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Topological Indices of Drugs Used in Brain Tumor Treatment with Their QSPR Analysis and M-polynomial

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Abstract: A brain tumor is a cell growth in or near the brain. A topological index of graph G is a numerical quantity that describes its topology. If it is applied to the molecular structure of chemical compounds, then it reflects the theoretical properties of the chemical compounds. This paper applies well-known degree-based topological Indices to the chemical structures of brain tumor drugs. Furthermore, QSPR analysis of the said topological indices is discussed, showing that these topological indices are highly correlated with the physical properties of brain tumor drugs. Finally, we calculate the M-polynomial of brain tumor drugs.

Keywords: topological indices; drugs; brain tumor; linear QSPR model; M-polynomial.

1. Introduction

Brain tumors can happen in the brain tissue. Brain tumors also can happen near the brain tissue. Nearby locations include nerves, the pituitary gland, the pineal gland, and the membranes covering the brain's surface. Brain tumors can begin in the brain. These are called primary brain tumors. Sometimes, cancer spreads to the brain from other parts of the body. These tumors are secondary brain tumors, also called metastatic brain tumors. Many different types of primary brain tumors exist. Some brain tumors aren't cancerous. These are called noncancerous brain tumors or benign brain tumors. Noncancerous brain tumors may grow over time and press on the brain tissue. Other brain tumors are brain cancers, also called malignant brain tumors. Brain cancers may grow quickly. The cancer cells can invade and destroy the brain tissue. General signs and symptoms caused by brain tumors may include headache, nausea, speech problems, eye problems, etc. For further details, see [1–4]. The eight medicines Everolimus (E), Belzutifan (B), Carmustine (C), Lomustine (L), Temozolomide (T), Dabrafenib mesylate (D), Trametinib dimethyl sulfoxide (Tr), and Bevacizumab (Be) are used to treat brain tumor.

A topological index is a mathematical measure of chemical compounds represented as molecular graphs. It is used in quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) studies to model chemical compounds' physicochemical, pharmacological, toxicological, biological, and other aspects of theoretical chemistry. Topological indices are used in biology, mathematics, bioinformatics, informatics, and other fields. There are several types of topological indices, including distance-based topological indices, degree-based topological indices, counting-related polynomials, and graph indices. Graph theory has given chemists many useful tools, such as topological indices.

Molecules and molecular compounds are frequently represented by molecular graphs. A molecular graph is a graph-theoretic representation of a chemical compound's structural formula. Zhao *et al*. [9] created the SS index and studied the physicochemical features of 67 different alkane isomers. Many algebraic graph polynomials were introduced in the past; some important ones are the Hosoya polynomial, Forgotten polynomial [10], Pi polynomial, Schultz polynomial, Modified Schultz polynomial [11], Matching polynomial [12], Tutte polynomial [13], and M-Polynomial. Nagarajan *et al*. and Priyadharsini *et al*. [14] calculated the status-based topological indices of COVID-19 drugs. Colakoglu *et al*. [15] calculated the topological indices of some potential drugs against COVID-19. A graph polynomial is an algebraic object associated with a graph that is usually invariant under graph isomorphism. In this work, we further discuss the QSPR analysis of said topological indices. We also show that the characteristics obtained are highly correlated with the characteristics of brain tumor drugs using linear regression. Furthermore, we derive the M-polynomial of brain tumor drugs.

2. Materials and Methods

The vertices of the molecular graph represent the atoms of the chemical structure, and the edges represent the bonds of the chemical structure. Consider G(V, E) a molecular graph with vertex and edge set, respectively. The degree of a vertex v is the number of edges incident on the vertex v and is expressed as $d_G(v) = \chi_N(v)$ for every $v \in V(G)$.

In 1972, I. Gutman and N. Trinajstic [16] defined the first and second Zagreb index of a graph as

$$M_1(G) = \sum_{v\in V(G)}[\chi_G(v)^2] = \sum_{uv\in E(G)}[\chi_G(u) + \chi_G(v)]$$
$$M_2(G) = \sum_{uv\in E(G)}[\chi_G(u)\chi_G(v)]$$

B. Furtula and I. Gutman defined the F-index as [17] in 2015:

$$F(G) = \sum_{v\in V(G)}[\chi_G(v)^3] = \sum_{uv\in E(G)}[\chi_G(u)^2 + \chi_G(v)^2]$$

In 2020, Abdu Alameri and Noman AI-Naggar [18] introduced the Y-index, which is defined as:

$$Y(G) = \sum_{v\in V(G)}[\chi_G(v)^4] = \sum_{uv\in E(G)}[\chi_G(u)^3 + \chi_G(v)^3]$$

In 2021, S. Nagarajan and G. Kayalvizhi defined the S-index as [19]:

$S(G) = \sum_{v\in V(G)}[\chi_G(v)^5] = \sum_{uv\in E(G)}[\chi_G(u)^4 + \chi_G(v)^4]$

S. Fajtlowicz defined the harmonic index graph as [20] in 1987:

$$H(G) = \sum_{uv\in E(G)} \frac{2}{\chi_G(u)+\chi_G(v)}$$

The modified second Zagreb index of a graph as [21]:

$$mM_2(G) = \sum_{uv\in E(G)} \frac{1}{\chi_G(u)\chi_G(v)}$$

So, the linear regression model is adequate to test and adopt for said analysis. The molecular structure of brain tumor drugs is represented in Figure 1.

