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Topological Indices of Antibiotic Drugs used in Pneumonia Treatment with their QSPR Analysis and M-polynomial

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Authors' contributions

This work was carried out in collaboration between both authors. Both authors read and approved the final manuscript.

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ABSTRACT

Chemical graph theory is the mathematical modeling of molecules. It is a branch of graph theory that studies all of the efects of connection in a chemical network. Pneumonia is an infection of one or both of the lungs caused by bacteria, viruses, or fungi. Antibiotic drugs such as Azithromycin, Amoxicillin, Ciprofloxacin, Erythromycin, Clarithromycin, Clindamycin, Levofloxacin, Sulfamethoxazole, Metronidazole, Moxifloxacin, Tetracycline, Cefotaxime are used to treat pneumonia. In this paper, various degree based topological indices of these drugs are calculated and different types of regression models predicting the physicochemical properties of these drugs in terms of proposed indices are obtained and analyzed. Furthermore, we calculate the M-polynomial of these drugs.

Keywords: Graph; vertex; polynomial; exponential.

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1. INTRODUCTION

Pneumonia is mostly spread when people infected cough, sneeze or talk, sending respiratory droplets into the air. The symptoms include fever, chills, chest pain, cough, shortness of breath, nausea and vomiting. There are many drugs used to treat of pneumonia. Gram-negative bacteria are widely accepted as the etiological agents of hospital-acquired pneumonia (HAP). Between 1986 and 2003, Acinetobacter species were the only Gram-negative bacteria that grew considerably as a cause of pneumonia in Intensive Care Units (ICUs) in the United States [1]. Community-acquired pneumonia (CAP) is a clinical and public health problem all over the world [2]. the bacterial etiology of CAP in adults hospitalized in various settings, as well as to evaluate the adequacy of empirical treatment recommendations given by clinical practice guidelines (CPGs) in connection to the bacteria found in CAP patients [3]. Identifying relevant risk factors for multidrug-resistant organisms or atypical infections during the initial evaluation of a patient coming from the community with pneumonia is critical [4-6]. Because a microbiological identification is found in around 30% of hospitalized patients with community pneumonia and normally takes 24-48 hours to be accessible, most patients are treated empirically [7]. As a result, the number of patients with pneumonia admitted to the hospital from the community who may not be totally immunocompetent is growing [8,9]. Determine the prevalence, type, microbiology, and intercorrelations of several risk variables for immunocompromise in community-dwelling hospitalized patients with pneumonia [10]. Highly active antiretroviral treatment (HAART) has significantly reduced HIV/AIDS morbidity and death. However, with an inpatient mortality rate of 10%, bacterial community acquired pneumonia (BCAP) remains one of the most common causes of morbidity in HIV-infected individuals [11]. Pneumonia is defined as an acute respiratory illness characterized by newly developed radiological pulmonary shadowing that can be segmental, lobar, or mutilobar [12]. The annual incidence of community acquired pneumonia (CAP) ranges between 4 million and 5 million cases, with 25% requiring hospitalization [13]. A graph polynomial is an algebraic object associated with a graph that is typically invariant under graph isomorphism. Many algebraic graph polynomials have been introduced in the past, including the Hosoya polynomial [14], the Forgotten polynomial [15], the Pi polynomial [16], the Schultz polynomial, the Modified Schultz polynomial [17], the Matching polynomial [18], the Tutte polynomial [19], and the M-Polynomial. Degree-based topological indices are particularly relevant in chemistry among these groups. There has been a lot of interest in exploiting graph invariants in QSPR and QSAR investigations in recent years. In [20] The Curvilinear and multilinear regression models predicting the properties of COVID 19 drugs in terms of proposed indices are obtained and analyzed. In [21] The results of the QSPR experiments, which were acquired using the polynomial regression technique, can contribute in the development of new drugs for the treatment of COVID-19. For further detail see [22-27]. A topological index (molecular descriptor) 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 the physicochemical, pharmacological, toxicological, biological, and other aspects of chemical compounds in theoretical chemistry. In this study, we construct topological indices of some drugs used in pneumonia treatment are computed for use in QSPR models. Many types of regression models are obtained for few physicochemical properties of these drugs. Finally, these models are compared and the best predictor index and models are obtained. Also, we derived the M-polynomial of pneumonia drugs.

