked. There are many cancers that affect the lungs, but we usually use the term 'lung cancer' for two main kinds: Non-small call Lung cancer and Small cell Lung cancer.

A molecular graph is a representation of the structural formula of a chemical compound cheminformatics of chemistry, Mathematics and information science. It studies Quantitative structure–activity (QSAR) and Quantitative structure –property (QSAR) relationships that are used to predict the biological activities and properties of different chemical compounds.

Topological indices (TIs) are commonly employed in the study of the physico-chemical properties of numerous medications. They are also known as numerical descriptor that are obtained using a molecular graph in order to comprehensively mention the chemical system. In this research, we calculated degree- based TIs for lung cancer drugs. These drugs are chemical compounds with well-defined topological indices analyzed using QSPR. This method's calculated feature has a strong correlation with lung cancer drugs characteristics using linear regression. Drug characteristics and TIs exhibit strong association.

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2. Material and Method

In drug structures, atoms denote vertices and the corresponding bonds connecting the atoms are termed edges. Graph G(V, E) is considered as simple, finite, and connected. Where as V and E represented in the chemical graph are termed as vertex and edge set respectively. Some of the Degree-Based Topological in- dices which we used in this work are defined as follows

- Definition: The First and Second Zagreb indices are proposed by Gutman and Trinajestic as

$$M_1(G) = \sum_{e=uv \in E(G)} [du + dv]$$

$$M_2(G) = \sum_{e=uv \in E(G)} [du \cdot dv]$$

- Definition: The Randic index is proposed by Milan Randic in, as

$$R(G) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{du \cdot dv}}$$

- Definition: The Reciprocal Randic index formulated by Gutman et al, as

$$RR(G) = \sum_{e=uv \in E(G)} \sqrt{du \cdot dv}$$

- Definition: The Reduced Reciprocal Randic index is proposed by Gutman et al,as

$$RR(G) = \sum_{e=uv \in E(G)} \sqrt{(du-1) \cdot (dv-1)}$$

- Definition: The Sum connectivity index is introduced by Zhou and Trinjstic in [3],

$$SCI(G) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{du + dv}}$$

as

- Definition: The Harmonic index is proposed by Fajtlowicz et el, in [5] as

$$H(G) = \sum_{e=uv \in E(G)} \frac{2}{du + dv}$$

- Definition: The Forgotten index is proposed by Furtula et al, in [4]as

$$F(G) = \sum_{e=uv \in E(G)} [(du)^2 + (dv)^2]$$

- Definition: The Y-index is proposed by Abdu Alameri et al, in [2]as

$$Y(G) = \sum_{e=uv \in E(G)} [(du)^3 + (dv)^3]$$

- Definition: The Inverse sum index is proposed by Vukicevic et el, as

$$ISI(G) = \sum_{e=uv \in E(G)} \frac{du \cdot dv}{du + dv}$$

3. Results and Discussion

The above defined ten topological in- dices are used the modeling of six Physical properties: Boiling point(BP), Enthalpy(E), Flash point(F), Molar refractivity(MR), and Polarizability(P) of 20 Lung cancer drugs: Alectinib, Brigatinib, Binimetinib, Encorafenib, Ceritinib, Crizotinib, Dacomitinib, Entrectinib, Pralsetinib, Gefitinib, Afatinib, Gemcitabine, Ipilimumab, Pembrolizumab, Sotorasib, Lortatinib, Paclitaxel, Tafinlar, Tepotinib, Docetaxel.

3.1. Regression models

The Equation below correlates physical features of medications used to treat Lung cancer with topological indices. We applied the following linear regression model:

$$P = A + b[TI],$$

where P is physical property of drug. A is constant, b is regression coefficient, and TI is topological index. SPSS software calculates constant A and regression coefficient for six physical properties and ten degree-based topological indices of 20 medicine's molecular structure. [6-13]

- Regression models for First zagreb index: M1(G)
  - Boiling point = 279.919+2.079 [M1(G)]
  - Enthalpy = 47.091+0.286 [M1(G)]
  - Flash point = 123.097+1.258 [M1(G)]
  - Molar refractivity = 19.682+0.598 [M1(G)]
  - Molar volume = 47.274+1.681[M1(G)]
  - Polarizability = 7.791+0.237[M1(G)]
- Regression models for Second zagreb index: M2(G)
  - Boiling point = 309.322+1.613 [M2(G)]
  - Enthalpy = 50.754+0.223 [M2(G)]
  - Flash point = 140.881+0.975 [M2(G)]
  - Molar refractivity =28.008+0.465 [M2(G)]
  - Molar volume = 70.236+1.308 [M2(G)]
  - Polarizability = 11.098+0.184 [M2(G)]
- Regression models for Randic index: R(G)
  - Boiling point=392.085+12.356 [R(G)]
  - Enthalpy=61.046+1.761 [R(G)]
  - Flash point= 190.916+7.473 [R(G)]
  - Molar refractivity= 50.717+3.668 [R(G)]
  - Molar volume = 132.154+10.405 [R(G)]
  - Polarizability= 20.117+1.454 [R(G)]
- Regression models for Reciprocal Randic index: RR(G)
  - Boiling point=260.137+4.572 [RR(G)]
  - Enthalpy=44.896+0.662 [RR(G)]
  - Flash point= 111.136+2.765 [RR(G)]
  - Molar refractivity= 14.229+1.313 [RR(G)]
  - Molar volume = 34.111+3.664 [RR(G)]
  - Polarizability= 5.632+0.521 [RR(G)]
- Regression models for Reduced Reciprocal Randic index: RRR(G)
  - Boiling point=295.836+8.017 [RRR(G)]
  - Enthalpy=49.653+1.093 [RRR(G)]
  - Flash point= 132.728+4.848 [RRR(G)]
  - Molar refractivity= 23.185+2.340 [RRR(G)]
  - Molar volume=59.264+6.525 [RRR(G)]
  - Polarizability= 9.182+0.928 [RRR(G)]
- Regression models for Sum Connectivity index: SCI(G)
  - Boiling point=314.452+15.418 [SCI(G)]
  - Enthalpy=51.773+2.146 [SCI(G)]
  - Flash point= 143.949+9.326 [SCI(G)]
  - Molar refractivity=38.205+4.148 [SCI(G)]
  - Molar volume=102.315+11.517 [SCI(G)]
  - Polarizability= 15.154+1.644 [SCI(G)]
- Regression models for Harmonic index: H(G)
  - Boiling point=231.213+10.823 [H(G)]
  - Enthalpy=40.763+1.478 [H(G)]
  - Flash point= 93.642+6.545 [H(G)]
  - Molar refractivity= 5.866+3.110 [H(G)]
  - Molar volume = 9.053+8.721 [H(G)]

- Polarizability= 1.096+1.260 [H(G)]

- Regression models for Forgotten index: F(G)
  - Boiling point = 322.677+0.693 [F(G)]
  - Enthalpy = 52.445+0.96 [F(G)]
  - Flash point = 148.971+0.419 [F(G)]
  - Molar refractivity = 32.810+0.197 [F(G)]
  - Molar volume = 83.192+0.557 [F(G)]
  - Polarizability = 12.067+0.080 [F(G)]
- Regression models for Y-index: Y(G)
  - Boiling point=378.336+0.208 [Y(G)]
  - Enthalpy=59.522+0.029 [Y(G)]
  - Flash point= 182.616+0.126 [Y(G)]
  - Molar refractivity= 49.678+0.059 [Y(G)]
  - Molar volume = 129.229+0.168 [Y(G)]
  - Polarizability= 19.688+0.023 [Y(G)]
- Regression models for Inverse sum index: ISI(G)
  - Boiling point=233.301+9.814 [ISI(G)]
  - Enthalpy=40.774+1.346 [ISI(G)]
  - Flash point= 94.905+5.935 [ISI(G)]
  - Molar refractivity = 6.516+2.819 [ISI(G)]
  - Molar volume = 9.225+7.942 [ISI(G)]
  - Polarizability= 2.569+1.118 [ISI(G)]

Table 1 Physical properties of drugs used for the treatment of Lung Cancer

Lung cancer drug	Boiling point	Enthalpy	Flash point	Refraction	Molar refractivity	Polar surface area	Polarizability	Surface tension	Molar volume
Alectinib	722.5	105.5	390.7	1.673	140.4	72	55.7	66.3	374.7
Brigatinib	781.8	113.8	426.6	1.641	160.1	96	63.5	65.0	443.6
Binimetinib.	-	-	-	1.652	96.6	88	38.3	51.2	264.1
Encorafenib	-	-	-	1.641	134.1	149	53.2	50.2	371.7
Ceritinib	720.7	105.3	389.6	1.595	151.5	114	60.1	52.5	446.0
Crizotinib	599.2	89.2	316.2	1.673	114.4	78	45.4	51.1	305.2
Dacomitinib	665.7	97.9	356.4	1.663	129.5	79	51.3	62.2	349.5
Entrectinib	717.5	104.8	387.7	1.672	156.6	86	62.1	62.8	418.1
Pralsetinib	799.1	116.2	437.1	1.683	144.5	136	57.3	52.4	381.0
Gefitinib	586.8	87.6	308.7	1.621	118.8	69	47.1	55.3	337.8
Afatinib	676.9	99.4	363.2	1.668	131.2	89	52.0	60.1	352.0
Gemcitabine	482.7	86.2	245.7	1.652	52.1	108	20.6	65.4	142.3
Ipilimumab	627.2	92.8	333.1	1.700	108.6	82	43.1	64.8	280.9
Pembrolizumab	235.0	45.3	95.9	1.555	43.7	22	17.3	42.2	136.2
Sotorasib	730.5	110.4	395.6	1.651	150.5	102	59.6	47.3	411.9
Lorlatinib	675.0	99.1	362.1	1.687	108.5	110	43.0	53.4	285.0
Paclitaxel	957.1	146.0	532.6	1.637	219.3	221	86.9	68.5	610.6
Dabrafenib	653.7	96.3	349.2	1.626	127.4	147	50.7	61.0	359.9
Tepotinib	626.5	92.7	332.7	1.660	144.5	95	57.3	52.1	391.6
Docetaxel	900.5	137.1	498.4	1.618	205.2	224	81.4	66.2	585.7

