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DEGREE BASED TOPOLOGICAL INDICES ON ANTIPLATELET DRUGS AND QSPR ANALYSIS AND M-POLYNOMIALS

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Abstract:
Chemical graph theory is an interdisciplinary field where the molecular structure of a chemical compound is analyzed as a graph and where related math ematical questions are investigated through graph theoretical and computational technique. A Topological index is a real number obtained from the chemical graph structure. It can be predict the physicochemical and biological properties of many anticancer medicines like blood, breast, lung and skin cancer. This can be done through degree-based Topological indices. Antiplatelet drugs are medications that prevent blood clots from forming. They work by stopping your platelets from sticking together. Antiplatelet drugs are used to avoid blood clots, which can cause heart attacks and strokes. This study defines Topological indices for Antiplatelet drugs in order to clarify their physical properties and chemical reactions. We also discuss a QSPR analysis of ten degree- based topological indices. Our findings suggest a different types of regression models predicting the physicochemical properties of these drugs. Finally we calculate the M-polynomial of these drugs.
Keywords: Topological index, Antiplatelet drugs, QSPR, Regression model

Introduction

Platelets or thrombocytes are small, colorless cell fragments in our blood that form clots and stop or prevent bleeding. Platelets are made in our bone marrow, the sponge-like tissue inside our bones. Bone marrow contains stem cells that develop into red blood cells, white blood cells, and platelets. When you are wounded, platelets arrive on the scene and group together to form a clot that stops the bleeding. This is a good thing when an injury involves a break in your skin. But platelets can also group when injury to a blood vessel comes from the inside, as many happen in an artery affected by atherosclerosis. In this situation, the platelets cause blood clots in an already injured artery. Antiplatelet medications can prevent this from happening. These drugs are sometimes used to prevent blood clots, heart attacks and strokes, but are primarily used to prevent the recurrence of blood clots after a heart attack or stroke. They can also help relieve symptoms such as chest pain, poor circulation and shortness of breath.

Antiplatelet medications are divided into oral and parenteral agents. Oral agents subdivide further based on the mechanism of action. Aspirin was the first antiplatelet medication and is a cyclooxygenase inhibitor. Other oral antiplatelet agents include clopidogrel, ticagrelor, prasugrel, pentoxifylline, cilostazol, and dipyridamole. Glycoprotein IIb/IIIa inhibitors such as tirofiban and eptifibatide are only available as parenteral agents and are used in acute coronary syndrome

Materials and Methods

In drugs, structure elements denote vertices, and corresponding bonds connecting the atoms are termed edges. Graph $\Re(\alpha,\beta)$ is considered as simple, finite, and connected, whereas V and E represented in chemical graph are termed as vertex and edge sets, respectively. Degree of vertex in graph $\Re$ is number of vertices adjacent to it and is denoted by ξ_α. Valence of a compound in chemistry and the degree of vertex in the graph are closely related concepts. Degree-based topological indices used are defined below

Definition.1. In 2013, G.H. Shirdel, H. Rezapour and A.M. Sayadi introduced the hyper-Zagreb index of a graph as: [3]

$$HM_1(\Re) = \sum_{\alpha\beta\in E(G)} (\xi_\alpha + \xi_\beta)^2$$

$$HM_2(\Re) = \sum_{\alpha\beta\in E(G)} (\xi_\alpha \cdot \xi_\beta)^2$$

Definition.2. Ranjini et al. introduced the redefined third Zagreb index in 2013, defined as [4]

$$\mathrm{Re}\,M_3(\Re) = \sum_{\alpha\beta\in E(\Re)} (\xi_\alpha \cdot \xi_\beta)\,(\xi_\alpha + \xi_\beta)$$

Defintion.3. In 2021, a Mathematical chemist Ivan Gutman introduced Sombor index as defined as [5]

$$S(\Re) = \sum_{\alpha\beta\in E(\Re)} \sqrt{(\xi_\alpha)^2 + (\xi_\beta)^2}$$

Defintion.4. Furtula et al. defined the augmented Zagreb index (AZI) as [6]

$$AZI(\Re) = \sum_{\alpha\beta\in E(\Re)} \left(\frac{\xi_\alpha \cdot \xi_\beta}{\xi_\alpha + \xi_\beta - 2} \right)^3$$

Defintion.5. Gutman et al. introduced the reciprocal Randić index as a variant of the Randić index.[7]

$$RR(\Re) = \sum_{\alpha\beta\in E(\Re)} \sqrt{\xi_\alpha \cdot \xi_\beta}$$

Defintion.6. Jamil et al. introduced the face index in graph theory as [8]

$$FI(\Re) = \sum_{h-f\in F(\Re)} \phi_n = \sum_{f\in F(\Re)} \phi(f)$$

Defintion.7. In 2015**,** Furtula and Gutman defined the F-index, also known as the "forgotten topological index defined as [9]

$$F(\Re) = \sum_{\alpha\beta\in E(\Re)} (\xi_\alpha)^2 + (\xi_\beta)^2$$

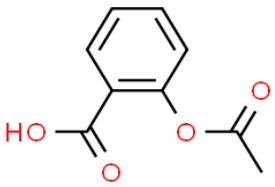
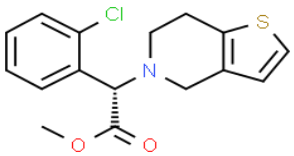
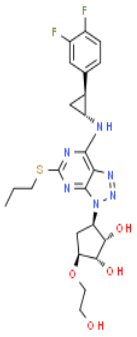
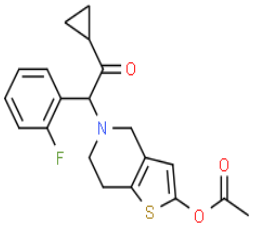
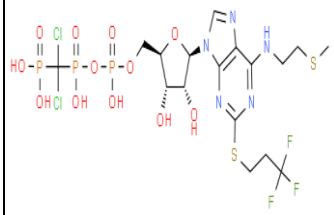
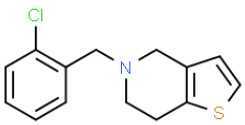
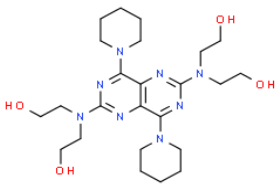
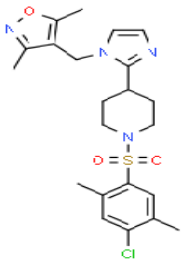
Defintion.8. Abdu Alameri, Noman Q. Al Naggar, and Mahmoud Al-Rumaima defined the Y-index in graph theory in 2020. The Y-index, also known as the Yemen index [2]