2. MATERIALS AND METHODS

Chemical structure is considered as graph, where elements are taken as vertices and bounds between them are taken as edges. Let G be a simple connected graph with vertex sets and edge sets are respectively. The degree of a vertex v is the number of edges incident on the vertex v and is expressed as $d_G(v) = \chi_G(v)$ for every $v \in V(G)$.

In 1972, I. Gutman and N. Trinajstic [28] 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 [29] 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 Al-Naggar [30] 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 [31]:

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

S. Fajtlowicz defined the harmonic index graph as [32] in 1987:

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

In 1998, E. Estrada [33] defined the Atom bond connectivity index as:

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

Zhao et al. [34] formulated the SS index which is defined as:

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

The physical property values are extracted from Chem Spider. The molecules of the pneumonia drug served as the materials for this work. The topological indices of twelve different pneumonia drug molecules are found by treating each molecule as a graph. We use the degree based vertex and edge partitions to calculate our proposed topological indices. Table 1 calculated the degree based topological indices for pneumonia drugs given in Fig. 1. The proposed indices are subjected to some types of regression analysis using SPSS.

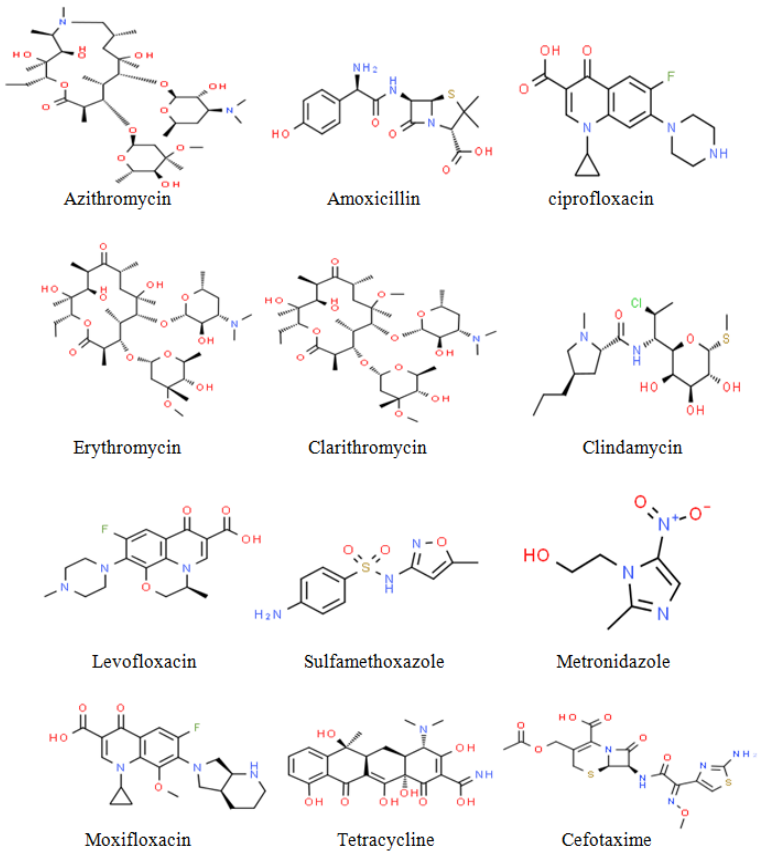

Fig. 1. Molecular structure of pneumonia drugs

3. QSPR ANALYSIS OF PNEUMONIA DRUGS

In this section, degree based topological indices and some physicochemical properties which are boiling point (BP), enthalpy of vaporization (EV), flash point (FP), molar refractivity (MR), complexity (C), polarizability (P), molecular weight (MW), molar volume (MV) of antibiotic drugs are analyzed. The physicochemical properties of these drugs are presented in Table 2. In general, R^2 depicts the strength of the relationship between the dependent and independent variables. We present the many regression models with value of $R^2 \geq 0.8$ for the physicochemical properties in terms of proposed indices. In Tables (4, 6, 8, 10, 12, 14), the value of p is less than or equal to 0.001 ($p < 0.05$), indicating the significance of the results. Consider the following regression models to obtain the relationship between the degree based topological indices and the physicochemical properties of these drugs.