Table 2 Lung cancer drug sand computed topological indices

Lung cancer drugs	M1(G)	M2(G)	R(G)	RR(G)	RRR(G)	SCI(G)	H(G)	F(G)	Y(G)	ISI(G)
Alectinib	202	251	16.878	98.447	53.938	18.002	43.085	548	1570	47.63
Brigatinib	223	266	19.234	107.78	56.971	20.999	47.019	595	1681	51.76
Binimetinib.	140	166	12.89	68.014	34.55	12.825	30.39	364	992	33.11
Encorafenib	186	214	16.852	88.72	42.187	17.324	41.133	504	1104	45.25
Ceritinib	200	235	18.032	96.402	46.284	18.734	43.415	532	1444	47.96
Crizotinib	160	190	14.428	77.95	40.798	26.588	34.73	414	1120	37.65
Dacomitinib	170	197	24.02	83.150	43.87	22.063	38.4	426	1118	40.902
Entrectinib	222	261	28.565	108.51	58.592	19.777	47.73	566	1516	50.45
Pralsetinib	210	248	19.262	101.81	53.586	26.135	46.011	606	1559	52.163
Gefitinib	160	186	24.296	74.891	42.041	22.941	36.396	398	1036	42.516
Afatinib	176	203	23.876	85.650	44.284	24.576	38.73	446	1184	41.45
Gemcitabine	92	108	13.28	44.22	20.899	12.748	21.399	244	680	24.316
Ipilimumab	136	157	15.642	65.482	32.455	17.273	29.733	356	976	32.45
Pembrolizumab	44	49	7.879	21.626	10.656	6.85	11.899	104	262	14.366
Sotorasib	221	268	23.321	107.427	55.213	28.577	47.399	585	1619	50.11
Lorlatinib	154	179	21.589	72.192	32.798	25.593	33.733	400	1090	35.616
Paclitaxel	348	436	45.954	167.87	88.358	42.997	70.801	982	2976	78.297
Dabrafenib	192	229	27.879	91.528	45.015	23.069	40.608	538	1620	45.797
Tepotinib	188	220	25.362	92.983	49.941	25.957	41.733	476	1246	44.45
Docetaxel	326	403	43.321	137.074	76.702	38.589	66.001	948	2978	73.097

Table 3 Correlation coefficients

Topological index	Correlation coefficients of Boiling point	Correlation coefficients of Enthalpy	Correlation coefficients of Flash point	Correlation coefficients of Molar refractivity	Correlation coefficients of Molar volume	Correlation coefficients of Polarizability
M1(G)	0.939	0.949	0.939	0.979	0.976	0.979
M2(G)	0.928	0.945	0.928	0.970	0.968	0.969
R(G)	0.754	0.790	0.754	0.831	0.837	0.831
RR(G)	0.941	0.943	0.941	0.980	0.971	0.980
RRR(G)	0.921	0.925	0.921	0.976	0.967	0.976
SCI(G)	0.817	0.837	0.818	0.831	0.819	0.830
H(G)	0.943	0.947	0.943	0.985	0.980	0.985
Y(G)	0.929	0.950	0.929	0.960	0.960	0.958
F(G)	0.894	0.928	0.894	0.924	0.930	0.924
ISI(G)	0.934	0.943	0.934	0.977	0.977	0.977

Table 4 Statistical parameter for the linear QSPR model for M1(G)

Physical property	N	A	b	r	r2	F	p	Std error of estimate
Boiling point	18	279.919	2.079	0.939	0.881	118.494	0.000	55.5988
Enthalpy	18	47.091	0.286	0.949	0.900	144.542	0.000	6.9146
Flashpoint	18	123.097	1.258	0.939	0.881	118.432	0.000	33.6322
Molar refractivity	20	19.682	0.598	0.979		411.985	0.000	8.6378
Molar volume	20	47.274	1.681	0.976	0.953	366.742	0.000	25.9007
Polarizability	20	7.791	0.237	0.979	0.958	414.732	0.000	3.4391

Table 5 Statistical parameter for the linear QSPR model for M2(G)

Physical property	N	A	b	r	r2	F	p	Std error of estimate
Boiling point	18	309.322	1.613	0.928	0.862	99.816	0.000	59.9145
Enthalpy	18	50.754	0.223	0.945	0.894	134.858	0.000	7.1331
Flashpoint	18	140.881	0.975	0.928	0.862	99.760	0.000	36.2433
Molar refractivity	20	28.008	0.465	0.970	0.940	282.400	0.000	10.4062
Molar volume	20	70.236	1.308	0.968	0.937	269.488	0.000	29.9630
Polarizability	20	11.098	0.184	0.969	0.940	280.591	0.000	4.1401

Table 6 Statistical parameter for the linear QSPR model for R(G)

Physical property	N	A	b	r	r2	F	p	Std error of estimate
Boiling point	18	392.085	12.356	0.754	0.568	21.038	0.000	105.947
Enthalpy	18	61.046	1.761	0.790	0.625	26.616	0.000	13.4207
Flashpoint	18	190.916	7.473	0.754	0.568	21.043	0.000	64.0697
Molar refractivity	20	50.717	3.668	0.831	0.691	40.298	0.000	23.6219
Molar volume	20	132.154	10.405	0.837	0.701	42.230	0.000	65.4617
Polarizability	20	20.117	1.454	0.831	0.690	40.110	0.000	9.3847

Table 7 Statistical parameter for the linear QSPR model for RR(G)

Physical property	N	A	b	r	r2	F	p	Std error of estimate
Boiling point	18	260.137	4.572	0.941	0.886	124.518	0.000	54.3939
Enthalpy	18	44.896	0.622	0.943	0.889	128.198	0.000	7.2959
Flashpoint	18	111.136	2.765	0.941	0.886	124.433	0.000	32.9057
Molar refractivity	20	14.229	1.313	0.980	0.960	435.973	0.000	8.4650
Molar volume	20	34.111	3.664	0.971	0.942	294.732	0.000	28.7282
Polarizability	20	5.632	0.521	0.980	0.960	430.791	0.000	3.3770

Table 8 Statistical parameter for the linear QSPR model for RRR(G)

Physical property	N	A	b	r	r2	F	p	Std error of estimate
Boiling point	18	295.836	8.017	0.921	0.849	89.908	0.000	62.6543
Enthalpy	18	49.653	1.093	0.925	0.855	94.297	0.000	8.3422
Flashpoint	18	132.728	4.848	0.921	0.849	89.849	0.000	37.9021
Molar refractivity	20	23.185	2.340	0.976	0.953	368.879	0.000	9.1697
Molar volume	20	59.264	6.525	0.967	0.935	257.607	0.000	30.6021
Polarizability	20	9.182	0.928	0.976	0.953	365.802	0.000	3.6517

Table 9 Statistical parameter for the linear QSPR model for SCI(G)

Physical property	N	A	b	r	r2	F	p	Std error of estimate
Boiling point	18	314.452	15.418	0.817	0.668	32.232	0.000	92.8432
Enthalpy	18	51.773	2.146	0.837	0.701	37.555	0.000	11.9718
Flashpoint	18	143.949	9.326	0.818	0.668	32.254	0.000	56.1355
Molar refractivity	20	38.205	4.148	0.831	0.690	40.023	0.000	23.6777
Molar volume	20	102.315	11.517	0.819	0.670	36.584	0.000	68.7643
Polarizability	20	15.154	1.644	0.830	0.689	39.872	0.000	9.4040

Table 10 Statistical parameter for the linear QSPR model for H(G)

Physical property	N	A	b	r	r2	F	p	Std error of estimate
Boiling point	18	231.213	10.823	0.943	0.889	128.055	0.000	53.7219
Enthalpy	18	40.763	1.478	0.947	0.898	140.316	0.000	7.0074
Flashpoint	18	93.642	6.545	0.943	0.889	127.989	0.000	32.4969
Molar refractivity	20	5.866	3.110	0.985	0.970	584.510	0.000	7.3478
Molar volume	20	9.053	8.721	0.980	0.961	448.056	0.000	23.5329
Polarizability	20	1.096	1.260	0.985	0.970	585.960	0.000	2.9725

Table 11 Statistical parameter for the linear QSPR model for F(G)

Physical property	N	A	b	r	r2	F	p	Std error of estimate
Boiling point	18	322.677	0.693	0.929	0.864	101.476	0.000	59.4923
Enthalpy	18	52.445	0.96	0.950	0.902	147.053	0.000	6.8611
Flashpoint	18	148.971	0.419	0.929	0.864	101.431	0.000	35.9845
Molar refractivity	20	32.810	0.197	0.960	0.921	209.391	0.000	11.9606
Molar volume	20	83.192	0.557	0.960	0.922	212.307	0.000	33.4767
Polarizability	20	12.067	0.080	0.958	0.918	202.210	0.000	4.9227