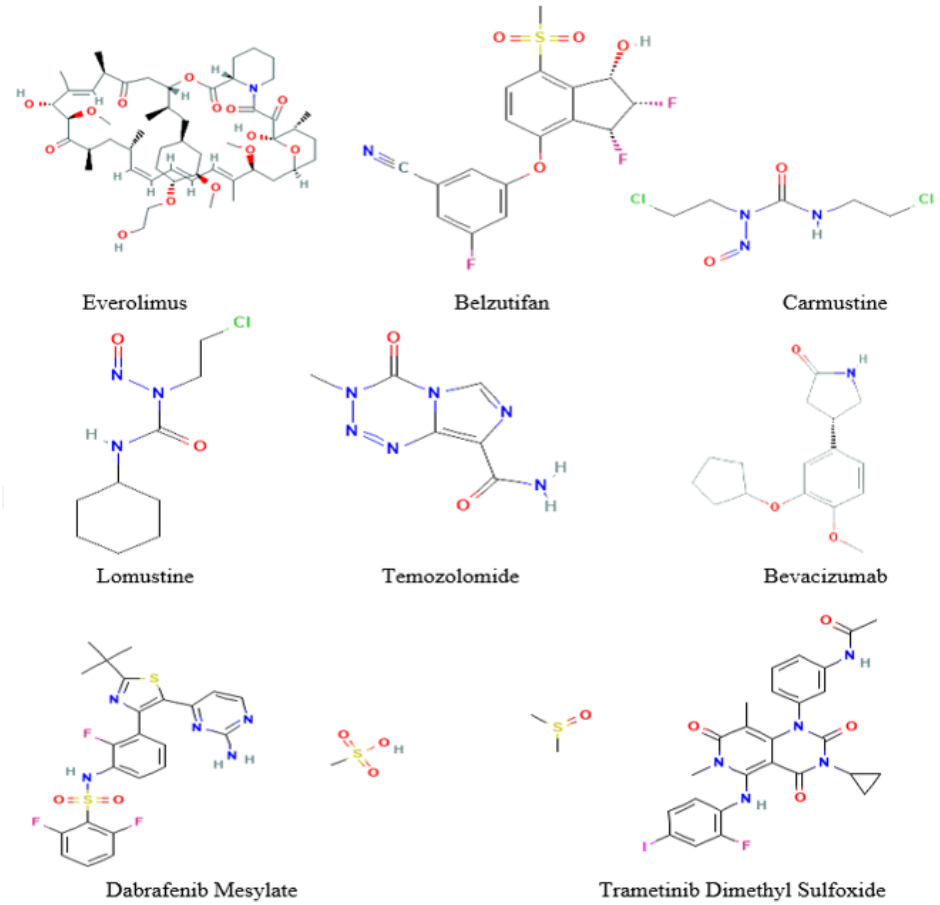

Figure 1. Molecular structure of drugs.

3. Results and Discussion

In this section, degree-based TIs are imposed on brain tumor drugs. The relation between QSPR analysis and topological indices shows that they are highly correlated regarding physicochemical properties used in brain tumors. The eight medicines Everolimus (E), Belzutifan (B), Carmustine (C), Lomustine (L), Temozolomide (T), Dabrafenib mesylate (D), Trametinib dimethyl sulfoxide (Tr), and Bevacizumab (Be) are used for this analysis of said disease. In drugs, structure elements denote vertices and corresponding bonds connecting the atoms are termed edges. Table 1 shows the topological indices values calculated from their chemical structure. The physical property values are extracted from Chem Spider. It is observed from data Table 2 that these data values are normally distributed. Tables 3–9 display the statistical parameters such as number of drugs considered, constant, regression coefficient, correlation coefficient, R- square, Fisher's statistic, significant value, and standard error denoted by N, A, b, r, r^2, F, p, and SE, respectively, for all the considered Topological indices and physical properties. Table 10 shows the association coefficient between five physicochemical properties and Topological indices. The graph of Topological indices and physico-chemical properties is shown in Figure 2 using MS - Excel. In each table, the value of p is less than or equal to 0.001 ($p \leq 0.05$), indicating the significance of the results. Hence, the study used regression analysis for the calculation purpose.

Table 1. Computed values of topological indices for brain tumor drugs.

Drug name	M_1	M_2	F	Y	S	mM_2	H
E	340	397	892	2488	7252	15.46	30.774
B	138	166	390	1170	3654	5.195	10.818

Drug name	M_1	M_2	F	Y	S	mM_2	H
C	52	56	126	328	894	3.39	5.868
L	66	72	156	390	1020	3.696	7.068
T	74	89	198	554	1590	3.057	6.268
D	206	237	586	1814	5962	8.126	16.705
Tr	218	262	586	1646	4738	8.89	20.267
Be	112	132	298	856	2626	4.614	9.754

Table 2. Physicochemical properties of brain tumor drugs.

Drug name	BP	MW	PSA	Com	MV
E	998.7	958.2	205	1810	811.2
B	505.8	383.3	96	675	244.7
C	309.6	214.05	65	156	146.4
L	354.07	233.69	62	219	173.1
T	526.6	194.15	106	315	98.4
D	-	615.7	210	910	-
Tr	-	693.5	138	1120	-
Be	472.7	-	-	-	-

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

Physical properties	N	A	b	r	r^2	F	p	SE
BP	6	239.504	2.213	0.966	0.934	56.565	0.002	70.738
MW	7	38.015	2.766	0.992	0.984	311.754	0.000	40.302
PSA	7	46.246	0.570	0.874	0.764	16.170	0.010	32.643
Com	7	-136.503	5.631	0.996	0.992	603.056	0.000	58.984
MV	5	-28.349	2.411	0.984	0.969	92.265	0.002	60.143

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

Physical properties	N	A	b	r	r^2	F	p	SE
BP	6	241.586	1.884	0.969	0.939	61.675	0.001	67.931
MW	7	43.558	2.336	0.991	0.981	263.244	0.000	43.795
PSA	7	47.741	0.428	0.867	0.752	15.201	0.011	33.417
Com	7	-127.749	4.769	0.997	0.995	932.337	0.000	47.507
MV	5	-22.564	2.034	0.978	0.957	67.302	0.004	70.010

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

Physical properties	N	A	b	r	r^2	F	p	SE
BP	6	242.319	0.832	0.966	0.933	55.840	0.002	71.166
MW	7	43.447	1.019	0.988	0.976	207.024	0.000	49.259
PSA	7	45.156	0.193	0.894	0.799	19.821	0.007	30.147
Com	7	-123.702	2.069	0.990	0.980	244.680	0.000	92.047
MV	5	-21.501	0.897	0.974	0.950	56.462	0.005	76.125

Table 6. Satistical specifications for the linear model of $Y(G)$.