p=a+bq (Linear)
$p=aq^2+bq+c$ (Quadratic)
$p=a+bq+cq^2+dq^3$ (Cubic)
p=a+b*ln(q) (Logarithmic)
$p=ab^q$ (Exponential)
$p=aq^b$ (Power)

Figs. 2-5 show the plots of the all regression models of physical properties against indices.

3.1 Linear Regression

Table 3 shows the square of correlation coefficient (R^2) 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 Y and MR, P, MW has the highest predicting with ABC and C has the highest predicting with M_2 and MV has the highest predicting with H. Over all indices, it is noticed that the ABC index are best suited for predicting the properties MR and P.

BP=406.6005+0.1765(Y)
EV=62.8804+0.0301(Y)
FP=199.6961+0.1067(Y)
MR=-4.5182+4.8371(ABC)
C=2.0655+3.5786(M_2)
P=-1.7874+1.9174(ABC)
MW=10.1079+18.0279(ABC)
MV=-85.3185+29.7927(H)

Table 4 shows best predictors, R^2 value, p value, F-statistic and standard error values in this models.

3.2 Quadratic Regression

Table 5 shows the square of correlation coefficient (R^2) obtained by quadratic regression model between Indices and physical properties of these drugs. In this model, the physical properties: BP, FP has the highest predicting with S and MR, P, MW, MV has the highest predicting with ABC and C has the highest predicting with F and EV has the highest predicting with Y. Over all indices, it is noticed that the ABC index is best suited for predicting the property MR.

$BP=-9.8751E\text{-}6(S)^2+0.1504(S)+240.6816$
$EV=-7.6826E\text{-}6(Y)^2+0.0542(Y)+47.8855$
$FP=-5.9688E\text{-}6(S)^2+0.0909(S)+99.4145$
$MR=0.0213(ABC)^2+3.6794(ABC)+8.8848$
$C=-0.0013(F)^2+2.8111(F)-246.8855$
$P=0.0083(ABC)^2+1.4676(ABC)+3.4197$
$MW=0.0139(ABC)^2+17.2704(ABC)+18.8779$
$MV=0.2656(ABC)^2+2.3290(ABC)+88.4448$

Table 6 shows best predictors, R^2 value, p value, F-statistic and standard error values in this models.

3.3 Cubic Regression

Table 7 shows the square of correlation coefficient (R^2) obtained by cubic regression model between Indices and physical properties of these drugs. In this model, the physical properties: BP, FP, MV has the highest predicting with S and MR, P, MW has the highest predicting with H and C has the highest predicting with M_1 and EV has the highest predicting with Y. Over all indices, it is noticed that the H index is best suited for predicting the property MW.

$BP=208.9067+0.1824(S)-1.8670E\text{-}5(S)^2+6.6989E\text{-}10(S)^3$
$EV=38.2224+0.0841(Y)-3.3179E\text{-}5(Y)^2+6.1015E\text{-}9(Y)^3$
$FP=80.1893+0.1103(S)-1.1290E\text{-}5(S)^2+4.0531E\text{-}10(S)^3$
$MR=48.0274-5.6383(H)+1.0937(H)^2-0.0249(H)^3$
$C=260.1410-5.3525(M_1)+0.0818(M_1)^2-0.0002(M_1)^3$
$P=18.9114-2.2126(H)+0.4325(H)^2-0.0099(H)^3$

$MW=212.2875-27.9363(H)+4.9214(H)^2-0.1172(H)^3$
$MV=-146.7244+0.3068(S)-7.7250E-5(S)^2+6.4447E-9(S)^3$

Table 8 shows best predictors, R^2 value, p value, F-statistic and standard error values in this models.