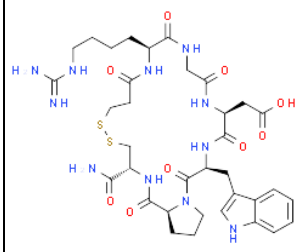
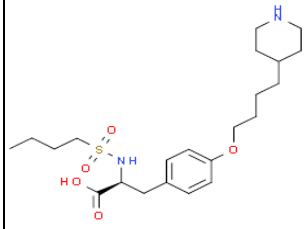
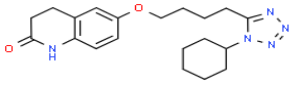
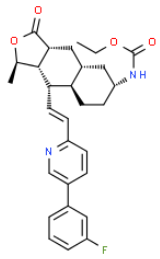
$$Y(\Re) = \sum_{\alpha\beta\in E(\Re)} (\xi_\alpha)^3 + (\xi_\beta)^3$$

Defintion.9. In 2024 we introduced the D-index as defined as

$$D(\Re) = \sum_{\alpha\beta\in E(\Re)} (\xi_\alpha)^5 + (\xi_\beta)^5$$

Figure:1 2D-molecular structure of Antiplatelet drugs

			
(a)Aspirin	(b)Clopidogrel	(c) Ticagrelor	(d)Prasugrel
			
(e) Cangrelor	(f) Ticlopidine	(g)Dipyridamole	(h) Abciximab

			
(i) Eptifibatide	(j) Tirofiban	(k) Cilostazol	(l)Vorapaxer

Qspr Analysis Of Antiplatelet Drugs[10-13]

This section analyzes degree-based topological indices as well as a few physicochemical properties of antibiotic medications, including their boiling point (BP), enthalpy of vaporization (EV), flash point (FP), molar refractivity (MR), complexity (C), polarizability (P), molecular weight (MW), and molar volume (MV). The physicochemical properties of these drugs are presented in Table 1. In regression analysis, the letter r refers to the correlation coefficient, which measures the relationship between the independent and dependent variables. The value of r can range from -1 to +1. The higher the r value, the better the relationship between the variables. We present the many regression models with value of $r \geq 0.09$ for the physicochemical properties in terms of proposed indices. In tables (4,6,8,10,12,14), we indicate the best predictor from 6 regression models. Consider the following regression models to obtain the relationship between the degree based topological indices and the physicochemical properties of these drugs.

$Y = p + qx\,(Linear)$

$Y = px^2 + qx + r\,(Quadratic)$

$Y = p + qx + rx^2 + sx^3\,(cubic)$

$Y = p + q^* In(x)\ \ (Logarithmic)$

$Y = pq^x\ \ (Exponential)$

$Y = ax^q\ \ (Power)$

Where Y is dependent variable. X represents independent variables and p,q,r,s are real numbers called coefficients

1. Linear Regression

Table 3 shows the correlation coefficient (r) obtained by linear regression model between Indices and physical properties of these drugs. In this model, the physical properties: BP, EV, FP has the highest predicting with AZI and MR, P, MV has the highest predicting with RR and PSA has the highest predicting with F .Over all indices, it is noticed that the RR index are best suited for predicting the properties MR and P.

BP = 131.194+ 1.937(AZI)
EV = 28.917 +0.264 (AZI)
FP = 24.718 +1.199 (AZI)
MR = 9.513 + 1.363(RR)
PSA= -101.414 + 0.560 (F)
P = 3.785 + 0.540 (RR)F
MV = 73.699 + 3.114 (RR)

Table 4 shows best predictors, r- value, p value, F-statistic and standard error values in this models.

2. Quadratic Regression

Table 5 shows the correlation coefficient (r) obtained by quadratic regression model between Indices and physical properties of these drugs. In this model, the physical properties BP, EV, FP has the highest predicting with AZI and MR, P, MV has the highest predicting with RR and PSA has the highest predicting with F .Over all indices, it is noticed that the RR index are best suited for predicting the properties MR and P.

$BP = 0.003(AZI)^2+0.551(AZI)+266.185$
$EV = 0.001\ (AZI)^2-0.040(AZI)+58.528$
$FP = 0.002(AZI)^2+0.450(AZI)+97.677$
$MR = 0.002(RR)^2+1.063(RR)+20.235$
$PSA = 0.001\ (F)^2-0.702\ (F)+139.995$
$P = 0.001(RR)^2+ 0.419(RR)+8.115$
$MV = -0.003(RR)^2+3.636\ (RR)+55.045$

Table 6 shows best predictors, r value, p value, F-statistic and standard error values in this models.

3. Cubic Regression

Table 7 shows the correlation coefficient (r) obtained by cubic regression model between Indices and physical properties of these drugs. In this model, the physical properties: BP, EV, FP has the highest predicting with AZI and MR, MV has the highest predicting with RR and PSA has the highest predicting with F and P has the highest predicting with S. Over all indices, it is noticed that the RR index is best suited for predicting the property MR.

$BP = 248.168+0.855(AZI)+0.002(AZI)^2+1.938E\text{-}6(AZI)^3$
$EV = 48.034+0.137(AZI)+0.000(AZI)^2+1.129E\text{-}6\ (AZI)^3$
$FP = 78.697+0.770(AZI)+0.000(AZI)^2+2.041E\text{-}6(AZI)^3$
$MR = -54.161+4.515(RR)-0.044(RR)^2-0.000(RR)^3$
$PSA= -21.588 +0.739(F)-0.002\ (F)^2-+2.834E\text{-}6(F)^3$
$P = -31.146+1.488\ (S)-0.010\ (S)^2+2.790E\text{-}5\ (S)^3$
$MV = -168.668+14.019\ (RR)-0.143\ (RR)^2+0.001\ (RR)^3$

Table 8 shows best predictors, r- value, p value, F-statistic and standard error values in this models.

4. Logarithmic Regression

Table 9 shows the correlation coefficient (r) obtained by logarithmic regression model between Indices and physical properties of these drugs. In this model, the physical properties: BP, FP ,MR,P has the highest predicting with S and MV has the highest predicting with RR and EV has the highest predicting with F and PSA has the highest predicting with D. Over all indices, it is noticed that the Sombar index is best suited for predicting the properties MR and P

$BP = -952.226+332.639*\ln(S)$
$EV = -166.426+43.714*\ln(F)$
$FP = -1008.157+287.630*\ln(S)$
$MR = -310.388+91.040*\ln(S)$
$PSA= -166.426+43.714*\ln(D)$
$P = -122.987+36.081*\ln(S)$
$MV = -600.239+214.165*\ln(RR)$

Table 10 shows best predictors, r-value, p value, F-statistic and standard error values in this models.