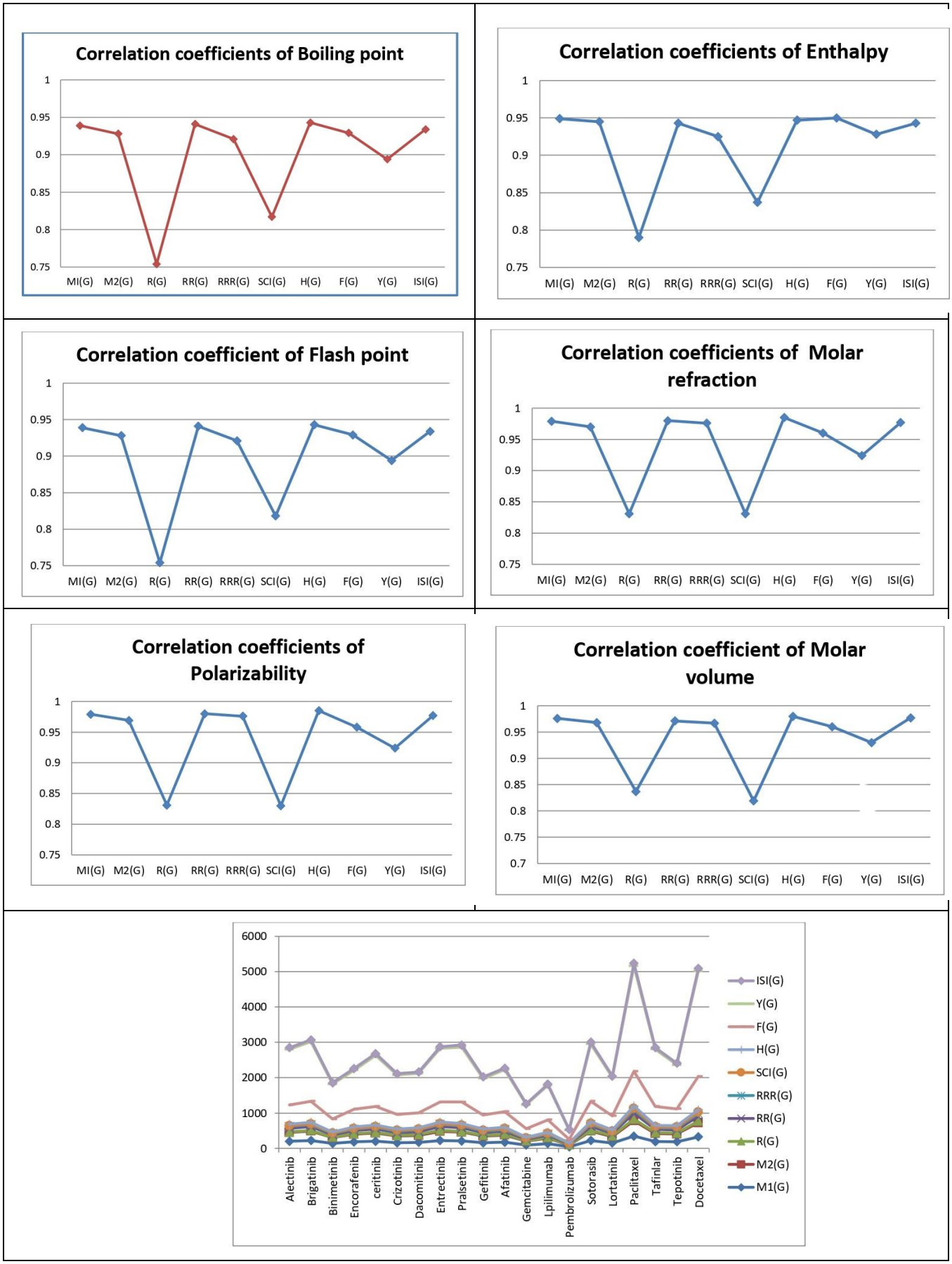


Figure 1 Medicine with topological indices

Table 12 Statistical parameter for the linear QSPR model for Y(G)

Physical property	N	A	b	r	r2	F	p	Std error of estimate
Boiling point	18	378.336	0.208	0.894	0.799	63.646	0.000	72.2495
Enthalpy	18	59.522	0.029	0.928	0.861	98.877	0.000	8.1742
Flashpoint	18	182.616	0.126	0.894	0.799	63.624	0.000	43.7003
Molar refractivity	20	49.678	0.059	0.924	0.853	104.619	0.000	16.2878
Molar volume	20	129.226	0.168	0.930	0.865	115.600	0.000	43.9355
Polarizability	20	19.688	0.023	0.924	0.853	104.333	0.000	6.4681

Table 13 Statistical parameter for the linear QSPR model for ISI(G)

Physical property	N	A	b	r	r2	F	p	Std error of estimate
Boiling point	18	233.301	9.814	0.934	0.873	110.120	0.000	57.4149
Enthalpy	18	40.774	1.346	0.943	0.890	129.081	0.000	7.2737
Flashpoint	18	94.905	5.935	0.934	0.873	110.083	0.000	34.7306
Molar refractivity	20	6.516	2.819	0.977	0.954	373.272	0.000	9.1180
Molar volume	20	9.225	7.942	0.977	0.954	375.815	0.000	25.6006
Polarizability	20	2.569	1.118	0.977	0.954	370.946	0.000	3.6255

Table 14 Comparison of actual and computed values for Boiling point from regression models

Name of drug	Boiling point of drug	Boiling point computed from regression model for									
		M1(G)	M2(G)	R(G)	RR(G)	RRR(G)	SCI(G)	H(G)	F(G)	Y(G)	ISI(G)
Alectinib	722.5	699.87	714.18	600.62	710.23	728.25	592.00	697.52	702.44	704.89	700.74
Brigatinib	781.8	743.53	738.38	629.74	752.90	752.57	638.21	740.09	735.01	727.98	741.27
Binimetinib.	-	570.97	577.08	551.35	571.09	572.82	512.18	560.12	574.92	584.67	558.24
Encorafenib	-	666.61	654.50	600.30	665.76	634.04	581.55	676.39	671.94	607.96	677.38
Ceritinib	720.7	695.71	688.37	614.88	700.88	666.89	603.29	701.09	691.35	678.68	703.98
Crizotinib	599.2	612.55	615.79	570.35	616.52	622.91	724.38	607.09	609.57	611.29	602.79
Dacomitinib	665.7	633.34	627.08	688.87	640.29	647.54	654.61	646.81	613.73	610.88	634.71
Entrectinib	717.5	741.45	730.31	745.03	756.24	765.56	619.37	747.79	714.91	693.66	728.41
Pralsetinib	799.1	716.509	709.34	630.08	725.61	725.43	717.40	729.19	742.63	702.60	745.22
Gefitinib	586.8	612.55	609.34	692.28	602.53	632.87	668.15	625.12	598.49	593.82	650.55
Afatinib	676.9	645.82	636.76	687.09	651.72	650.86	693.36	650.38	631.75	624.60	640.09
Gemcitabine	482.7	471.18	483.52	556.17	462.31	463.38	511.00	462.81	491.76	519.77	471.93
Ipilimumab	627.2	562.66	562.56	585.35	559.52	556.02	580.76	553.01	569.38	581.34	551.76
Pembroli zumab	235.0	371.39	388.35	489.43	359.01	381.26	420.06	359.99	394.74	432.83	374.28
Sotorasib	730.5	739.37	741.60	680.23	751.29	738.47	755.05	744.21	728.08	715.08	725.08

Lorlatinib	675.0	600.08	598.04	658.83	590.19	558.77	709.04	596.30	599.87	605.05	582.83
Paclitaxel	957.1	1003.41	1012.5	959.89	1027.63	1004.20	977.37	997.49	1001.8	997.34	1001.7
Dabrafenib	653.7	679.08	619.01	736.55	678.60	656.72	670.12	670.71	695.51	715.29	682.75
Tepotinib	626.5	670.77	609.34	705.45	685.25	696.21	714.65	682.88	652.54	637.50	669.53
Docetaxel	900.5	957.67	959.36	927.35	886.83	910.75	909.41	945.54	979.64	997.76	950.67

Table 15 Comparison of actual and computed values for Enthalpy from regression models

Name of drug	**Enthalpy of drug**	**Enthalpy computed from regression model for**									
		M1(G)	**M2(G)**	**R(G)**	**RR(G)**	**RRR(G)**	**SCI(G)**	**H(G)**	**F(G)**	**Y(G)**	**ISI(G)**
Alectinib	105.5	104.86	106.72	90.76	106.13	108.60	90.40	104.44	578.52	105.05	104.88
Brigatinib	113.8	110.86	110.07	94.91	111.93	111.92	96.83	110.25	623.64	108.27	110.44
Binimetinib	-	87.13	87.77	83.74	87.20	87.41	79.29	85.67	401.88	88.29	85.34
Encorafenib	-	100.28	98.47	90.72	100.07	95.76	88.95	101.55	536.28	91.53	101.68
Ceritinib	105.3	104.29	103.15	92.800	104.85	100.24	91.97	104.93	563.16	101.39	105.32
Crizotinib	89.2	92.85	93.12	86.45	93.38	94.24	108.83	92.09	449.88	92.00	91.45
Dacomitinib	97.9	95.71	94.68	103.34	96.61	97.60	99.12	97.51	455.64	91.94	95.82
Entrectinib	104.8	110.58	108.95	111.34	112.38	113.69	94.21	111.30	595.80	103.48	108.67
Pralsetinib	116.2	107.15	106.05	94.96	108.22	108.22	107.85	108.76	634.20	104.73	110.98
Gefitinib	87.6	92.58	92.23	103.83	91.47	95.60	101.00	94.55	434.52	89.56	98.00
Afatinib	99.4	97.42	96.02	103.09	98.17	98.05	104.51	98.00	480.60	93.85	96.56
Gemcitabine	86.2	73.40	74.83	84.43	72.40	72.49	79.13	72.39	286.68	79.24	73.50
Ipilimumab	92.8	85.98	85.76	88.59	85.62	85.12	88.84	84.70	394.20	87.82	84.45
Pembroli zumab	45.3	59.67	61.68	74.92	58.34	61.30	66.47	58.34	152.28	67.12	60.11
Sotorasib	110.4	110.29	110.51	102.11	111.71	110.00	113.09	110.81	614.04	106.47	108.22
Lorlatinib	99.1	91.13	90.67	99.06	89.79	85.50	106.69	90.62	436.44	91.13	88.71
Paclitaxel	146.0	146.61	147.98	141.97	149.31	146.22	144.04	145.40	995.16	145.82	146.16
Dabrafenib	96.3	102.00	101.82	110.14	101.82	98.85	101.27	100.78	568.92	106.50	102.41
Tepotinib	92.7	100.859	99.81	105.70	102.73	104.23	107.51	102.44	509.40	95.65	100.60
Docetaxel	137.1	140.32	140.62	137.33	130.15	133.48	134.58	138.31	962.52	145.88	139.16