3.4 Logarithmic Regression

Table 9 shows the square of correlation coefficient (R^2) obtained by logarithmic regression model between Indices and physical properties of these drugs. In this model, the physical properties: BP, FP has the highest predicting with S and MR, P, MW, MV has the highest predicting with H and C, EV has the highest predicting with Y. Over all indices, it is noticed that the Y index is best suited for predicting the property C.

$BP=-1151.8066+219.7110*\ln(S)$
$EV=-170.4144+38.7496*\ln(Y)$
$FP=-742.7535+132.8714*\ln(S)$
$MR=-172.1730+112.0253*\ln(H)$
$C=-3504.8689+596.1933*\ln(Y)$
$P=-68.2636+44.4131*\ln(H)$
$MW=-622.0350+420.3687*\ln(H)$
$MV=-634.7948+378.4903*\ln(H)$

Table 10 shows best predictors, R^2 value, p value, F-statistic and standard error values in this models.

3.5 Exponential Regression

Table 11 shows the square of correlation coefficient (R^2) obtained by exponential regression model between Indices and physical properties of these drugs. In this model, the physical properties: EV has the highest predicting with F and MR, P, MW has the highest predicting with SS and C has the highest predicting with M_2 and MV has the highest predicting with ABC. Over all indices, it is noticed that the ABC index is best suited for predicting the property MV.

$EV=66.1783*0.0301^{(F)}$
$MR=35.8646*0.0295^{(SS)}$
$C=201.3868*0.0057^{(M_2)}$
$P=14.2065*0.0295^{(SS)}$
$MW=151.5764*0.0280^{(SS)}$
$MV=89.8245*0.0481^{(ABC)}$

Table 12 shows best predictors, R^2 value, p value, F-statistic and standard error values in this models.

3.6 Power Regression

Table 13 shows the square of correlation coefficient (R^2) 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 Y and MR, P, MW, MV has the highest predicting with H and C has the highest predicting with M_2. Over all indices, it is noticed that the H index is best suited for predicting the property MR.

$BP=40.9584(Y)^{0.3864}$
$EV=6.6801(Y)^{0.3843}$
$FP=14.3804(Y)^{0.4444}$
$MR=7.1604(H)^{1.0461}$
$C=1.8184(M_2)^{1.1259}$
$P=2.8312(H)^{1.0471}$
$MW=32.5993(H)^{0.9955}$
$MV=15.4377(H)^{1.1511}$

Table 14 shows best predictors, R^2 value, p value, F-statistic and standard error values in this models.

Table 1. Degree based topological indices values of Pneumonia drugs

Drugs	M_1	M_2	F	Y	S	ABC	H	SS
Azithromycin	294	354	826	2502	7978	42.6388	25.0097	62.2259
Amoxicillin	136	161	384	1156	3624	19.9493	11.0524	28.4254
Ciprofloxacin	134	164	354	974	2754	19.2061	11.1667	29.2164
Erythromycin	270	324	778	2406	7786	39.002	21.643	55.9685
Clarithromycin	274	330	786	2422	7818	39.5502	22.243	57.0454
Clindamycin	136	161	362	1012	2906	20.2412	12.0001	29.4475
Levofloxacin	146	180	394	1106	3178	20.7579	11.8334	31.3981
Sulfamethoxazole	88	100	240	712	2256	13.2028	7.5191	18.8439
Metronidazole	56	64	144	392	1104	8.6921	5.3667	12.3751
Moxifloxacin	166	207	444	1234	3516	23.3272	13.5334	35.9936
Tetracycline	186	239	550	1722	5590	25.4167	13.7286	38.1027
Cefotaxime	156	186	412	1140	3244	23.0292	13.5667	33.9512