5. Exponential regression

Table 11 shows the square of correlation coefficient (r) obtained by Exponential regression model between indices and physical properties of these drugs. In this model, the physical properties: BP, EV, PSA has the highest predicting with AZI and FP, MR, MV has the highest predicting with RR and P has the highest predicting with S . Over all indices, it is noticed that AZI index is best suited for predicting the property BP.

$BP = 332.750*0.002(AZI)$
$EV = 32.155*0.004(AZI)$
$FP = 121.332*0.012(RR)$
$MR = 40.794*0.013(RR)$
$PSA = 23.222*0.006(AZI)$
$P = 16.836*0.008(S)$
$MV = 131.478*0.011(RR)$

Table 12 shows best predictors, r value, p value, F-statistic and standard error values in this models.

6. Power Regression

Table 13 shows the correlation coefficient () obtained by power regression model between Indices and physical properties of these drugs. In this model, the physical properties: BP, EV, FP has the highest predicting with S and MR, P, , MV has the highest predicting with RR and PSA has the highest predicting with AZI. Over all indices, it is noticed that the RR index is best suited for predicting the property MR and P.

$BP=415.552(S)^{0.038}$

$EV=8.524(S)^{0.504}$

$FP=38..943(S)^{0.413}$

$MR=2.276(RR)^{0.903}$

$PSA=1.8184(AZI)^{1.1259}$

$P=0.908(RR)^{0.901}$

$MV=0.199(RR)^{1.140}$

Table 14 shows best predictors, r-value, p value, F-statistic and standard error values in this models

Table:1 Physical Properties of Antiplatelet Drugs

Drugs	**BP**	**Enthalpy**	**FP**	**Index of Refraction**	**MR**	**PSA**	**Polarizability**	**ST**	**MV**
Aspirin	321.4	59.5	131.2	1.551	44.5	64	17.7	49.9	139.6
Clopidogrel	423.7	67.8	210	1.617	85.5	58	33.9	52.8	244.3
Ticagrelor	777.6	118.7	424	1.744	126.3	164	50.1	63.3	311.9
Prasugrel	493.5	76.1	252.3	1.619	97.2	75	38.5	56.8	271.1
Cangrelor	979.0	149.5	545.9	1.722	147.1	336	58.3	96.0	371.9
Ticlopidine	367.3	61.4	175.9	1.638	74.4	31	29.5	51.5	207.1
Dipyridamole	806.5	122.9	441.5	1.670	139.4	145	55.3	81.6	373.0
Abciximab	658.0	96.9	351.7	1.651	122.8	90	48.7	49.5	336.0
Eptifibatide	-	-	-	1.735	208.0	374	82.5	75.9	518.5
Tirofiban	611.7	95.5	323.7	1.532	118.3	113	46.9	46.1	381.7
Cilostazol	664.7	97.7	355.8	1.676	102.9	82	40.8	54.9	273.8
Vorapaxar	676.0	99.3	362.6	1.594	133.7	78	53.0	53.1	394.2

Table :2 Computed Values of Antiplatelet Drugs Using Topological Indices

S. no	Drugs	$HM_1(G$	$HM_2(G$	$ReM_3(G$	S(G)	AZI(G)	RR(G)	FI(G)	F(G)	Y(G)	D(G)
1	Aspirin	284	390	324	44.041	92.281	28.726	39	152	328	3240
2	Clopidogrel	542	847	666	79.194	191.702	53.923	87	280	746	5810
3	Ticagrelor	988	1598	1236	141.418	335.406	95.847	138	512	1408	11236
4	Prasugrel	710	1106	872	102.724	233.843	69.221	100	370	1006	8062
5	Cangrelor	1241	2012	1530	175.761	401.018	109.585	135	693	2245	29803
6	Ticlopidine	434	627	516	64.673	90.156	44.226	79	219	563	4139
7	Dipyridamole	880	1351	1074	130.272	335.734	89.848	138	450	1166	8702
8	Abciximab	874	1435	1092	124.133	269.606	81.881	122	464	1346	12890
9	Eptifibatide	1356	1941	1590	205.090	487.015	136.572	160	714	1902	14862
10	Tirofiban	666	851	742	103.595	230.88	68.48	80	356	970	8962
11	Cilostazol	677	993	810	100.946	248.937	69.575	102	342	872	6320
12	Vorapaxar	962	1475	1174	140.099	325.23	95.853	151	500	1346	10634

Table:3 r obtained by Linear Regression Model Between Topological Indices and Physical Properties of Drugs

Index\Property	BP	Enthalpy	FP	MR	PSA	P	MV
$HM_1(G)$	0.941	0.921	0.945	0.947	0.857	0.947	0.882
$HM_2(G)$	0.913	0.895	0.918	0.889	0.815	0.889	0.808
$ReM_3(G)$	0.929	0.908	0.933	0.923	0.833	0.923	0.851
S(G)	0.951	0.930	0.955	0.967	0.868	0.967	0.909
AZI(G)	**0.955**	**0.934**	**0.958**	0.958	0.847	0.958	0.902
RR(G)	0.943	0.915	0.948	**0.975**	0.837	**0.975**	**0.920**
FI(G)	0.823	0.775	0.833	0.886	0.623	0.886	0.832
F(G)	0.937	0.923	0.940	0.932	**0.874**	0.931	0.868
Y(G)	0.907	0.923	0.940	0.932	0.874	0.931	0.868
D(G)	0.803	0.822	0.799	0.631	0.797	0.630	0.571

Table:4 Best Predictor from Linear Regression Model

Properties	R	BP	P	F	SE
BP	0.955	AZI	0.001	99.406	62.394
EV	0.934	AZI	0.001	61.378	10.545
FP	0.958	AZI	0.001	99.246	37.663
MR	0.975	RR	0.001	195.409	9.552
PSA	0.874	F	0.001	32.412	55.874
P	0.975	RR	0.001	94.701	3.794
MV	0.920	RR	0.001	54.943	41.167

Table:5. r obtained by Quadratic Regression Model Between Topological Indices and Physical Properties of Drugs