Physical properties	N	A	b	r	r^2	F	p	SE
BP	6	246.131	0.292	0.961	0.924	48.445	0.002	76.017
MW	7	54.108	0.347	0.977	0.954	103.866	0.000	68.745
PSA	7	44.261	0.068	0.916	0.839	26.063	0.004	26.948
Com	7	-98.708	0.703	0.975	0.950	95.009	0.000	145.440
MV	5	-13.737	0.313	0.963	0.927	38.350	0.008	91.287

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

Physical properties	N	A	b	r	r^2	F	p	SE
BP	6	250.851	0.098	0.952	0.906	38.547	0.003	84.398
MW	7	73.159	0.111	0.955	0.911	51.288	0.001	95.604
PSA	7	44.434	0.023	0.936	0.876	35.419	0.002	23.624
Com	7	-55.560	0.223	0.947	0.897	43.512	0.001	208.822
MV	5	-4.979	0.104	0.951	0.903	28.077	0.013	105.300

Table 8. Statistical specifications for the linear model of $mM_2(G)$.

Physical properties	N	A	b	r	r^2	F	p	SE
BP	6	238.938	48.962	0.945	0.982	33.088	0.005	90.395
MW	7	30.212	64.439	0.980	0.960	120.551	0.000	64.014
PSA	7	48.471	11.350	0.824	0.679	10.596	0.023	38.031

Physical properties	N	A	b	r	r^2	F	p	SE
Com	7	-151.488	131.037	0.983	0.966	140.401	0.000	120.620
MV	5	-48.330	55.700	0.999	0.998	1216.846	0.000	16.807

Table 9. Statistical specifications for the linear model of *H(G)*.

Physical properties	N	A	b	r	r^2	F	p	SE
BP	6	237.613	24.689	0.955	0.912	41.340	0.003	81.757
MW	7	30.882	31.466	0.993	0.985	338.529	0.000	38.699
PSA	7	49.151	5.502	0.829	0.687	10.984	0.021	37.567
Com	7	-146.848	63.752	0.992	0.984	303.080	0.000	82.865
MV	5	-41.135	27.625	0.997	0.993	444.236	0.000	27.758

Table 10. Correlation coefficient between physicochemical properties and Topological indices of brain tumor drugs.

Indices	BP	MW	PSA	Com	MV
M_1	0.966	0.992	0.874	0.996	0.984
M_2	0.969	0.991	0.867	0.997	0.978
F	0.966	0.988	0.894	0.990	0.974
Y	0.961	0.977	0.916	0.975	0.963
S	0.952	0.955	0.936	0.947	0.951
mM_2	0.945	0.980	0.824	0.983	0.999
H	0.955	0.993	0.829	0.992	0.997

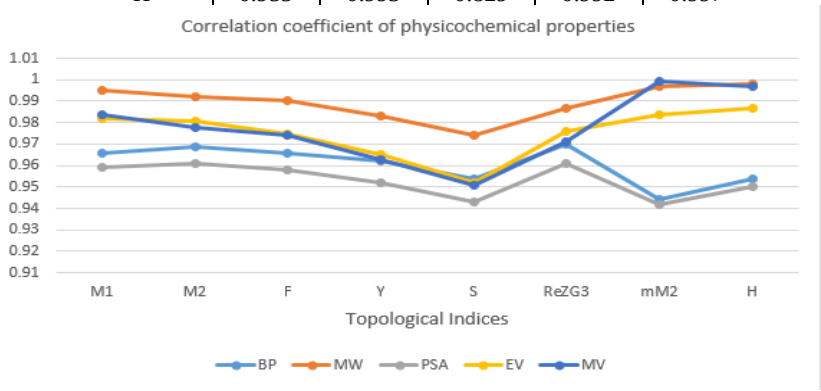

Figure 2. Topological indices and physicochemical properties of brain tumor drugs

3.1. Regression model.

The following equation is used to correlate the physical properties of various drugs used to treat brain tumors with some topological indices. We have used the following linear regression model:

$$P = A + b\,(TI) \qquad (1)$$

Where P, A, b, TI ⟶ is the physical property of the drug, constant, regression coefficient, and topological index. All data tables are calculated using SPSS software version-26 to obtain accurate results. Using equation (1), the following is the linear regression model for the defined degree-based topological indices:

1. **Regression models for $M_1(G)$**

BP=239.504+2.213[M_1(G)]
MW=38.015+2.766[M_1(G)]
PSA=46.246+0.510[M_1(G)]
Com=-136.503+5.631[M_1(G)]
MV=-28.349+2.411[M_1(G)]

2. **Regression models for $M_2(G)$**

BP=241.586+1.884[M_2(G)]
MW=43.558+2.336[M_2(G)]
PSA=47.741+0.428[M_2(G)]
Com=-127.749+4.769[M_2(G)]

MV=-22.564+2.034[M_2(G)]

3. **Regression models for $F(G)$**

BP=242.319+0.832[F(G)]
MW=43.447+1.019[F(G)]
PSA=45.156+0.193[F(G)]
Com=-123.702+2.069[F(G)]
MV=-21.501+0.897[F(G)]

4. **Regression models for $Y(G)$**

BP=246.131+0.292[Y(G)]
MW=54.108+0.347[Y(G)]
PSA=44.261+0.068[Y(G)]
Com=-98.708+0.703[Y(G)]
MV=-13.737+0.313[Y(G)]