Table 2. Various physicochemical properties of Pneumonia drugs

Drugs	BP	EV	FP	MR	C	P	MW	MV
Azithromycin	822.1	136.0	451.0	197.6	1150	78.3	749.0	632.7
Amoxicillin	743.2	113.7	403.3	91.5	590	36.3	365.4	236.2
Ciprofloxacin	581.8	91.5	305.6	83.3	571	33.0	331.34	226.8
Erythromycin	818.4	135.4	448.8	189.2	1180	75.0	733.9	607.2
Clarithromycin	805.5	133.4	440.9	194.0	1190	76.9	748.0	631.9
Clindamycin	628.1	106.5	333.6	107.9	502	42.8	425.0	327.2
Levofloxacin	571.5	90.1	299.4	91.1	634	36.1	361.4	244.0
Sulfamethoxazole	482.1	74.7	245.4	62.5	346	24.8	253.28	173.1
Metronidazole	405.4	69.3	199.0	41.0	170	16.2	171.15	117.9
Moxifloxacin	636.4	98.8	338.7	101.8	727	40.4	401.4	285.0
Tetracycline	738.2	113.0	400.2	106.9	971	42.4	444.4	266.3
Cefotaxime	-	-	-	106.0	833	42.0	455.5	252.8

Table 3. R^2 obtained by linear regression model between topological indices and physicochemical properties of these drugs

Index/property	BP	EV	FP	MR	C	P	MW	MV
M_1	0.8268	0.8797	0.8268	0.9671	0.9334	0.9672	0.9681	0.9175
M_2	0.8306	0.8715	0.8306	0.9450	0.9467	0.9451	0.9483	0.8877
F	0.8422	0.8889	0.8422	0.9590	0.9377	0.9591	0.9607	0.9104
Y	0.8461	0.8895	0.8462	0.9453	0.9264	0.9454	0.9468	0.9016
S	0.8382	0.8798	0.8382	0.9253	0.9030	0.9254	0.9257	0.8883
ABC	0.8176	0.8826	0.8176	0.9811	0.9158	0.9811	0.9804	0.9379
H	0.7844	0.8612	0.7844	0.9797	0.8873	0.9790	0.9756	0.9407
SS	0.8118	0.8683	0.8118	0.9666	0.9255	0.9666	0.9668	0.9168

Table 4. Best predictor from linear regression model

Property	R^2	Best predictor	P	F	SE
BP	0.8461	Y	0.001	49.4959	58.1058
EV	0.8895	Y	0.001	72.4848	8.1887
FP	0.8462	Y	0.001	49.5072	35.1370
MR	0.9811	ABC	0.001	520.4602	7.4316
C	0.9467	M_2	0.001	177.4693	80.8500
P	0.9811	ABC	0.001	520.3882	2.9460
MW	0.9804	ABC	0.001	499.7440	28.2659
MV	0.9407	H	0.001	158.5248	46.7276

Table 5. R^2 obtained by quadratic regression model between topological indices and physicochemical properties of these drugs

Index/property	BP	EV	FP	MR	C	P	MW	MV
M_1	0.8774	0.8911	0.8773	0.9729	0.9587	0.9728	0.9697	0.9518
M_2	0.8646	0.8760	0.8645	0.9570	0.9618	0.9569	0.9540	0.9347
F	0.8990	0.9019	0.8989	0.9639	0.9656	0.9638	0.9620	0.9436
Y	0.9174	0.9078	0.9173	0.9481	0.9614	0.9481	0.9472	0.9296
S	0.9247	0.9034	0.9246	0.9271	0.9437	0.9271	0.9258	0.9131
ABC	0.8858	0.9037	0.8857	0.9831	0.9511	0.9830	0.9804	0.9616
H	0.8612	0.8920	0.8611	0.9792	0.9339	0.9791	0.9765	0.9532
SS	0.8592	0.8790	0.8591	0.9725	0.9499	0.9724	0.9685	0.9504