Index\Property	BP	Enthalpy	FP	MR	PSA	P	MV
HM_1 (G)	0.942	0.928	0.945	0.947	0.958	0.947	0.886
HM_2 (G)	0.913	0.901	0.918	0.890	0.935	0.889	0.818
$ReM_3(G)$	0.929	0.915	0.933	0.923	0.953	0.923	0.855
S(G)	0.952	0.940	0.955	0.967	0.949	0.967	0.912
AZI(G)	0.966	0.961	0.966	0.964	0.937	0.964	0.920
RR(G)	0.949	0.934	0.951	0.977	0.914	0.976	0.920
FI(G)	0.793	0.778	0.833	0.894	0.695	0.894	0.837
F(G)	0.938	0.924	0.942	0.933	0.964	0.933	0.881
Y(G)	0.919	0.904	0.924	0.901	0.913	0.900	0.868
D(G)	0.878	0.869	0.880	0.889	0.814	0.888	0..882

Table:6 Best Predictor from Quadratic Regression Model

Properties	R	BP	P	F	SE
BP	0.966	AZI	0.001	56.700	57.584
EV	0.961	AZI	0.001	48.936	8.598
FP	0.966	AZI	0.001	55.741	35.848
MR	0.977	RR	0.001	92.411	9.834
PSA	0.964	F	0.001	59.696	32.114
P	0.976	RR	0.001	92.237	3.902
MV	0.920	RR	0.001	84.946	43.231

Table:7. r obtained by Cubic Regression Model Between Topological Indices and Physical Properties of Drugs

Index\Property	BP	Enthalpy	FP	MR	PSA	P	MV
HM_1 (G)	0.942	0.928	0.946	0.965	0.961	0.965	0.911
HM_2 (G)	0.917	0.904	0.923	0.941	0.953	0.896	0.828
$ReM_3(G)$	0.931	0.916	0.935	0.941	0.968	0.941	0.879
S(G)	0.952	0.940	0.956	0.981	0.950	0.981	0.933
AZI(G)	0.967	0.962	0.966	0.970	0.938	0.970	0.916
RR(G)	0.949	0.935	0.952	0.986	0.918	0.986	0.936
FI(G)	0.863	0.826	0.868	0.924	0.700	0.924	0.891
F(G)	0.938	0.924	0.942	0.944	0.970	0.943	0.896
Y(G)	0.919	0.905	0.925	0.915	0.922	0.915	0.877
D(G)	0.900	0.887	0.906	0.896	0.871	0.896	0.882

Table:8 Best Predictor from Cubic Regression Model

Properties	R	BP	P	F	SE
BP	0.967	AZI	0.001	33.100	61.538
EV	0.962	AZI	0.001	28.878	9.142
FP	0.966	AZI	0.001	32.585	38.285
MR	0.986	RR	0.001	95.853	7.963
PSA	0.970	F	0.001	42.184	31.370
P	0.981	S	0.001	68.428	3.716
MV	0.936	RR	0.001	19.013	41.137

Table:9 r obtained By Logarithmic Regression Model Between Topological Indices and Physical Properties of Drugs

Index\Property	BP	Enthalpy	FP	MR	PSA	P	MV
HM_1 (G)	0.910	0.871	0.921	0.926	0.735	0.926	0.886
HM_2 (G)	0.886	0.847	0.898	0.880	0.694	0.879	0.823
$ReM_3(G)$	0.898	0.856	0.908	0.905	0.710	0.904	0.856
S(G)	0.919	0.880	0.929	0.944	0.752	0.944	0.909
AZI(G)	0.900	0.862	0.906	0.901	0.712	0.901	0.872
RR(G)	0.903	0.859	0.914	0.943	0.721	0.942	0.909
FI(G)	0.823	0.736	0.810	0.849	0.543	0.848	0.805
F(G)	0.918	0.883	0.927	0.924	0.756	0.923	0.885
Y(G)	0.900	0.867	0.911	0.889	0.734	0.889	0.854
D(G)	0.889	0.887	0.892	0.802	0.774	0.802	0.771

Table:10 Best Predictor from Logarithmic Regression Model

Properties	R	BP	P	F	SE
BP	0.919	S	0.001	48.621	83.584
EV	0.883	F	0.001	31.786	13.852
FP	0.929	S	0.001	56.357	48.470
MR	0.944	S	0.001	81.842	14.285
PSA	0.774	D	0.001	14.909	72.908
P	0.944	S	0.001	81.311	5.680
MV	0.909	RR	0.001	47.737	43.661

Table:11. r obtained by Exponential Regression Model Between Topological Indices and Physical Properties of Drugs

Index\Property	BP	Enthalpy	FP	MR	PSA	P	MV
HM_1 (G)	0.939	0.928	0.937	0.928	0.879	0.929	0.875
HM_2 (G)	0.903	0.895	0.901	0.889	0.846	0.889	0.820
$ReM_3(G)$	0.925	0.913	0.923	0.915	0.862	0.916	0.854
S(G)	0.953	0.942	0.951	0.938	0.887	0.938	0.891
AZI(G)	0.965	0.954	0.959	0.931	0.905	0.931	0.886
RR(G)	0.957	0.937	0.959	0.950	0.864	0.951	0.904
FI(G)	0.856	0.812	0.871	0.916	0.673	0.916	0.860
F(G)	0.926	0.922	0.920	0.911	0.891	0.911	0.859
Y(G)	0.882	0.886	0.874	0.859	0.874	0.859	0.805
D(G)	0.737	0.769	0.716	0.632	0.781	0.632	0.584

Table:12 Best Predictor from Exponential Regression Model

Properties	R	BP	P	F	SE
BP	0.965	AZI	0.001	120.936	0.097
EV	0.954	AZI	0.001	91.641	0.094
FP	0.959	RR	0.001	103.460	0.124
MR	0.950	RR	0.001	92.859	0.128
PSA	0.905	AZI	0.001	45.045	0.320
P	0.938	S	0.001	73.617	0.141
MV	0.904	RR	0.001	44.753	0.155

Table:13. r obtained by Power Regression Model Between Topological Indices and Physical Properties of Drugs

Index\Property	BP	Enthalpy	FP	MR	PSA	P	MV
HM_1 (G)	0.942	0.904	0.957	0.968	0.798	0.968	0.924
HM_2 (G)	0.913	0.875	0.929	0.935	0.759	0.934	0.876
$ReM_3(G)$	0.928	0.889	0.944	0.955	0.775	0.955	0.904
S(G)	0.952	0.916	0.966	0.978	0.815	0.978	0.940
AZI(G)	0.941	0.908	0.947	0.934	0.834	0.934	0.905
RR(G)	0.944	0.902	0.962	0.982	0.788	0.982	0.944
FI(G)	0.844	0.782	0.875	0.928	0.597	0.927	0.873
F(G)	0.943	0.911	0.955	0.961	0.819	0.961	0.920
Y(G)	0.923	0.890	0.937	0.944	0.791	0.944	0.903
D(G)	0.878	0.874	0.875	0.840	0.824	0.840	0.807