Table 16 Comparision of actual and computed values for Flash point from regression models

Name of drug	Flash point of drug	Flash point computed from regression model for									
		M1(G)	M2(G)	R(G)	RR(G)	RRR(G)	SCI(G)	H(G)	F(G)	Y(G)	ISI(G)
Alectinib	390.7	377.21	385.60	317.04	383.34	394.21	311.83	375.63	378.58	380.43	377.58
Brigatinib	426.6	403.63	400.23	334.65	409.14	408.92	339.78	401.38	398.27	394.42	402.10
Binimetinib.	-	299.21	302.73	287.24	299.19	300.22	263.55	292.54	301.48	307.60	291.41
Encorafenib	-	357.08	349.53	316.85	356.44	337.25	305.51	362.85	360.14	321.72	363.46
Ceritinib	389.6	374.69	370.00	325.66	377.68	357.11	318.66	377.79	371.87	364.56	379.54
Crizotinib	316.2	324.37	326.13	298.73	326.66	330.51	391.90	320.94	322.43	323.73	318.35
Dacomitinib	356.4	336.95	332.95	370.41	341.04	345.40	349.70	344.97	324.95	323.48	337.65
Entrectinib	387.7	402.37	395.35	404.38	411.16	416.78	328.38	406.03	386.12	373.63	394.32
Pralsetinib	437.1	387.27	382.68	334.86	392.64	392.51	387.68	394.78	402.88	379.05	404.49
Gefitinib	308.7	324.37	322.23	372.48	318.20	336.54	357.89	331.85	315.73	313.15	347.23
Afatinib	363.2	344.50	338.00	369.34	347.95	347.41	373.14	374.12	335.84	331.8	340.91
Gemcitabine	245.7	238.83	246.18	290.15	233.40	234.04	262.83	233.69	251.20	268.29	239.22
Ipilimumab	333.1	294.18	293.95	307.80	292.19	290.06	305.03	288.24	298.13	305.59	287.49
Pembroli zumab	95.9	178.44	188.65	249.79	170.93	184.38	207.83	171.52	192.54	215.62	180.16
Sotorasib	395.6	401.11	402.18	365.19	408.17	400.40	410.45	403.86	394.08	386.61	392.30
Lorlatinib	362.1	316.82	315.40	352.25	310.74	291.73	382.62	314.42	316.57	319.95	306.61
Paclitaxel	532.6	560.88	565.98	534.33	575.29	561.08	544.93	557.03	560.42	557.59	559.59
Dabrafenib	349.2	364.63	364.15	399.25	364.21	350.96	359.09	359.42	374.39	386.73	366.71
Tepotinib	332.7	359.60	355.38	380.44	368.23	374.84	386.23	366.78	348.41	339.61	358.71
Docetaxel	498.4	533.20	533.80	514.65	490.14	504.57	503.83	525.61	546.18	557.84	528.73

Table 17 Comparison of actual and computed values for Molar refractivity from regression models

Name of drug	Molar Refractivity of drug	Molar Refractivity computed from regression model for									
		M1(G)	M2(G)	R(G)	RR(G)	RRR(G)	SCI(G)	H(G)	F(G)	Y(G)	ISI(G)
Alectinib	140.4	140.47	144.72	112.62	143.48	149.39	112.87	139.86	140.76	142.30	140.78
Brigatinib	160.1	153.03	151.69	121.26	155.74	156.49	125.30	152.09	150.02	148.85	152.42
Binimetinib.	96.6	103.40	105.19	97.99	103.53	104.03	91.40	100.37	104.51	108.20	99.85
Encorafenib	134.1	130.91	127.51	112.53	130.71	121.90	110.06	133.78	132.09	114.81	134.07
Ceritinib	151.5	139.28	137.28	116.85	140.80	131.48	115.91	140.88	137.61	134.87	141.71
Crizotinib	114.4	115.36	116.35	103.63	116.57	118.65	148.49	113.87	114.36	115.75	112.65
Dacomitinib	129.5	121.34	119.61	138.82	123.40	125.84	129.72	125.29	115.55	115.64	121.81
Entrectinib	156.6	152.43	149.37	155.49	156.70	160.29	120.23	154.30	144.31	139.12	148.73

Pralsetinib	144.5	145.26	143.32	121.37	147.905	148.57	146.61	148.96	152.19	141.65	153.56
Gefitinib	118.8	115.36	114.49	139.83	112.56	121.56	133.36	119.05	111.21	110.80	126.36
Afatinib	131.2	124.93	122.40	138.29	126.68	126.80	140.14	126.31	120.67	119.53	123.36
Gemcitabine	52.1	74.69	78.22	99.42	72.28	72.08	91.08	72.41	80.87	89.79	75.06
Ipilimumab	108.6	101.01	101.01	108.09	100.20	99.12	109.85	98.33	102.94	107.26	97.99
Pembroli zumab	43.7	45.99	50.79	79.61	42.62	48.12	66.61	42.87	53.29	65.13	47.01
Sotorasib	150.5	151.84	152.62	136.25	155.28	152.38	156.74	153.27	148.05	145.19	147.77
Lorlatinib	108.5	111.77	111.24	129.90	109.01	97.59	144.36	110.77	111.61	113.98	106.91
Paclitaxel	219.3	227.78	230.74	219.27	234.64	229.94	216.55	226.05	226.26	225.26	227.23
Dabrafenib	127.4	134.49	134.49	152.97	134.40	128.52	133.89	132.15	138.79	145.25	135.61
Tepotinib	144.5	132.10	130.30	143.74	136.31	140.04	145.87	135.65	126.58	123.19	131.82
Docetaxel	205.2	214.63	215.40	209.61	194.20	202.66	198.27	211.12	219.56	225.38	212.57

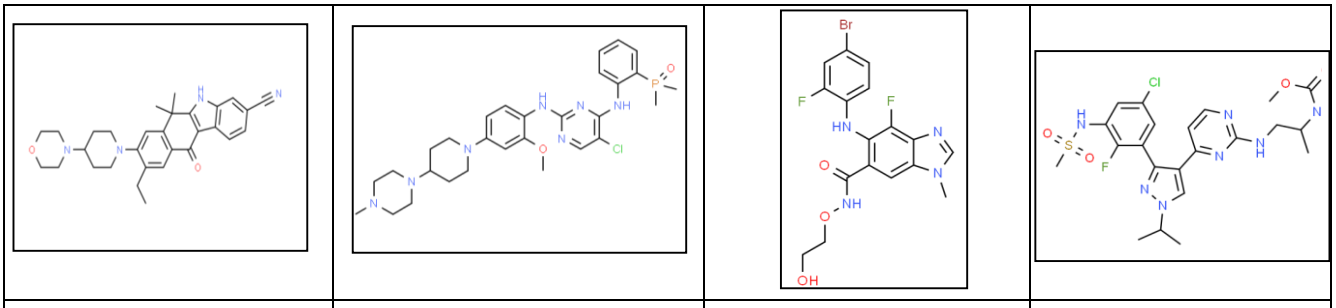
Table 18 Comparison of actual and computed values for Molar volume from regression models

Name of drug	**Molar Volume Of drug**	**Molar volume computed from regression model for**									
		M1(G)	**M2(G)**	**R(G)**	**RR(G)**	**RRR(G)**	**SCI(G)**	**H(G)**	**F(G)**	**Y(G)**	**ISI(G)**
Alectinib	374.7	386.83	398.54	307.76	394.82	411.20	309.64	384.79	388.42	392.98	387.50
Brigatinib	443.6	422.13	418.16	332.28	429.01	430.99	344.16	419.10	414.60	411.63	420.30
Binimetinib.	264.1	282.61	287.36	266.27	283.31	284.70	250.02	274.08	285.94	295.88	272.18
Encorafenib	371.7	359.94	350.14	307.49	359.18	334.53	301.83	367.77	363.92	314.69	368.60
Ceritinib	446.0	383.47	377.61	319.77	387.32	361.26	318.07	387.67	379.51	371.81	390.12
Crizotinib	305.2	316.23	318.75	282.27	319.71	325.47	408.52	311.93	313.79	317.38	308.24
Dacomitinib	349.5	333.04	327.91	382.08	338.77	345.51	356.41	343.93	317.13	317.05	334.06
Entrectinib	418.1	420.45	411.62	429.37	431.69	441.57	330.08	425.30	398.45	383.91	409.89
Pralsetinib	381.0	400.28	394.62	332.57	407.14	408.91	403.31	410.31	420.73	391.13	423.50
Gefitinib	337.8	316.23	313.52	384.95	308.51	333.58	366.52	326.46	304.87	303.27	346.88
Afatinib	352.0	343.13	335.76	380.58	347.93	348.21	385.35	346.81	331.61	328.13	338.42
Gemcitabine	142.3	201.92	211.5	270.33	196.13	195.62	249.13	195.67	219.1	243.46	202.34
Ipilimumab	280.9	275.89	275.59	294.90	274.03	271.03	301.24	268.35	281.48	293.19	266.94
Pembroli zumab	136.2	121.23	134.32	214.13	113.34	128.79	181.20	112.82	141.12	173.24	123.31
Sotorasib	411.9	418.77	420.78	374.80	427.72	419.52	431.43	422.41	409.03	401.21	407.19
Lorlatinib	285.0	306.14	304.36	356.78	298.62	273.27	397.06	303.23	305.99	312.34	292.08
Paclitaxel	610.6	632.26	640.52	610.30	649.18	635.79	597.51	626.50	630.16	629.19	631.05
Dabrafenib	359.9	370.02	369.76	422.23	369.46	352.98	368.00	363.19	382.85	401.38	372.94
Tepotinib	391.6	363.30	357.99	396.04	374.80	385.12	401.26	373.00	348.32	338.55	362.24