Table 6. Best predictor from quadratic regression model

Property	R^2	Best predictor	P	F	SE
BP	0.9247	S	0.001	49.1018	43.1233
EV	0.9078	Y	0.001	39.3969	7.9343
FP	0.9246	S	0.001	49.0703	26.0873
MR	0.9831	ABC	0.001	261.1800	7.4253
C	0.9656	F	0.001	126.1748	68.4753
P	0.9830	ABC	0.001	259.9630	2.9501
MW	0.9804	ABC	0.001	225.5761	29.7500
MV	0.9616	ABC	0.001	112.6593	39.6280

Table 7. R^2 obtained by cubic regression model between topological indices and physicochemical properties of these drugs

Index/property	BP	EV	FP	MR	C	P	MW	MV
M_1	0.8775	0.8911	0.8774	0.9741	0.9762	0.9740	0.9698	0.9537
M_2	0.8672	0.8795	0.8671	0.9635	0.9723	0.9634	0.9570	0.9428
F	0.8991	0.9028	0.8990	0.9744	0.9757	0.9744	0.9675	0.9590
Y	0.9176	0.9102	0.9175	0.9745	0.9639	0.9745	0.9657	0.9654
S	0.9258	0.9086	0.9257	0.9708	0.9437	0.9709	0.9605	0.9678
ABC	0.8860	0.9046	0.8859	0.9831	0.9719	0.9830	0.9818	0.9616
H	0.8614	0.8931	0.8613	0.9849	0.9489	0.9848	0.9857	0.9635
SS	0.8595	0.8790	0.8594	0.9725	0.9689	0.9724	0.9694	0.9505

Table 8. Best predictor from cubic regression model

Property	R^2	Best predictor	P	F	SE
BP	0.9258	S	0.001	29.0934	45.7690
EV	0.9102	Y	0.001	23.6550	8.3715
FP	0.9257	S	0.001	29.0750	27.6877
MR	0.9849	H	0.001	174.4423	7.4256
C	0.9762	M_1	0.001	109.5617	60.3300
P	0.9848	H	0.001	173.0597	2.9549
MW	0.9857	H	0.001	183.6255	26.9948
MV	0.9678	S	0.001	80.0485	38.5081

Table 9. R^2 obtained by logarithmic regression model between topological indices and physicochemical properties of these drugs

Index/property	BP	EV	FP	MR	C	P	MW	MV
M_1	0.8756	0.8707	0.8755	0.8664	0.9335	0.8669	0.8816	0.7720
M_2	0.8651	0.8489	0.8650	0.8322	0.9295	0.8327	0.8490	0.7328
F	0.8954	0.8811	0.8953	0.8615	0.9409	0.8620	0.8773	0.7664
Y	0.9113	0.8903	0.9112	0.8600	0.9417	0.8606	0.8753	0.7675
S	0.9163	0.8902	0.9163	0.8534	0.9310	0.8540	0.8673	0.7661
ABC	0.8806	0.8902	0.8805	0.8967	0.9326	0.8972	0.9106	0.8077
H	0.8567	0.8848	0.8566	0.9122	0.9198	0.9125	0.9240	0.8290
SS	0.8591	0.8601	0.8590	0.8663	0.9257	0.8668	0.8809	0.7730