Table:14 Best Predictor from Power Regression Model

Properties	R	BP	P	F	SE
BP	0.952	S	0.001	86.590	0.113
EV	0.916	S	0.001	46.830	0.126
FP	0.966	S	0.001	125.787	0.117
MR	0.982	RR	0.001	275.030	0.077
PSA	0.834	AZI	0.001	22.848	0.415
P	0.982	RR	0.001	274.891	0.077
MV	0.944	RR	0.001	81.939	0.120

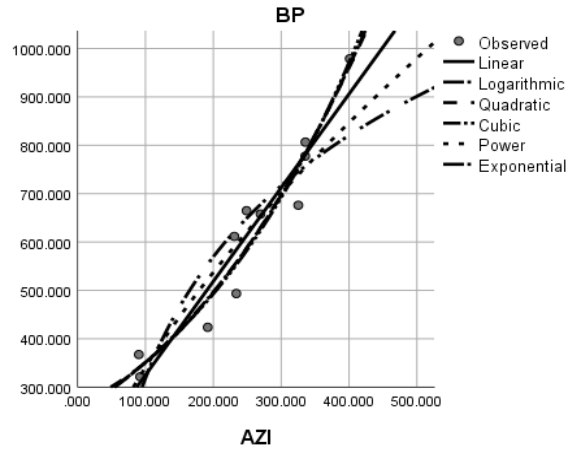


Fig:2 Regression curves for BP

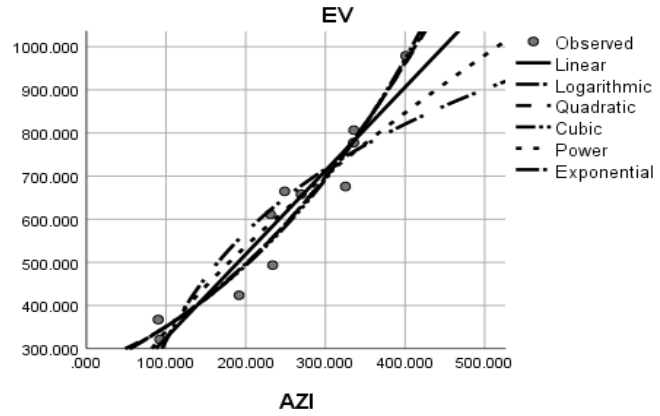


Fig:3 Regression curves for EV

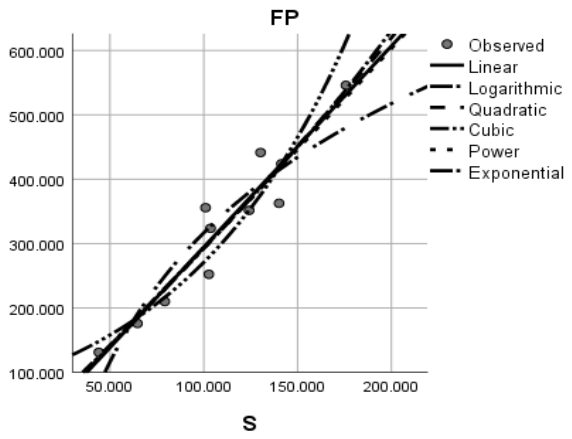


Fig:4 Regression curves for FP

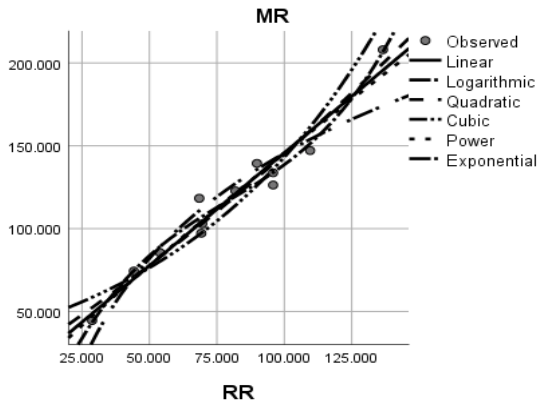


Fig:5 Regression curves for MR

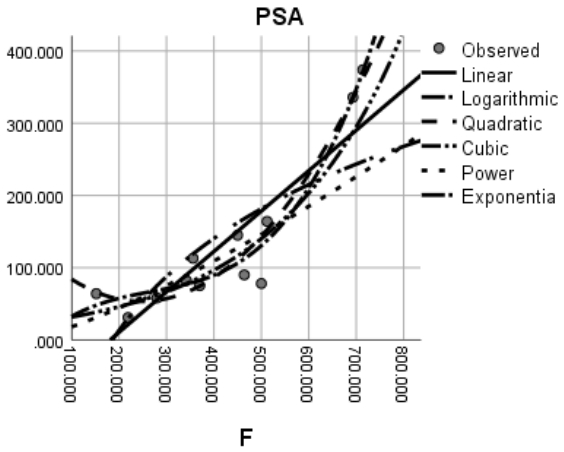


Fig:6 Regression curves for PSA

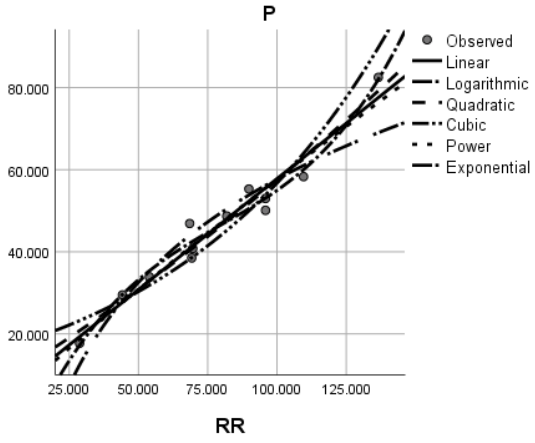


Fig:7 Regression curves for BP

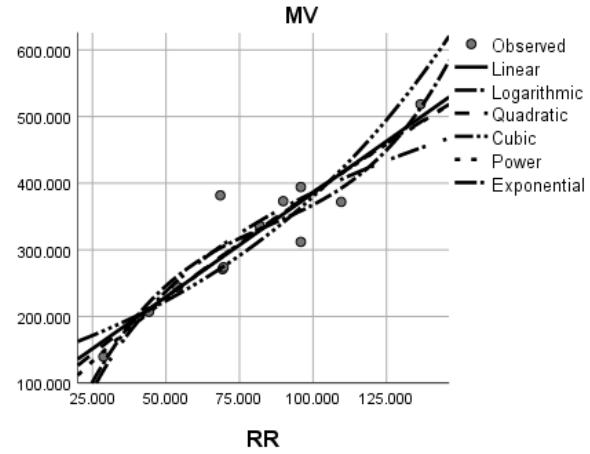


Fig:8 Regression curves for MV

M-Polynomial Of a Antiplatelet Drugs[14]

The M-polynomial of a graph is a function that represents the number of edges in a graph based on the degrees of the vertices.