5. **Regression models for $S(G)$**

BP=250.851+0.098[S(G)]
MW=73.159+0.111[S(G)]
PSA=44.434+0.023[S(G)]
Com=-55.560+0.223[S(G)]
MV=-4.979+0.104[S(G)]

6. **Regression models for $mM_2(G)$**

BP=238.938+48.962[mM_2(G)]
MW=30.212+64.439[mM_2(G)]
PSA=48.471+11.350[mM_2(G)]
Com=-151.488+131.037[mM_2(G)]
MV=-48.330+55.700[mM_2(G)]

7. **Regression models for $H(G)$**

BP=237.613+24.689[H(G)]
MW=30.882+31.466[H(G)]
PSA=49.151+5.502[H(G)]
Com=-146.848+63.752[H(G)]
MV=-41.135+27.625[H(G)]

Tables 11-15 compare the physicochemical properties of the experimental and theoretical derived values of the models.

Table 11. Comparison of actual and computed values for BP from regression models.

Drugs name	BP of drugs	BP computed from regression model for M_1	BP computed from regression model for M_2	BP computed from regression model for F	BP computed from regression model for Y	BP computed from regression model for S	BP computed from regression model for mM_2	BP computed from regression model for H
E	998.7	991.924	989.534	984.463	972.627	961.547	995.891	997.392
B	505.8	544.898	554.33	566.799	587.771	608.943	493.296	504.699
C	309.6	354.58	347.09	347.151	341.907	338.463	404.919	382.488
L	354.07	385.562	377.234	372.111	360.011	350.811	419.902	412.115
T	526.6	403.266	409.262	407.055	407.899	406.671	388.615	392.364
D	-	695.382	688.094	729.871	775.819	835.127	636.803	650.043
Tr	-	721.938	735.194	729.871	726.763	715.175	674.210	737.985
Be	472.7	487.36	490.274	490.255	496.083	508.199	464.849	478.429

Table 12. Comparison of actual and computed values for MW from regression models.

Drugs name	MW of drugs	MW computed from the regression model for M_1	MW computed from regression model for M_2	MW computed from regression model for F	MW computed from the regression model for Y	MW computed from regression model for S	MW computed from regression model for mM_2	MW computed from regression model for H
E	958.2	978.455	970.95	952.395	917.444	878.131	1026.438	999.216
B	383.3	419.723	431.334	440.857	460.098	478.753	364.972	371.281

Drugs name	MW of drugs	MW computed from the regression model for M_1	MW computed from regression model for M_2	MW computed from regression model for F	MW computed from the regression model for Y	MW computed from regression model for S	MW computed from regression model for mM_2	MW computed from regression model for H
C	214.05	181.847	174.374	171.841	167.924	172.393	248.660	215.524
L	233.69	220.571	211.75	202.411	189.438	186.379	268.378	253.283
T	194.15	242.699	251.462	245.209	246.346	249.649	227.202	228.110
D	615.7	607.811	597.19	640.581	683.566	734.941	553.843	556.522
Tr	693.5	641.003	655.59	640.581	625.27	599.077	603.074	668.603
Be	-	347.807	351.91	347.109	351.14	364.645	327.533	337.801

Table 13. Comparison of actual and computed values for PSA from regression models.

Drugs name	PSA of drugs	PSA computed from regression model for M_1	PSA computed from regression model for M_2	PSA computed from regression model for F	PSA computed from regression model for Y	PSA computed from regression model for S	PSA computed from regression model for mM_2	PSA computed from regression model for H
E	205	219.646	217.657	217.312	213.445	211.23	223.942	218.469
B	96	116.626	118.789	120.426	123.821	128.476	107.434	108.672
C	65	72.766	71.709	69.474	66.565	64.996	86.948	81.437
L	62	79.906	78.557	75.264	70.781	67.894	90.421	88.039
T	106	83.986	85.833	83.37	81.933	81.004	83.168	83.638
D	210	151.306	149.177	158.254	167.613	181.56	140.701	141.062
Tr	138	157.426	159.877	158.254	156.189	153.408	149.373	160.660
Be	-	103.366	104.237	102.67	102.469	104.832	100.839	102.818

Table 14. Comparison of actual and computed values for Com from regression models.

Drugs name	Com of drugs	Com computed from regression model for M_1	Com computed from regression model for M_2	Com computed from regression model for F	Com computed from regression model for Y	Com computed from regression model for S	Com computed from regression model for mM_2	Com computed from regression model for H
E	1810	1778.037	1765.544	1721.846	1650.356	1561.636	1874.344	1815.056
B	675	640.575	663.905	683.208	723.802	759.282	529.249	542.821
C	156	156.309	139.315	136.992	131.876	143.802	292.727	227.248
L	219	235.143	215.619	199.062	175.462	171.9	332.825	303.751
T	315	280.191	296.692	285.96	290.754	299.01	249.092	252.749
D	910	1023.483	1002.504	1088.732	1176.534	1273.966	913.318	918.129
Tr	1120	1091.055	1121.729	1088.732	1058.43	1001.014	1013.430	1145.214
Be	-	494.169	501.759	492.86	503.06	530.06	453.116	474.989

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

Drugs name	MV of drugs	MV computed from regression model for M_1	MV computed from regression model for M_2	MV computed from regression model for F	MV computed from regression model for Y	MV computed from regression model for S	MV computed from regression model for mM_2	MV computed from regression model for H
E	811.2	791.391	784.934	778.623	765.007	749.229	812.792	808.997
B	244.7	304.369	315.08	328.329	352.473	375.037	241.032	257.712
C	146.4	97.023	91.34	91.521	88.927	87.997	140.493	120.968
L	173.1	130.777	123.884	118.431	108.333	101.101	157.537	154.118
T	98.4	150.065	158.462	156.105	159.665	160.381	121.945	132.018
D	-	468.317	459.494	504.141	554.045	615.069	404.288	420.340
Tr	-	497.249	510.344	504.141	501.461	487.773	446.843	518.740
Be	-	241.683	245.924	245.805	254.191	268.125	208.669	228.319

Figures 3-7 depict the linear regression of the first Zagreb index against physical properties by using SPSS software.