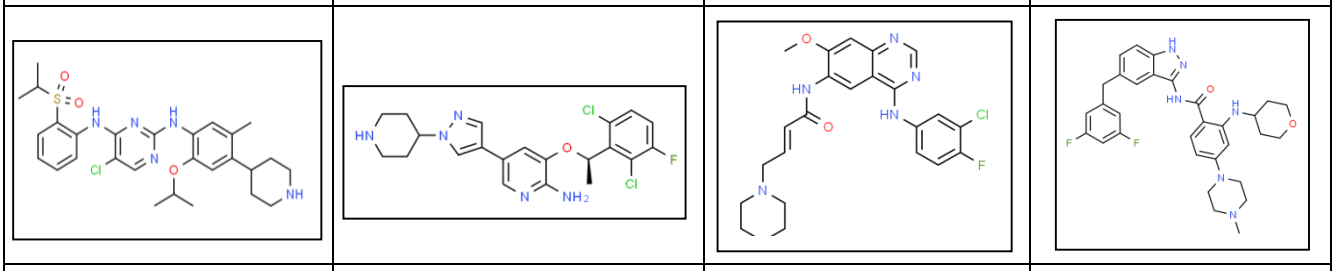
Docetaxel	585.7	595.28	597.36	582.90	539.35	559.74	546.74	584.64	611.22	629.53	589.76

Table 19 Comparison of actual and computed values for Polarizability from regression models

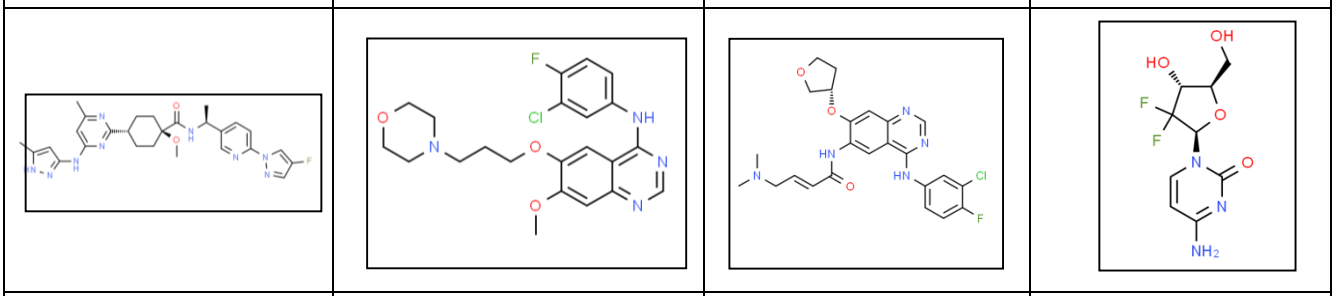
Name of drug	**Polari-zability of drug**	**Polarizability computed from regression model for**									
		M1(G)	**M2(G)**	**R(G)**	**RR(G)**	**RRR(G)**	**SCI(G)**	**H(G)**	**F(G)**	**Y(G)**	**ISI(G)**
Alectinib	55.7	55.66	57.28	44.65	56.92	59.23	44.74	55.38	55.90	55.79	55.81
Brigatinib	63.5	60.64	60.04	48.08	61.78	62.05	49.67	60.33	59.66	58.35	60.43
Binimetinib.	38.3	40.97	41.64	38.85	41.06	41.24	36.23	39.38	41.18	42.50	39.58
Encorafenib	53.2	51.87	50.47	44.61	51.85	48.33	43.63	52.92	52.38	45.08	53.15
Ceritinib	60.1	55.19	54.33	46.33	55.85	52.13	45.95	55.79	54.62	52.9	56.18
Crizotinib	45.4	45.71	46.05	41.09	46.24	47.04	58.86	44.85	45.18	45.44	44.66
Dacomitinib	51.3	48.08	47.34	55.04	48.95	49.89	51.42	49.48	45.66	45.40	48.29
Entrectinib	62.1	60.40	59.12	61.65	62.16	63.55	47.66	61.23	57.34	54.55	58.97
Pralsetinib	57.3	57.56	56.73	48.12	58.67	58.90	58.11	59.06	60.54	55.54	60.88
Gefitinib	47.1	45.71	45.32	55.44	44.65	48.19	52.86	46.95	43.90	43.51	50.10
Afatinib	52.0	49.503	48.45	54.83	50.25	50.27	55.55	49.89	47.74	46.92	48.91
Gemcitabine	20.6	29.59	30.97	39.42	28.67	28.57	36.11	28.05	31.58	35.32	29.75
Ipilimumab	43.1	40.02	39.98	42.86	39.74	39.30	43.55	38.55	40.54	42.13	38.84
Pembroli zumab	17.3	18.21	20.11	31.57	16.89	19.07	26.41	16.08	20.38	25.71	18.63
Sotorasib	59.6	60.16	60.41	54.02	61.60	60.41	62.13	60.81	58.86	56.92	58.59
Lorlatinib	43.0	44.28	44.03	51.50	43.24	39.61	57.22	43.59	44.06	44.75	42.38
Paclitaxel	86.9	90.26	91.32	86.93	93.09	91.17	85.84	90.30	90.62	88.13	90.10
Dabrafenib	50.5	53.29	53.23	60.65	53.31	50.95	53.07	52.26	55.10	56.94	53.77
Tepotinib	57.3	52.34	51.57	56.99	54.07	55.52	57.82	53.67	50.14	48.34	52.26
Docetaxel	81.4	85.05	85.25	83.10	77.04	80.36	78.59	84.25	87.90	88.18	84.29



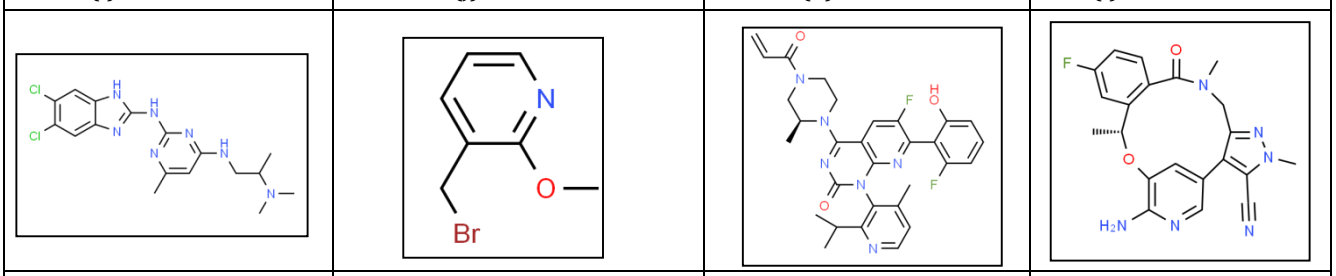
(a) Alectinib | (b) Brigatinib | (c) Binimetinib | (d) Encorafenib



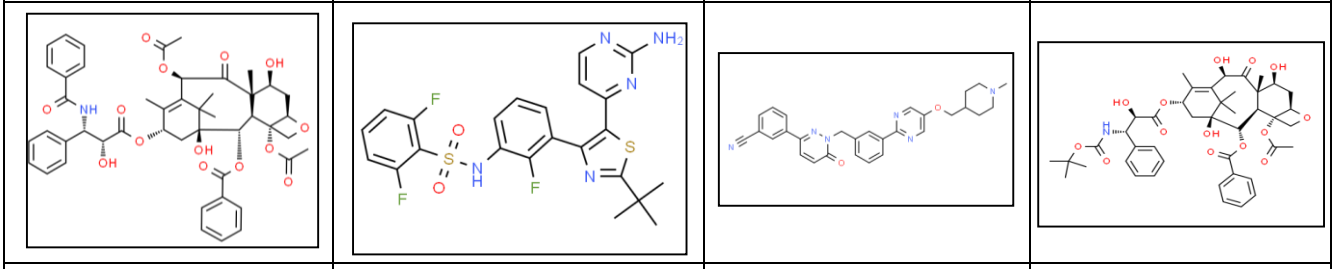
(e) Ceritinib | (f) Crizotinib | (g) Dacomitinib | (h) Entrectinib



(i) Pralsetinib | (j) Gefitinib | (k) Afatinib | (l) Gemcitabine



(m) Ipilimumab | (n) Pembrolizumab | (o) Sotorasib | (p) Lortatinib



(q) Paclitaxel | (r) Dabrafinib | (s) Tepotinib | (t) Docetaxel

Figure 2 Molecular structure of Lung cancer drugs

4. NM-polynomial of Lung cancer drugs

Verma and Mondal defined the Neighborhood NM-polynomial in 2019.[1,14]

$$NM(G:x,y)=\sum_{\psi\le i\le j\le\Psi}\chi_{ij}(G)x^i y^j$$

Where ψ=min {dx|x∈VG}
Ψ=max {dx|x∈VG}

χ_{ij} denotes the number of edges uv∈E(G), where {du, dv} = {i, j }. Here du , dv denotes the degree of the vertices u and v respectively. In this section we expressed the NM-polynomial of molar graphs of Alectinib, Brigatinib, Binimetinib, Encorafenib, Ceritinib, Crizotinib, Dacomitinib, Entrectinib, Pralsetinib, Gefitinib, Afatinib, Gemcitabine, Ipilimumab, Pembrolizumab, Sotorasib, Lortatinib, Paclitaxel, Tafinlar, Tepotinib, Docetaxel.