The M-polynomial of a graph $\Re$ is

$$M(\Re : x, y) = \sum_{\delta \le i \le j \le \Delta} \lambda_{ij}(\Re)\, x^i\, y^j$$

Where $\lambda_{ij}(\Re)$ is the number of edges $\alpha\beta \in E(\Re)$ such that $\xi_\alpha, \xi_\beta = i, j$. The degrees of the vertices $\alpha \text{ and } \beta$ are denoted by $\xi_\alpha \text{ and } \xi_\beta$ respectively. The minimum degree is δ and the maximum degree is Δ

Theorem .1: Let A be the graph of Aspirin. The M-polynomial of A is

$M(A : x, y) = 4x\, y^3 + 3x^2\, y^2 + 4x^2\, y^3 + 2x^3\, y^3$

Proof: The edge partitions of Aspirin as follows

$|E_{1,3}| = 4, |E_{2,2}| = 3, |E_{2,3}| = 4, |E_{3,3}| = 2$ from the definition of M-polynomial

$$M(A : x, y) = \sum_{\delta \le i \le j \le \Delta} \lambda_{ij}(A)\, x^i\, y^j$$

$$M(A : x, y) = \lambda_{13}(A)\, x^1\, y^3 + \lambda_{22}(A)\, x^2\, y^2 + \lambda_{23}(A)\, x^2\, y^3 + \lambda_{33}(A)\, x^3\, y^3$$

$$= 4x\, y^3 + 3x^2\, y^2 + 4x^2\, y^3 + 2x^3\, y^3$$

Theorem.2: Let C be the graph of Clopidogrel. The M-polynomial of C is

$M(C:x,y)=xy^2+3xy^3+6x^2y^2+9x^2y^3+5x^3y^3$

Proof: The edge partitions of Clopidogrel as follows

$|E_{1,2}|=1, |E_{1,3}|=2, |E_{2,2}|=6, |E_{2,3}|=9, |E_{3,3}|=5$ from the definition of M-polynomial

$$M(C:x,y)=\sum_{\delta\le i\le j\le\Delta}\lambda_{ij}(C)x^iy^j$$

$$M(C:x,y)=\lambda_{12}(C)x^1y^2+\lambda_{13}(C)x^1y^3+\lambda_{22}(C)x^2y^2+\lambda_{23}(C)x^2y^3+\lambda_{33}(C)x^3y^3$$
$$=xy^2+2xy^3+6x^2y^2+9x^2y^3+5x^3y^3$$

Theorem.3: Let T be the graph of Ticagrelor. The M-polynomial of T is

$M(T:x,y)=2xy^2+4xy^3+6x^2y^2+18x^2y^3+10x^3y^3$

Proof: The edge partitions of Ticagrelor as follows

$|E_{1,2}|=2, |E_{1,3}|=4, |E_{2,2}|=6, |E_{2,3}|=18, |E_{3,3}|=10$ from the definition of M-polynomial

$$M(T:x,y)=\sum_{\delta\le i\le j\le\Delta}\lambda_{ij}(T)x^iy^j$$

$$M(T:x,y)=\lambda_{12}(T)x^1y^2+\lambda_{13}(T)x^1y^3+\lambda_{22}(T)x^2y^2+\lambda_{23}(T)x^2y^3+\lambda_{33}(T)x^3y^3$$
$$=2xy^2+4xy^3+6x^2y^2+18x^2y^3+10x^3y^3$$

Theorem.4: Let P be the graph of Prasugrel. The M-polynomial of P is

$M(P:x,y)=4xy^3+5x^2y^2+14x^2y^3+6x^3y^3$

Proof: The edge partitions of Prasugrel as follows

$|E_{1,3}|=4, |E_{2,2}|=5, |E_{2,3}|=14, |E_{3,3}|=6$ from the definition of M-polynomial

$$M(P:x,y)=\sum_{\delta\le i\le j\le\Delta}\lambda_{ij}(P)x^iy^j$$

$$M(P:x,y)=\lambda_{13}(P)x^1y^3+\lambda_{22}(P)x^2y^2+\lambda_{23}(P)x^2y^3+\lambda_{33}(P)x^3y^3$$
$$=4xy^3+5x^2y^2+14x^2y^3+6x^3y^3$$

Theorem.5: Let Ca be the graph of Cangrelor. The M-polynomial of Ca is

$M(Ca:x,y)=xy^2+2xy^3+12xy^4+7x^2y^2+12x^2y^3+4x^2y^4+6x^3y^3+2x^4y^4$

Proof: The edge partitions of Cangrelor as follows

$|E_{1,2}|=1, |E_{1,3}|=2, |E_{1,4}|=12, |E_{2,2}|=7, |E_{2,3}|=12, |E_{2,4}|=4, |E_{3,3}|=6, |E_{4,4}|=2$ from the definition of M-polynomial

$$M(Ca:x,y)=\sum_{\delta\le i\le j\le\Delta}\lambda_{ij}(Ca)x^iy^j$$

$$M(Ca:x,y)=\lambda_{12}(Ca)x^1y^2+\lambda_{13}(Ca)x^1y^3+\lambda_{14}(Ca)x^1y^4+\lambda_{22}(Ca)x^2y^2+\lambda_{23}(Ca)x^2y^3$$
$$+\lambda_{24}(Ca)x^2y^4+\lambda_{33}(Ca)x^3y^3+\lambda_{44}(Ca)x^4y^4$$
$$=xy^2+2xy^3+12xy^4+7x^2y^2+12x^2y^3+4x^2y^4+6x^3y^3+2x^4y^4$$