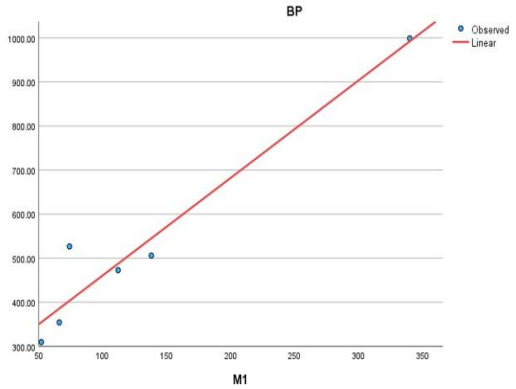

Figure 3. Linear regression plot for M_1 index against BP.

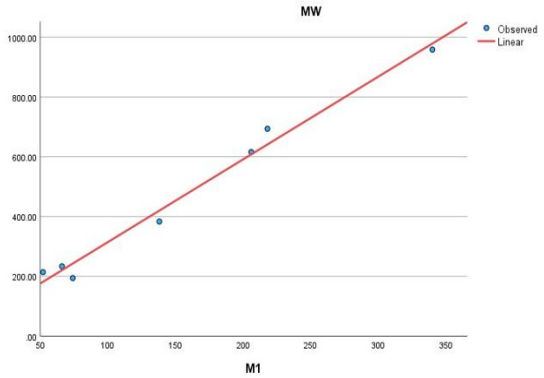

Figure 4. Linear regression plot for M_1 index against MW.

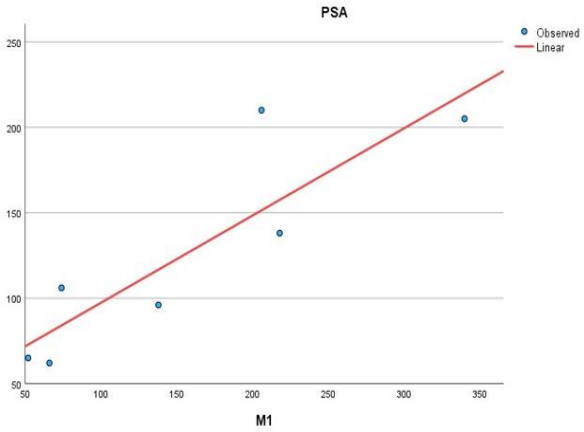

Figure 5. Linear regression plot for M_1 index against PSA.

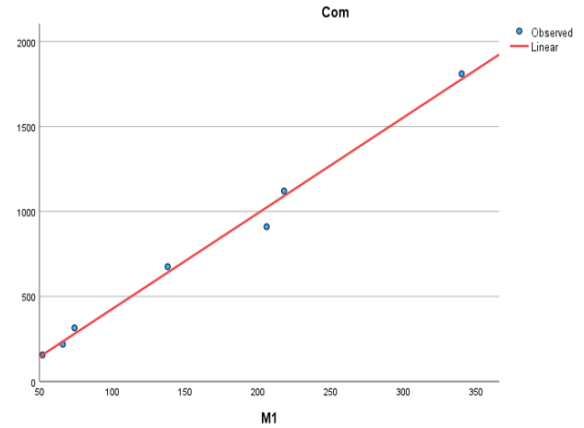

Figure 6. Linear regression plot for M_1 index against Com.

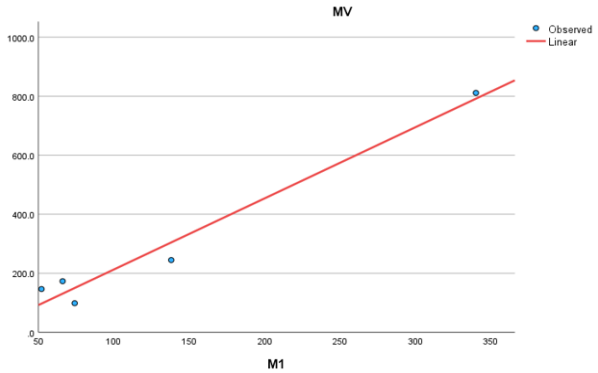

Figure 7. Linear regression plot for M_1 index against MV.

3. M-Polynomial of brain tumor drugs

Fath-Tabar [15] defined the first, second, and third Zagreb polynomials. Numerous algebraic polynomials, such as the Wiener polynomial [16], have potential applications in mathematical chemistry, such as calculating distance-based TIs. The M-polynomial performs the same function, providing formulas that are close enough to degree-based topological indices. It is the most general polynomial that has been devised to date. The definition of an M-polynomial is [17]:

$$M(G;x,y)=\sum_{a\leq b} n_{ab}(G)x^a y^b$$

Where, $n_{ab}(G)$ is the number of edges of G, such that $ij \in E(G)$and $\{\chi_i,\chi_j\}=\{a,b\}$. In this section, we expressed the M-polynomials of brain tumor drugs such as everolimus (E), belzutifan (B), carmustine (C), lomustine (L), temozolomide (T), dabrafenib mesylate (D), trametinib dimethyl sulfoxide (Tr), bevacizumab (Be). Figure 8-15 depicts the 3D surface plot for the M-polynomial of brain tumor drugs using Matlab.