3.2. Theorem4.1

Let A be the graph of Alectinib. Then NM-polynomial of A is

$$NM(A:x,y)=xy^2+2xy^3+2xy^4+7x^2y^2+17x^2y^3+9x^3y^3+2x^3y^4$$

Proof: The edge partitions of Alectinib as follows

$$|E_{1,2}|=1,\ |E_{1,3}|=2,\ |E_{1,4}|=2,\ |E_{2,2}|=7,|E_{2,3}|=17,\ |E_{3,3}|=9,\ |E_{3,4}|=2$$

From definition of NM-polynomial

$$NM(A:x,y)=\sum_{\psi\le i\le j\le\Psi}\chi_{ij}(A)x^i y^j$$

$$NM(A:x,y)=\chi_{12}(A)x^1y^2+\chi_{13}(A)x^1y^3+\chi_{14}(A)x^1y^4+\chi_{22}(A)x^2y^2+\chi_{23}(A)x^2y^3+\chi_{33}(A)x^3y^3+\chi_{34}(A)x^3y^4$$

$$=\quad xy^2+2xy^3+2xy^4+7x^2y^2+17x^2y^3+9x^3y^3+2x^3y^4$$

3.3. Theorem 4.2

Let B be the graph of Brigatinib. Then NM-polynomial of B is

$$NM(B:x,y)=3xy^3+3xy^4+8x^2y^2+23x^2y^3+7x^3y^3+x^3y^4$$

Proof: The edge partitions of Brigatinib as follows

$$|E_{1,3}|=3,\ |E_{1,4}|=3,\ |E_{2,2}|=8,\ |E_{2,3}|=23,\ |E_{3,3}|=7,\ |E_{3,4}|=1$$

From definition of NM-polynomial

$$NM(B:x,y)=\sum_{\psi\le i\le j\le\Psi}\chi_{ij}(B)x^i y^j$$

$$NM(B:x,y)=\chi_{13}(B)x^1y^3+\chi_{14}(B)x^1y^4+\chi_{22}(B)x^2y^2+\chi_{23}(B)x^2y^3+\chi_{33}(B)x^3y^3+\chi_{34}(B)x^3y^4$$

$$=3xy^3+3xy^4+8x^2y^2+23x^2y^3+7x^3y^3+x^3y^4$$

3.4. Theorem 4.3

Let Bi be the graph of Binimetinib. Then NM-polynomial of Bi is

$$NM(Bi:x,y) = 5xy^3 + 11x^2y^3 + xy^2 + 5x^2y^2 + 7x^3y^3$$

Proof: The edge partitions of Binimetinib as follows

$$|E_{1,3}|=5, |E_{2,3}|=11, |E_{1,2}|=1, |E_{2,2}|=5, |E_{3,3}|=7,$$

From definition of NM-polynomial

$$NM(Bi:x,y) = \sum_{\psi \le i \le j \le \Psi} \chi_{ij}(Bi) x^i y^j$$

$$NM(Bi:x,y) = \chi_{13}(Bi)x^1y^3 + \chi_{22}(Bi)x^2y^2 + \chi_{23}(Bi)x^2y^3 + \chi_{33}(Bi)x^3y^3 + \chi_{12}(Bi)x^1y^2$$

$$= 5xy^3 + 11x^2y^3 + xy^2 + 5x^2y^2 + 7x^3y^3$$

3.5. Theorem 4.4

Let E be the graph of Encorfenib. Then NM-polynomial of E is

$$NM(E:x,y) = xy^2 + 6xy^3 + 3xy^4 + 18x^2y^3 + 6x^3y^3 + x^2y^4 + 3x^2y^2$$

Proof: The edge partitions of Encorfenib as follows

$$|E_{1,2}|=1, |E_{1,3}|=6, |E_{1,4}|=3, |E_{2,3}|=18, |E_{3,3}|=6, |E_{2,4}|=1, |E_{2,2}|=3$$

From definition of NM-polynomial

$$NM(E:x,y) = \sum_{\psi \le i \le j \le \Psi} \chi_{ij}(E) x^i y^j$$

$$NM(E:x,y) = \chi_{12}(E)x^1y^2 + \chi_{13}(E)x^1y^3 + \chi_{14}(E)x^1y^4 + \chi_{22}(E)x^2y^2 + \chi_{23}(E)x^2y^3 + \chi_{33}(E)x^3y^3 + \chi_{24}(E)x^2y^4$$

$$= xy^2 + 6xy^3 + 3xy^4 + 18x^2y^3 + 6x^3y^3 + x^2y^4 + 3x^2y^2$$

3.6. Theorem 4.5

Let C be the graph of Ceritinib. Then NM-polynomial of C is

$$NM(C:x,y) = 6xy^3 + 2xy^4 + 18x^2y^3 + 5x^3y^3 + 8x^2y^2 + 2x^3y^4$$

Proof: The edge partitions of Ceritinib as follows

$$|E_{1,3}|=6, |E_{1,4}|=2, |E_{2,3}|=18, |E_{3,3}|=5, |E_{2,2}|=8, |E_{3,4}|=2,$$

From definition of NM-polynomial

$$NM(C:x,y) = \sum_{\psi \le i \le j \le \Psi} \chi_{ij}(C) x^i y^j$$

$$NM(C:x,y) = \chi_{13}(C)x^1y^3 + \chi_{14}(C)x^1y^4 + \chi_{22}(C)x^2y^2 + \chi_{23}(C)x^2y^3 + \chi_{33}(C)x^3y^3 + \chi_{34}(C)x^3y^4$$

$$= 6xy^3 + 2xy^4 + 18x^2y^3 + 5x^3y^3 + 8x^2y^2 + 2x^3y^4$$

3.7. Theorem 4.6

Let Cr be the graph of Crizotinib. Then NM-polynomial of Cr is

$$NM(Cr:x,y) = 5xy^3 + 14x^2y^3 + 7x^2y^2 + 7x^3y^3$$

Proof: The edge partitions of Crizotinib as follows

$$|E_{1,3}|=5, |E_{2,3}|=14, |E_{3,3}|=7, |E_{2,2}|=7,,$$

From definition of NM-polynomial

$$NM(Cr:x,y) = \sum_{\psi \le i \le j \le \Psi} \chi_{ij}(Cr)x^i y^j$$

$$NM(Cr:x,y) = \chi_{13}(Cr)x^1y^3 + \chi_{22}(Cr)x^2y^2 + \chi_{23}(Cr)x^2y^3 + \chi_{33}(Cr)x^3y^3$$

$$= 5xy^3 + 14x^2y^3 + 7x^2y^2 + 7x^3y^3$$

3.8. Theorem 4.7

Let D be the graph of Dacomitinib. Then NM-polynomial of D is

$$NM(D:x,y) = xy^2 + 3xy^3 + 9x^2y^2 + 19x^2y^3 + 4x^3y^3$$

Proof: The edge partitions of Dacomitinib as follows

$$|E_{1,2}|=1, |E_{1,3}|=3, |E_{2,2}|=9, |E_{2,3}|=19, |E_{3,3}|=4,$$

From definition of NM-polynomial

$$NM(D:x,y) = \sum_{\psi \le i \le j \le \Psi} \chi_{ij}(D)x^i y^j$$

$$NM(D:x,y) = \chi_{12}(D)x^1y^2 + \chi_{13}(D)x^1y^3 + \chi_{22}(D)x^2y^2 + \chi_{23}(D)x^2y^3 + \chi_{33}(D)x^3y^3$$

$$= xy^2 + 3xy^3 + 9x^2y^2 + 19x^2y^3 + 4x^3y^3$$

3.9. Theorem 4.8

Let En be the graph of Entrectinib. Then NM-polynomial of En is

$$NM(En:x,y) = 4xy^3 + 9x^2y^2 + 28x^2y^3 + 5x^3y^3$$

Proof: The edge partitions of Entrectinib as follows

$$|E_{1,3}|=4, |E_{2,2}|=9, |E_{2,3}|=28, |E_{3,3}|=5,$$

From definition of NM-polynomial

$$NM(En:x,y) = \sum_{\psi \le i \le j \le \Psi} \chi_{ij}(En)x^i y^j$$

$$NM(En:x,y) = \chi_{13}(En)x^1y^3 + \chi_{22}(En)x^2y^2 + \chi_{23}(En)x^2y^3 + \chi_{33}(En)x^3y^3$$