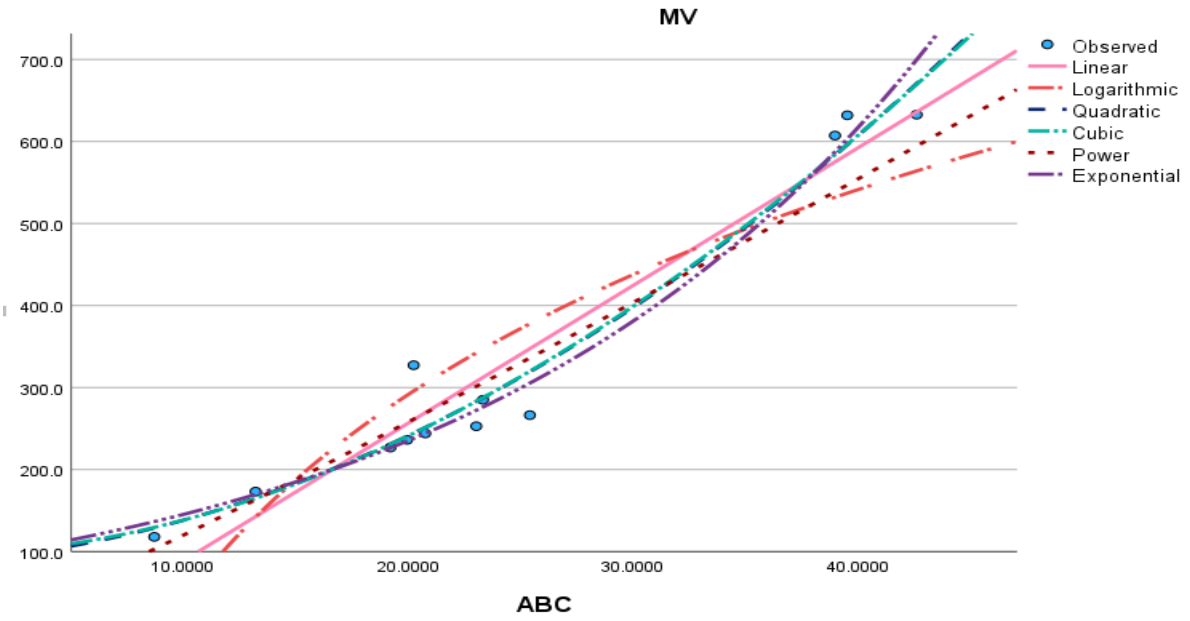

Fig. 2. Regression curves for MV against ABC

Table 10. Best predictor from logarithmic regression model

Property	R^2	Best predictor	P	F	SE
BP	0.9163	S	0.001	98.5659	42.8494
EV	0.8903	Y	0.001	73.0427	8.1608
FP	0.9163	S	0.001	98.5212	25.9193
MR	0.9122	H	0.001	103.8725	16.0399
C	0.9417	$_{Y}$	0.001	161.4676	84.5384
P	0.9125	H	0.001	104.2974	6.3461
MW	0.9240	H	0.001	121.5199	55.6471
MV	0.8290	H	0.001	48.4896	79.3170