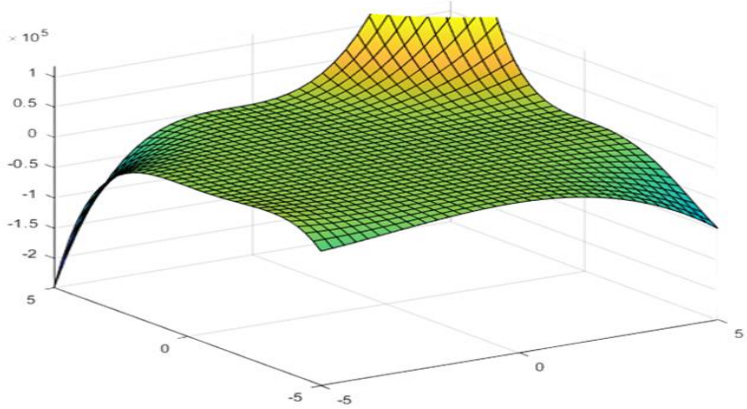

Figure 8. M-polynomial of Everolimus.

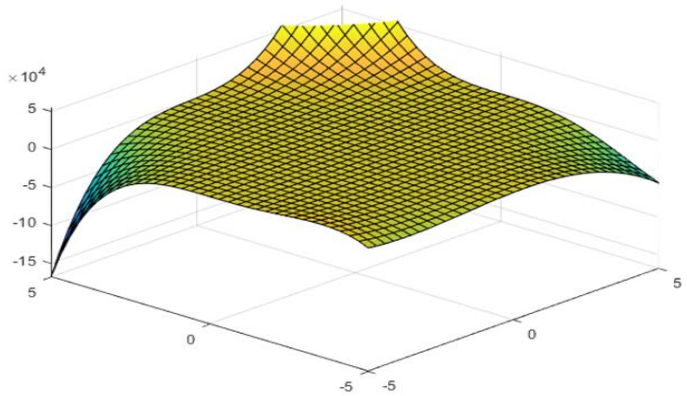

Figure 9. M-polynomial of Belzutifan.

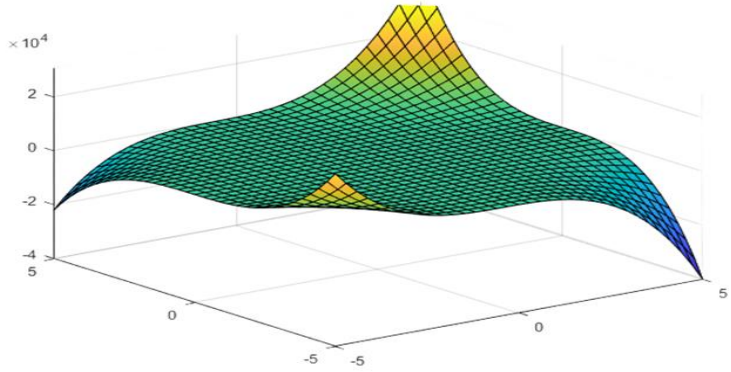

Figure 10. M-polynomial of Carmustine.

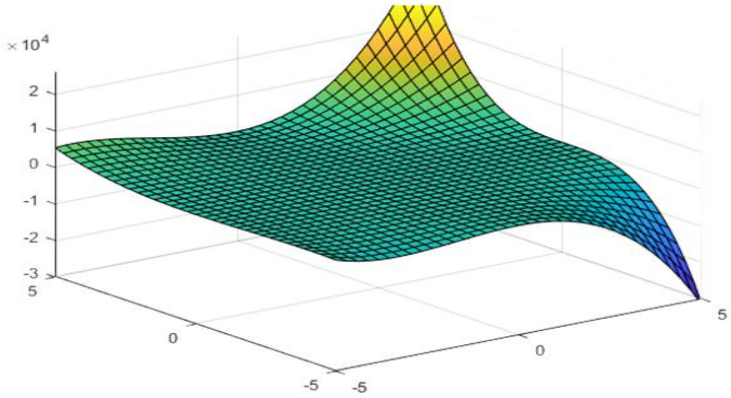

Figure 11. M-polynomial of Lomustine.

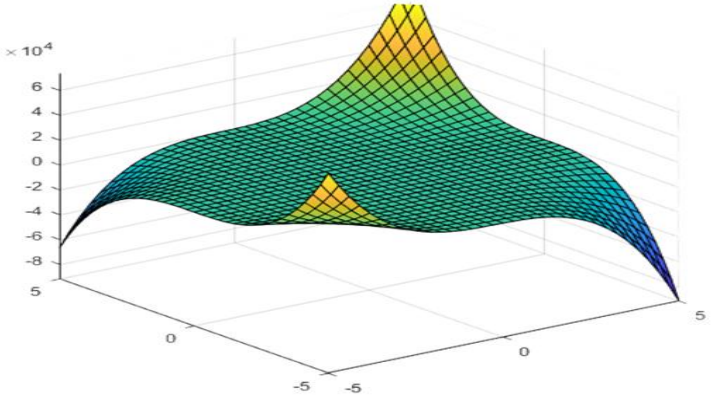

Figure 12. M-polynomial of Termozolomide.

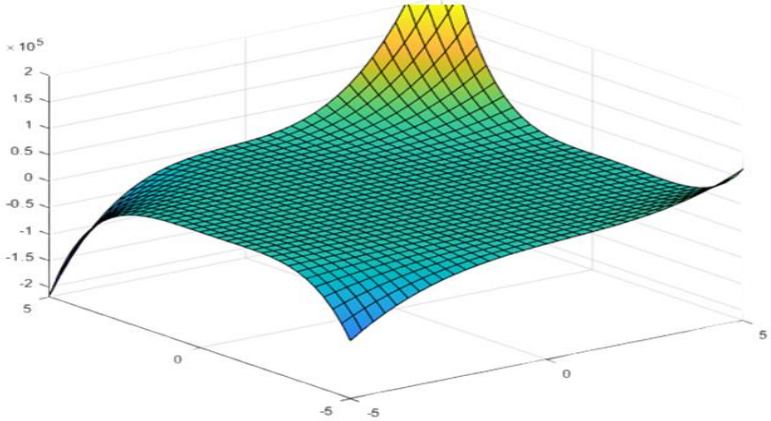

Figure 13. M-polynomial of Dabrafenib Mesylate.