$$=4xy^3+9x^2y^2+28x^2y^3+5x^3y^3$$

3.10. Theorem 4.9

Let P be the graph of Pralsetinib. Then NM-polynomial of P is

$$NM(P:x,y)=5xy^3+xy^2+6x^2y^2+24x^2y^3+3x^2y^4+3x^3y^3+x^3y^4$$

Proof: The edge partitions of Pralsetinib as follows

$$|E_{1,3}|=5,\ |E_{1,2}|=1,\ |E_{2,2}|=6,\ |E_{2,3}|=24,|E_{3,3}|=3,\ |E_{3,4}|=1,\ |E_{2,4}|=3$$

From definition of NM-polynomial

$$NM(P:x,y)=\sum_{\psi\le i\le j\le\Psi}\chi_{ij}(P)x^iy^j$$

$$NM(P:x,y)=\chi_{12}(P)x^1y^2+\chi_{13}(P)x^1y^3+\chi_{24}(P)x^2y^4+\chi_{22}(P)x^2y^2+\chi_{23}(P)x^2y^3+\chi_{33}(P)x^3y^3+\chi_{34}(P)x^3y^4$$

$$=5xy^3+xy^2+6x^2y^2+24x^2y^3+3x^2y^4+3x^3y^3+x^3y^4$$

3.11. Theorem 4.10

Let G be the graph of Gefitinib. Then NM-polynomial of G is

$$NM(G:x,y)=xy^2+2xy^3+10x^2y^2+17x^2y^3+4x^3y^3$$

Proof: The edge partitions of Gefitinib as follows

$$|E_{1,2}|=1,|E_{1,3}|=2,|E_{2,2}|=10,|E_{2,3}|=17,|E_{3,3}|=4$$

From definition of NM-polynomial

$$NM(G:x,y)=\sum_{\psi\le i\le j\le\Psi}\chi_{ij}(G)x^iy^j$$

$$NM(G:x,y)=\chi_{12}(G)x^1y^2+\chi_{13}(G)x^1y^3+\chi_{22}(G)x^2y^2+\chi_{23}(G)x^2y^3+\chi_{33}(G)x^3y^3$$

$$=xy^2+2xy^3+10x^2y^2+17x^2y^3+4x^3y^3$$

3.12. Theorem 4.11

Let Af be the graph of Afatinib. Then NM-polynomial of Af is

$$NM(Af:x,y)=5xy^3+8x^2y^2+20x^2y^3+4x^3y^3$$

Proof: The edge partitions of Afatinib as follows

$$|E_{1,3}|=5,|E_{2,2}|=8,\ |E_{2,3}|=20,\ |E_{3,3}|=4$$

From definition of NM-polynomial

$$NM(Af:x,y)=\sum_{\psi\le i\le j\le\Psi}\chi_{ij}(Af)x^iy^j$$

$$NM(Af:x,y)=\chi_{13}(Af)x^1y^3+\chi_{22}(Af)x^2y^2+\chi_{23}(Af)x^2y^3+\chi_{33}(Af)x^3y^3$$

$$=5xy^3+8x^2y^2+20x^2y^3+4x^3y^3$$

3.13. Theorem 4.12

Let Ge be the graph of Gemcitabine. Then NM-polynomial of Ge is

$$NM(Ge:x,y)=xy^2+5xy^3+x^2y^2+7x^2y^3+5x^3y^3$$

Proof: The edge partitions of Gemcitabine as follows

$$|E_{1,2}|=1,|E_{1,3}|=5,|E_{2,2}|=1,|E_{2,3}|=7,|E_{3,3}|=5$$

From definition of NM-polynomial

$$NM(Ge:x,y)=\sum_{\psi\le i\le j\le\Psi}\chi_{ij}(Ge)x^iy^j$$

$$NM(Ge:x,y)=\chi_{12}(Ge)x^1y^2\chi_{13}(Ge)x^1y^3+\chi_{22}(Ge)x^2y^2+\chi_{23}(Ge)x^2y^3+\chi_{33}(Ge)x^3y^3$$

$$=5xy^3+8x^2y^2+20x^2y^3+4x^3y^3$$

3.14. Theorem 4.13

Let I be the graph of Ipilimumab. Then NM-polynomial of I is

$$NM(I:x,y)=6xy^3+x^2y^2+18x^2y^3+3x^3y^3$$

Proof: The edge partitions of Ipilimumab as follows

$$|E_{1,3}|=6,|E_{2,2}|=1,|E_{2,3}|=18,|E_{3,3}|=3$$

From definition of NM-polynomial

$$NM(I:x,y)=\sum_{\psi\le i\le j\le\Psi}\chi_{ij}(I)x^iy^j$$

$$NM(I:x,y)=\chi_{13}(I)x^1y^3+\chi_{22}(I)x^2y^2+\chi_{23}(I)x^2y^3+\chi_{33}(I)x^3y^3$$

$$=6xy^3+x^2y^2+18x^2y^3+3x^3y^3$$

3.15. Theorem 4.14

Let Pe be the graph of Pembrolizumab. Then NM-polynomial of Pe is

$$NM(Pe:x,y)=2xy^2+3x^2y^2+4x^2y^3+x^3y^3$$

Proof: The edge partitions of Pembrolizumab as follows

$$|E_{1,2}|=2,|E_{2,2}|=3,|E_{2,3}|=4,|E_{3,3}|=1$$

From definition of NM-polynomial

$$NM(Pe:x,y)=\sum_{\psi\le i\le j\le\Psi}\chi_{ij}(Pe)x^iy^j$$

$$NM(Pe:x,y)=\chi_{12}(Pe)x^1y^2+\chi_{22}(Pe)x^2y^2+\chi_{23}(Pe)x^2y^3+\chi_{33}(Pe)x^3y^3$$

$$=2xy^2+3x^2y^2+4x^2y^3+x^3y^3$$

3.16. Theorem 4.15

Let S be the graph of Sotorasib. Then NM-polynomial of S is

$$NM(S:x,y)=2xy^2+8xy^3+6x^2y^2+15x^2y^3+14x^3y^3$$

Proof: The edge partitions of Sotorasib as follows

$$|E_{1,2}|=2,|E_{1,3}|=8,|E_{2,2}|=6,|E_{2,3}|=15,|E_{3,3}|=14$$

From definition of NM-polynomial

$$NM(S:x,y)=\sum_{\psi\le i\le j\le\Psi}\chi_{ij}(S)x^iy^j$$

$$NM(S:x,y)=\chi_{12}(S)x^1y^2\chi_{13}(S)x^1y^3+\chi_{22}(S)x^2y^2+\chi_{23}(S)x^2y^3+\chi_{33}(S)x^3y^3$$

$$=2xy^2+8xy^3+6x^2y^2+15x^2y^3+14x^3y^3$$

3.17. Theorem 4.16

Let L be the graph of Lortatinib. Then NM-polynomial of L is

$$NM(L:x,y)=7xy^3+5x^2y^2+14x^2y^3+6x^3y^3$$

Proof: The edge partitions of Lortatinib as follows

$$|E_{1,3}|=7,|E_{2,2}|=5,|E_{2,3}|=14,|E_{3,3}|=6$$

From definition of NM-polynomial

$$NM(L:x,y)=\sum_{\psi\le i\le j\le\Psi}\chi_{ij}(L)x^iy^j$$

$$NM(L:x,y)=\chi_{13}(L)x^1y^3+\chi_{22}(L)x^2y^2+\chi_{23}(L)x^2y^3+\chi_{33}(L)x^3y^3$$

$$=7xy^3+5x^2y^2+14x^2y^3+6x^3y^3$$

3.18. Theorem 4.17

Let Pa be the graph of Paclitaxel. Then NM-polynomial of Pa is

$$NM(Pa:x,y)=10xy^3+3xy^4+13x^2y^2+20x^2y^3+10x^3y^3+4x^2y^4+7x^3y^4+x^4y^4$$

Proof: The edge partitions of Paclitaxel as follows

$$|E_{1,3}|=10,|E_{1,4}|=3,|E_{2,3}|=20,|E_{3,3}|=10,|E_{2,2}|=13,|E_{2,4}|=4|E_{3,4}|=7,|E_{4,4}|=1$$

From definition of NM-polynomial

$$NM(Pa:x,y)=\sum_{\psi\le i\le j\le\Psi}\chi_{ij}(Pa)x^i y^j$$

$$NM(Pa:x,y)=\chi_{13}(Pa)x^1y^3+\chi_{14}(Pa)x^1y^4+\chi_{22}(Pa)x^2y^2+\chi_{23}(Pa)x^2y^3+\chi_{24}(Pa)x^2y^4+$$
$$+\chi_{33}(Pa)x^3y^3+\chi_{34}(Pa)x^3y^4+\chi_{44}(Pa)x^4y^4$$
$$=10xy^3+3xy^4+13x^2y^2+20x^2y^3+10x^3y^3+4x^2y^4+7x^3y^4+x^4y^4$$

3.19. Theorem 4.18

Let Da be the graph of Dabrafinib. Then NM-polynomial of Da is

$$NM(Da:x,y)=4xy^3+5xy^4+6x^2y^2+13x^2y^3+7x^3y^3+x^2y^4+2x^3y^4$$

Proof: The edge partitions of Dabrafinib as follows

$$|E_{1,3}|=4,|E_{1,4}|=5,|E_{2,3}|=13,|E_{3,3}|=7,|E_{2,2}|=6,|E_{2,4}|=1|E_{3,4}|=2$$

From definition of NM-polynomial

$$NM(Da:x,y)=\sum_{\psi\le i\le j\le\Psi}\chi_{ij}(Da)x^i y^j$$

$$NM(Da:x,y)=\chi_{13}(Da)x^1y^3+\chi_{14}(Da)x^1y^4+\chi_{22}(Da)x^2y^2+\chi_{23}(Da)x^2y^3+\chi_{24}(Da)x^2y^4+$$
$$+\chi_{33}(Da)x^3y^3+\chi_{34}(Da)x^3y^4$$
$$=4xy^3+5xy^4+6x^2y^2+13x^2y^3+7x^3y^3+x^2y^4+2x^3y^4$$