Theorem.6: Let Ti be the graph of Ticlopidine. The M-polynomial of Ti is

$M(Ti:x,y)=xy^3+6x^2y^2+10x^2y^3+2x^3y^3$

Proof: The edge partitions of Ticlopidine as follows

$|E_{1,3}|=1, |E_{2,2}|=6, |E_{2,3}|=10, |E_{3,3}|=2$ from the definition of M-polynomial

$$M(Ti:x,y)=\sum_{\delta\le i\le j\le\Delta}\lambda_{ij}(Ti)x^iy^j$$

$$M(Ti:x,y)=\lambda_{13}(Ti)\,x^1y^3+\lambda_{22}(Ti)\,x^2y^2+\lambda_{23}(Ti)\,x^2y^3+\lambda_{33}(Ti)\,x^3y^3$$
$$=xy^3+6x^2y^2+10x^2y^3+2x^3y^3$$

Theorem.7: Let D be the graph of Dipyridamole. The M-polynomial of D is
$M(D:x,y)=4xy^2+12x^2y^2+15x^2y^3+7x^3y^3$
Proof: The edge partitions of Dipyridamole as follows
$|E_{1,2}|=4,|E_{2,2}|=12,|E_{2,3}|=15,|E_{3,3}|=7$ from the definition of M-polynomial

$$M(D:x,y)=\sum_{\delta\le i\le j\le\Delta}\lambda_{ij}(D)\,x^iy^j$$
$$M(D:x,y)=\lambda_{13}(D)\,x^1y^3+\lambda_{22}(D)\,x^2y^2+\lambda_{23}(D)\,x^2y^3+\lambda_{33}(D)\,x^3y^3$$
$$=4xy^2+12x^2y^2+15x^2y^3+7x^3y^3$$

Theorem.8: Let Ab be the graph of Abciximab. The M-polynomial of Ab is
$M(Ab:x,y)=5xy^3+2xy^4+5x^2y^2+14x^2y^3+2x^3y^4+6x^3y^3+2x^3y^4$
Proof: The edge partitions of Abciximab as follows
$|E_{1,3}|=5,|E_{1,4}|=2,|E_{2,2}|=5,|E_{2,3}|=14,|E_{3,3}|=6,|E_{3,4}|=2$ from the definition of M-polynomial

$$M(Ab:x,y)=\sum_{\delta\le i\le j\le\Delta}\lambda_{ij}(Ab)\,x^iy^j$$
$$M(Ab:x,y)=\lambda_{13}(Ab)\,x^1y^3+\lambda_{14}(Ab)\,x^1y^4+\lambda_{22}(Ab)\,x^2y^2+\lambda_{23}(Ab)\,x^2y^3$$
$$+\lambda_{34}(Ab)\,x^3y^4+\lambda_{33}(Ab)\,x^3y^3$$
$$=5xy^3+2xy^4+5x^2y^2+14x^2y^3+2x^3y^4+6x^3y^3+2x^3y^4$$

Theorem.9: Let E be the graph of Eptifibatide. The M-polynomial of E is
$M(E:x,y)=12xy^3+15x^2y^2+24x^2y^3+9x^3y^3$
Proof: The edge partitions of Eptifibatide as follows
$|E_{1,3}|=12,|E_{2,2}|=15,|E_{2,3}|=24,|E_{3,3}|=9$ from the definition of M-polynomial

$$M(E:x,y)=\sum_{\delta\le i\le j\le\Delta}\lambda_{ij}(E)\,x^iy^j$$
$$M(E:x,y)=\lambda_{13}(E)\,x^1y^3+\lambda_{22}(E)\,x^2y^2+\lambda_{23}(E)\,x^2y^3+\lambda_{33}(E)\,x^3y^3$$
$$=12xy^3+15x^2y^2+24x^2y^3+9x^3y^3$$

Theorem.10: Let T be the graph of Tirofiban. The M-polynomial of T is
$M(\mathrm{T}:x,y)=xy^2+2xy^3+2xy^4+12x^2y^2+11x^2y^3+x^3y^3+2x^2y^4$
Proof: The edge partitions of Tirofiban as follows
$|E_{1,2}|=1,|E_{1,3}|=2,|E_{1,4}|=2,|E_{2,2}|=12,|E_{2,3}|=11,|E_{2,4}|=2,|E_{3,3}|=1$ from the definition of M-polynomial

$$M(\mathrm{T}:x,y)=\sum_{\delta\le i\le j\le\Delta}\lambda_{ij}(\mathrm{T})\,x^iy^j$$
$$M(\mathrm{T}:x,y)=\lambda_{12}(\mathrm{T})\,x^1y^2+\lambda_{13}(\mathrm{T})\,x^1y^3+\lambda_{14}(\mathrm{T})\,x^1y^4+\lambda_{22}(\mathrm{T})\,x^2y^2+\lambda_{23}(\mathrm{T})\,x^2y^3$$
$$+\lambda_{24}(\mathrm{T})\,x^2y^4+\lambda_{33}(\mathrm{T})\,x^3y^3$$
$$=xy^2+2xy^3+2xy^4+12x^2y^2+11x^2y^3+x^3y^3+2x^2y^4$$

Theorem.11: Let Ci be the graph of Cilostazol. The M-polynomial of Ci is
$M(Ci:x,y)=xy^3+12x^2y^2+13x^2y^3+4x^3y^3$
Proof: The edge partitions of Cilostazol as follows

$|E_{1,3}|=1, |E_{2,2}|=12, |E_{2,3}|=13, |E_{3,3}|=4$ from the definition of M-polynomial

$$M(Ci:x,y)=\sum_{\delta\le i\le j\le\Delta}\lambda_{ij}(Ci)\,x^i\,y^j$$

$$M(Ci:x,y)=\lambda_{13}(Ci)\,x^1\,y^3+\lambda_{22}(Ci)\,x^2\,y^2+\lambda_{23}(Ci)\,x^2\,y^3+\lambda_{33}(Ci)\,x^3\,y^3$$
$$=x\,y^3+12x^2\,y^2+13x^2\,y^3+4x^3\,y^3$$