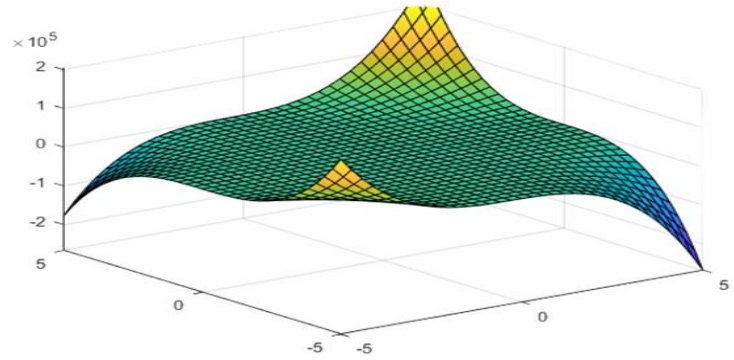

Figure 14. M-polynomial of Trametinib Dimethyl Sulfoxide.

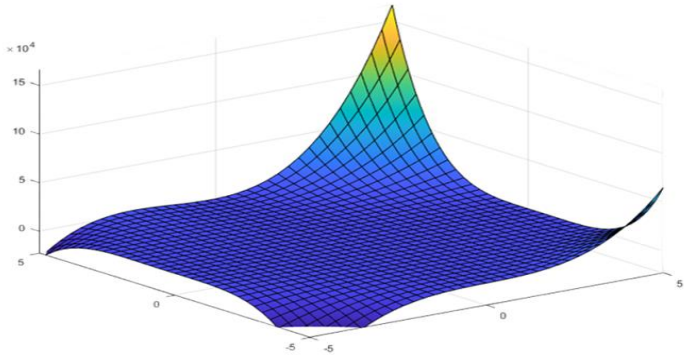

Figure 15. M-polynomial of Bevacizumab.

Theorem 4.1:

Let E be the graph of everolimus.

Then M-polynomial of E is:

$$M(E;x,y) = 4xy^2 + 13xy^3 + xy^4 + 11x^2y^2 + 27x^2y^3 + x^2y^4 + 12x^3y^3 + 2x^3y^4.$$

Proof:

The edge partitions of everolimus are as follows:

$$|E_{2,2}| = 11, |E_{2,3}| = 27, |E_{3,3}| = 12, |E_{1,3}| = 13, |E_{1,2}| = 4, |E_{3,4}| = 2, |E_{2,4}| = 1, |E_{1,4}| = 1.$$

From the definition of M-polynomial

$M(E;x,y) = \sum_{a\leq b} n_{ab}(E)x^a y^b$

$$M(E;x,y) = \sum_{1\leq 2} n_{12}(E)x^1y^2 + \sum_{1\leq 3} n_{13}(E)x^1y^3 + \sum_{1\leq 4} n_{14}(E)x^1y^4 + \sum_{2\leq 2} n_{22}(E)x^2y^2 + \sum_{2\leq 3} n_{23}(E)x^2y^3 + \sum_{2\leq 4} n_{24}(E)x^2y^4 + \sum_{3\leq 3} n_{33}(E)x^3y^3 + \sum_{3\leq 4} n_{34}(E)x^3y^4$$

We get the entire result.

Theorem 4.2:

Let B be the graph of belzutifan.

Then M-polynomial of B is:

$$M(B;x,y) = 5xy^3 + 3xy^4 + x^2y^2 + 10x^2y^3 + 7x^3y^3 + x^3y^4.$$

Proof:

The edge partitions of belzutifan are as follows:

$|E_{2,2}| = 1, |E_{2,3}| = 10, |E_{3,3}| = 7, |E_{1,3}| = 5, |E_{3,4}| = 1, \ |E_{1,4}| = 3$

From the definition of M-polynomial

$$M(B;x,y) = \sum_{a\leq b} n_{ab}(B)x^a y^b$$

$$M(B;x,y) = \sum_{1\leq 3} n_{13}(B)x^1y^3 + \sum_{1\leq 4} n_{14}(B)x^1y^4 + \sum_{2\leq 2} n_{22}(B)x^2y^2 + \sum_{2\leq 3} n_{23}(B)x^2y^3 + \sum_{3\leq 3} n_{33}(B)x^3y^3 + \sum_{3\leq 4} n_{34}(B)x^3y^4$$

We get the entire result.

Theorem 4.3:

Let C be the graph of carmustine.

Then M-polynomial of C is:

$$M(C;x,y) = 3xy^2 + 2xy^3 + 2x^2y^2 + 3x^2y^3 + 2x^3y^3$$

Proof:

The edge partitions of carmustine are as follows:

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

From the definition of M-polynomial

$$M(C;x,y) = \sum_{a\leq b} n_{ab}(C)x^a y^b$$

$$M(C;x,y) = \sum_{1\leq 2} n_{12}(C)x^1y^2 + \sum_{1\leq 3} n_{13}(C)x^1y^3 + \sum_{2\leq 2} n_{22}(C)x^2y^2 + \sum_{2\leq 3} n_{23}(C)x^2y^3 + \sum_{3\leq 3} n_{33}(C)x^3y^3$$

We get the entire result.

Theorem 4.4:

Let L be the graph of lomustine.

Then M-polynomial of L is:

$$M(L;x,y) = 2xy^2 + xy^3 + 5x^2y^2 + 6x^2y^3 + x^3y^3$$

Proof:

The edge partitions of lomustine are as follows:

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

From the definition of M-polynomial

$$M(L;x,y) = \sum_{a\leq b} n_{ab}(L)x^a y^b$$

$$M(L;x,y) = \sum_{1\leq 2} n_{12}(L)x^1y^2 + \sum_{1\leq 3} n_{13}(L)x^1y^3 + \sum_{2\leq 2} n_{22}(L)x^2y^2 + \sum_{2\leq 3} n_{23}(L)x^2y^3 + \sum_{3\leq 3} n_{33}(L)x^3y^3$$

We get the entire result.