3.20. Theorem 4.19

Let T be the graph of Tepotinib. Then NM-polynomial of T is

$$NM(T:x,y)=3xy^3+10x^2y^2+24x^2y^3+3x^3y^3$$

Proof: The edge partitions of Tepotinib as follows

$$|E_{1,3}|=3,|E_{2,2}|=10,|E_{2,3}|=24,|E_{3,3}|=3$$

From definition of NM-polynomial

$$NM(T:x,y)=\sum_{\psi\le i\le j\le\Psi}\chi_{ij}(T)x^i y^j\quad NM(T:x,y)=\chi_{13}(T)x^1y^3+\chi_{22}(T)x^2y^2+\chi_{23}(T)x^2y^3+\chi_{33}(T)x^3y^3$$

$$=3xy^3+10x^2y^2+24x^2y^3+3x^3y^3$$

3.21. Theorem 4.20

Let Do be the graph of Docetaxel. Then NM-polynomial of Do is

$$NM(Do:x,y)=10xy^3+7xy^4+9x^2y^2+16x^2y^3+9x^3y^3+4x^2y^4+7x^3y^4+x^4y^4$$

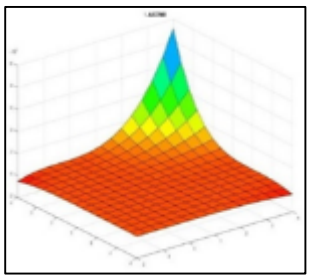
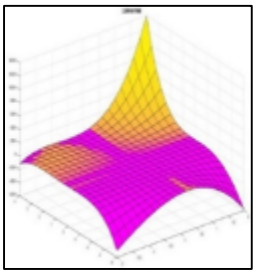
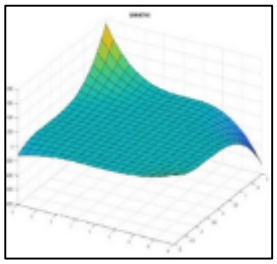
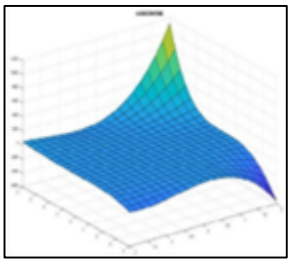
Proof: The edge partitions of Docetaxel as follows

$$|E_{1,3}|=10,|E_{1,4}|=7,|E_{2,3}|=16,|E_{3,3}|=9,|E_{2,2}|=9,|E_{2,4}|=4|E_{3,4}|=7,|E_{4,4}|=1$$

From definition of NM-polynomial

$$NM(Do:x,y)=\sum_{\psi\le i\le j\le\Psi}\chi_{ij}(Do)x^{i}y^{j}$$

$$NM(Do:x,y)=\chi_{13}(Do)x^{1}y^{3}+\chi_{14}(Do)x^{1}y^{4}+\chi_{22}(Do)x^{2}y^{2}+\chi_{23}(Do)x^{2}y^{3}+\chi_{24}(Do)x^{2}y^{4}+$$
$$+\chi_{33}(Do)x^{3}y^{3}+\chi_{34}(Do)x^{3}y^{4}+\chi_{44}(Do)x^{4}y^{4}$$
$$=10xy^{3}+7xy^{4}+9x^{2}y^{2}+16x^{2}y^{3}+9x^{3}y^{3}+4x^{2}y^{4}+7x^{3}y^{4}+x^{4}y^{4}$$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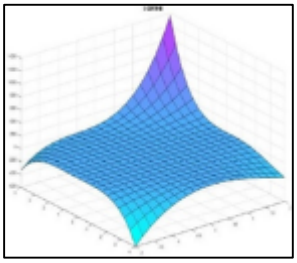	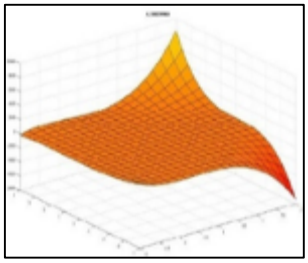	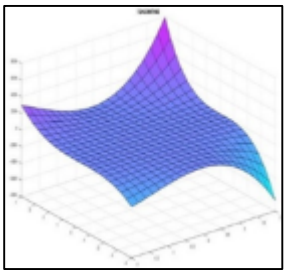	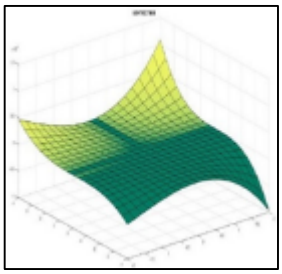
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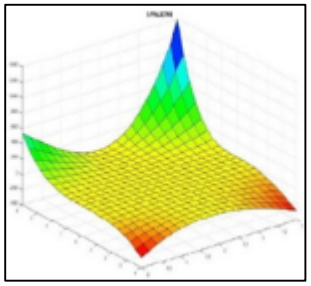	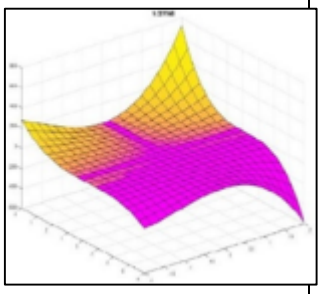	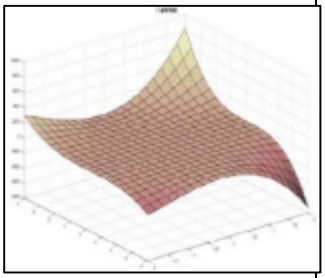	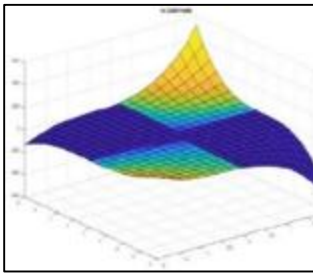
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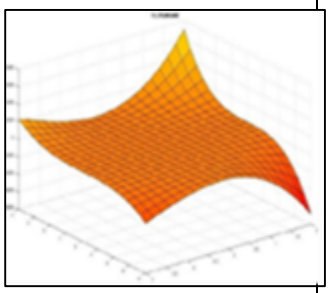	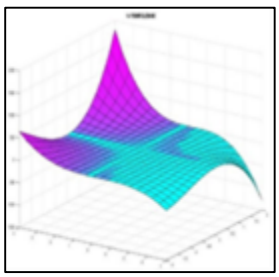	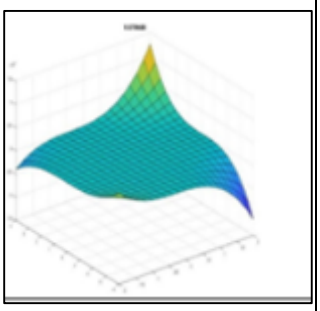	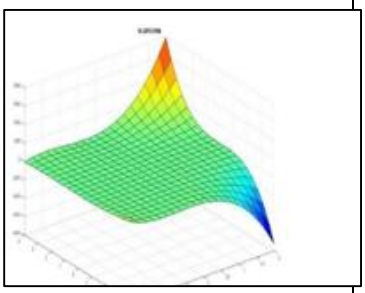
((m)) Ipilimumab	((n)) Pembrolizumab	((o))Sotorasib	((p))Lortatinib

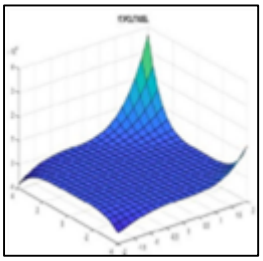	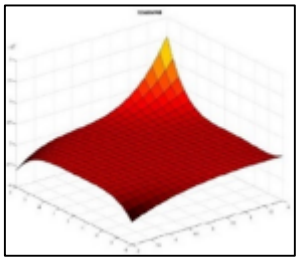	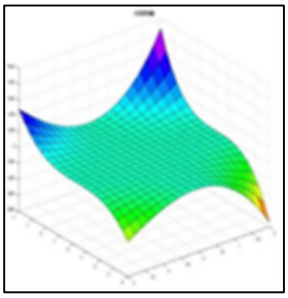	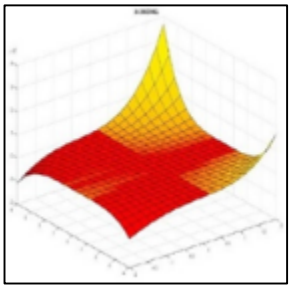
((q))Paclitaxel	((r))Dabrafinib	((s))Tepotinib	((t))Docetaxel

Figure 3 NM-Polynomials for Lung cancer drugs

4. Conclusion

This study examines drugs used to treat Lung cancer and computes several numerical descriptors. To design a new medicine , its important to understand its structure. QSPR modeling with TI's can provide this information. This work aims to use topological indices to acquire data about structure topology in a cost effective and time efficient manner. 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 H(G) with r=0.943. Also Enthalpy has the highest correlation with F(G) with r=0.950, and FP has a good correlation with H(G) with r=0.943. While MR with H(G) has high correlation with r=0.985, MV with H(G) has r=0.980 and polarizability with H(G) has r=0.985. The results show strong correlation coefficients between physical attributes and topological indices. The study indicates that MR and Polarizability has a strong association with all topological indices. The work guides chemists and pharmacists in developing new drugs for treating various diseases. TI's are often used for anticipating physicochemical qualities. The indices are utilized in prediction studies for models designed for soil absorption, boiling point, viscosity, organic solvent densities, and data retention via chromotography. We also derived the NM-polynomials of these drugs.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

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