Theorem.12: Let V be the graph of Vorapaxar. The M-polynomial of V is

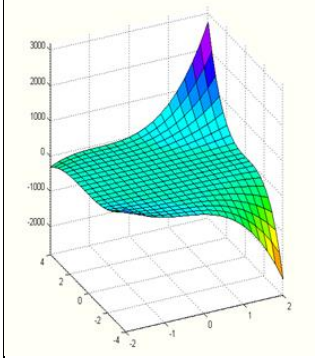
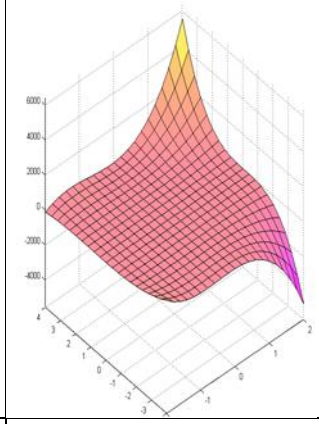
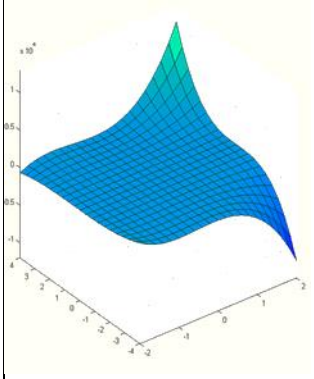
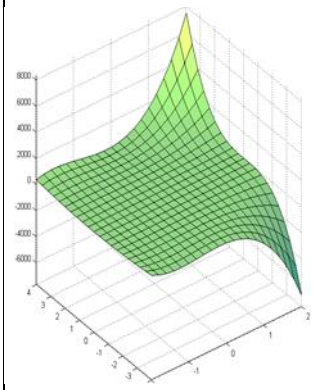
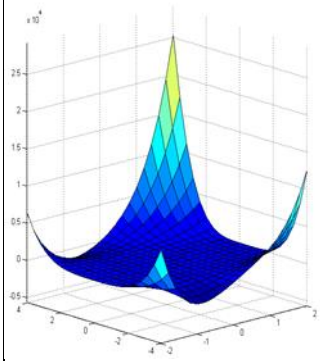
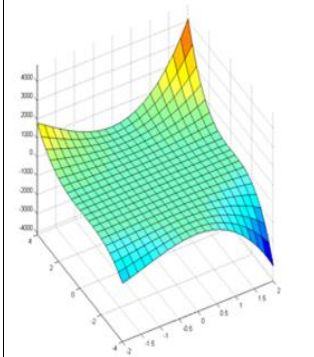
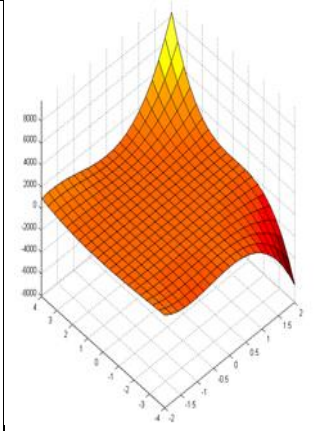
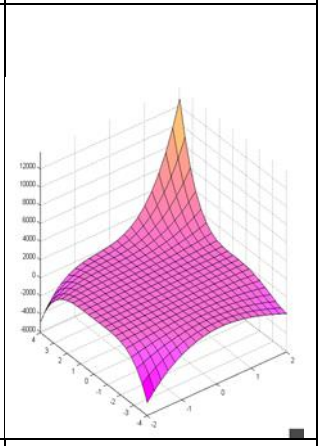
$$M(V:x,y)=xy^2+4x\,y^3+7x^2\,y^2+21x^2\,y^3+10x^3\,y^3$$

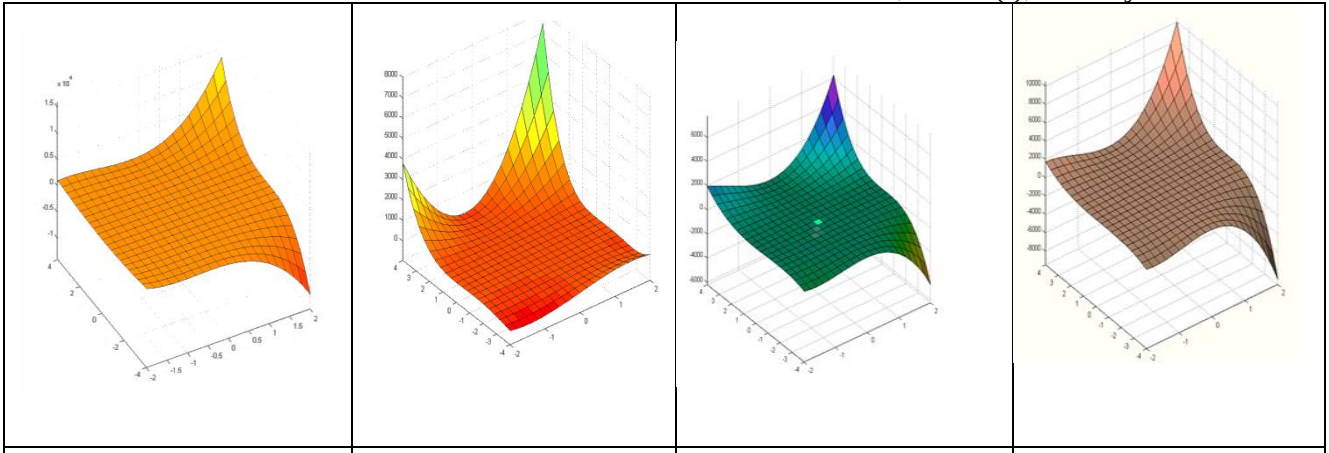
Proof: The edge partitions of Vorapaxar as follows

$|E_{1,2}|=1, |E_{1,3}|=4, |E_{2,2}|=7, |E_{2,3}|=21, |E_{3,3}|=7$ from the definition of M-polynomial

$$M(V:x,y)=\sum_{\delta\le i\le j\le\Delta}\lambda_{ij}(V)\,x^i\,y^j$$

$$M(\mathrm{V}:x,y)=\lambda_{12}(\mathrm{V})x^1y^2+\lambda_{13}(\mathrm{V})\,x^1\,y^3+\lambda_{22}(\mathrm{V})\,x^2\,y^2+\lambda_{23}(\mathrm{V})\,x^2\,y^3+\lambda_{33}(\mathrm{V})\,x^3\,y^3$$
$$=xy^2+4x\,y^3+7x^2\,y^2+21x^2\,y^3+10x^3\,y^3$$

			
(a)Aspirin	(b)Clopidogrel	(c) Ticagrelor	(d)Prasugrel
			
(e) Cangrelor	(f) Ticlopidine	(g)Dipyridamole	(h) Abciximab



(i) Eptifibatide	(j) Tirofiban	(k) Cilostazol	(l)Vorapaxer

Figure:9. M-polynomial of Antiplatelet drugs

Conclusion

In the case of developing countries, topological indices are applied in order to assess the medicinal properties of drugs. We carried out a study where we calculated a number of graph-theoretic indices including structural analysis of the drug. Also, we calculated intercorrelation of defined topological indices and correlation between these indices and Antiplatelet medicines. Theoretical results presented in this article are of great value in perspective of developing new drug intended for decrease our body's ability to form blood clots.

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