Theorem 4.5:

Let T be the graph of temozolomide.

Then M-polynomial of T is:

$$M(T;x,y) = 4xy^3 + 2x^2y^2 + 4x^2y^3 + 5x^3y^3$$

Proof:

The edge partitions of temozolomide are as follows:

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

From the definition of M-polynomial

$$M(T; x, y) = \sum_{a \le b} n_{ab}(T) x^a y^b$$

$$M(T; x, y) = \sum_{1 \le 3} n_{13}(T) x^1 y^3 + \sum_{2 \le 2} n_{22}(T) x^2 y^2 + \sum_{2 \le 3} n_{23}(T) x^2 y^3 + \sum_{3 \le 3} n_{33}(T) x^3 y^3$$

We get the entire result.

Theorem 4.6:

Let D be the graph of dabrafenib mesylate.

Then M-polynomial of D is:

$$M(D; x, y) = 3xy^3 + 9xy^4 + 7x^2y^2 + 13x^2y^3 + x^2y^4 + 6x^3y^3 + 2x^3y^4$$

Proof:

The edge partitions of dabrafenib mesylate are as follows:

$$|E_{2,2}| = 7, |E_{2,3}| = 13, |E_{3,3}| = 6, |E_{1,3}| = 3, |E_{3,4}| = 2, |E_{2,4}| = 1, |E_{1,4}| = 9$$

From the definition of M-polynomial

$$M(D; x, y) = \sum_{a \le b} n_{ab}(D) x^a y^b$$

$$M(D; x, y) = \sum_{1 \le 3} n_{13}(D) x^1 y^3 + \sum_{1 \le 4} n_{14}(D) x^1 y^4 + \sum_{2 \le 2} n_{22}(D) x^2 y^2 + \sum_{2 \le 3} n_{23}(D) x^2 y^3 + \sum_{2 \le 4} n_{24}(D) x^2 y^4 + \sum_{3 \le 3} n_{33}(D) x^3 y^3 + \sum_{3 \le 4} n_{34}(D) x^3 y^4$$

We get the entire result.

Theorem 4.7:

Let Tr be the graph of trametinib dimethyl sulfoxide.

Then M-polynomial of Tr is:

$$M(Tr; x, y) = 12xy^3 + 4x^2y^2 + 14x^2y^3 + 14x^3y^3$$

Proof:

The edge partitions of trametinib dimethyl sulfoxide are as follows:

$$|E_{2,2}| = 4, |E_{2,3}| = 14, |E_{3,3}| = 14, |E_{1,3}| = 12$$

From the definition of M-polynomial

$$M(Tr; x, y) = \sum_{a \le b} n_{ab}(Tr) x^a y^b$$

$$M(Tr; x, y) = \sum_{1 \le 3} n_{13}(Tr) x^1 y^3 + \sum_{2 \le 2} n_{22}(Tr) x^2 y^2 + \sum_{2 \le 3} n_{23}(Tr) x^2 y^3 + \sum_{3 \le 3} n_{33}(Tr) x^3 y^3$$

We get the entire result.

Theorem 4.8:

Let Be be the graph of bevacizumab.

Then M-polynomial of Be is:

$$M(\text{Be}; x, y) = xy^2 + xy^3 + xy^4 + 5x^2y^2 + 11x^2y^3 + 2x^2y^4 + x^3y^3 + x^3y^4$$

Proof:

The edge partitions of bevacizumab are as follows:

$$|E_{2,2}| = 5, |E_{2,3}| = 11, |E_{3,3}| = 1, |E_{1,3}| = 1, |E_{1,2}| = 1, |E_{3,4}| = 1, |E_{2,4}| = 2, |E_{1,4}| = 1$$

From the definition of M-polynomial

$$M(\text{Be}; x, y) = \sum_{a \le b} n_{ab}(\text{Be}) x^a y^b$$

$$M(\mathrm{Be};x,y)=\sum_{1\le 2} n_{12}(\mathrm{Be})x^1y^2+\sum_{1\le 3} n_{13}(\mathrm{Be})x^1y^3+\sum_{1\le 4} n_{14}(\mathrm{Be})x^1y^4+\sum_{2\le 2} n_{22}(\mathrm{Be})x^2y^2+\sum_{2\le 3} n_{23}(\mathrm{Be})x^2y^3+\sum_{2\le 4} n_{24}(\mathrm{Be})x^2y^4+\sum_{3\le 3} n_{33}(\mathrm{Be})x^3y^3+\sum_{3\le 4} n_{34}(\mathrm{Be})x^3y^4$$

We get the entire result.

4. Conclusion

From statistical parameters used in linear QSPR models and topological indices, it is obvious that BP has the highest correlation with $M_1(G)$ with r = 0.966. Also, MW has the highest correlation with H(G) having r = 0.993, and PSA has a maximum correlation with S(G) with r = 0.936, while Com with $M_2(G)$ has a high correlation with r = 0.997, MV with $mM_2(G)$ has r = 0.999. The obtained results have good correlation coefficients between physical properties and their respective topological indices. Overall, MV has the highest correlation with $mM_2(G)$ from all topological indices. It is observed that the correlation coefficient is more than 0.8. In this article, we computed topological indices and compared them to a linear QSPR model for drugs used to treat brain tumors. The results gained in this manner will be useful in generating new pharmaceuticals to obtain preventive measures for the aforementioned disease in the pharmaceutical business. The correlation coefficient contributes significantly to the range of topological indices for these drugs. We also derived the M-polynomial of drugs.

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Conflicts of Interest

The authors declare no conflict of interest.

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