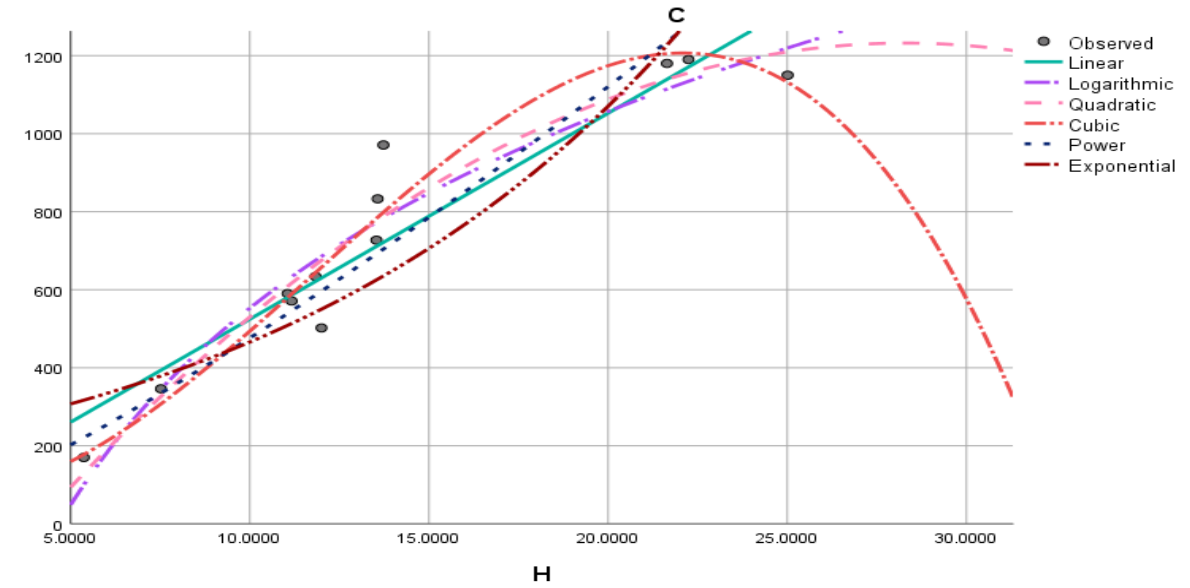

Fig. 3. Regression curves for C against H

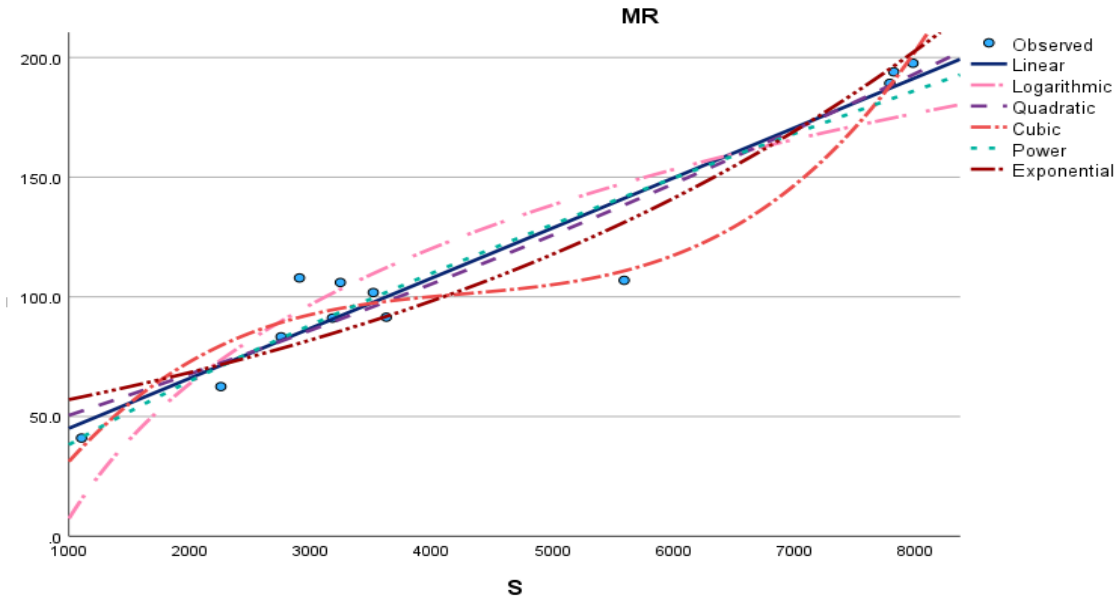

Fig. 4. Regression curves for MR against S

Table 11. R^2 obtained by exponential regression model between topological indices and physicochemical properties of these drugs

Index/property	BP	EV	FP	MR	C	P	MW	MV
M_1	0.7889	0.8458	0.7822	0.9364	0.8066	0.9358	0.9291	0.9360
M_2	0.7976	0.8443	0.7916	0.9282	0.8279	0.9276	0.9226	0.9182
F	0.7995	0.8521	0.7920	0.9208	0.7977	0.9202	0.9145	0.9207
Y	0.7963	0.8470	0.7878	0.8932	0.7693	0.8926	0.8873	0.8972
S	0.7811	0.8307	0.7715	0.8573	0.7298	0.8566	0.8513	0.8670
ABC	0.7758	0.8433	0.7686	0.9388	0.7829	0.9381	0.9304	0.9462
H	0.7428	0.8204	0.7357	0.9305	0.7556	0.9296	0.9205	0.9443
SS	0.7769	0.8361	0.7707	0.9398	0.8067	0.9391	0.9318	0.9394

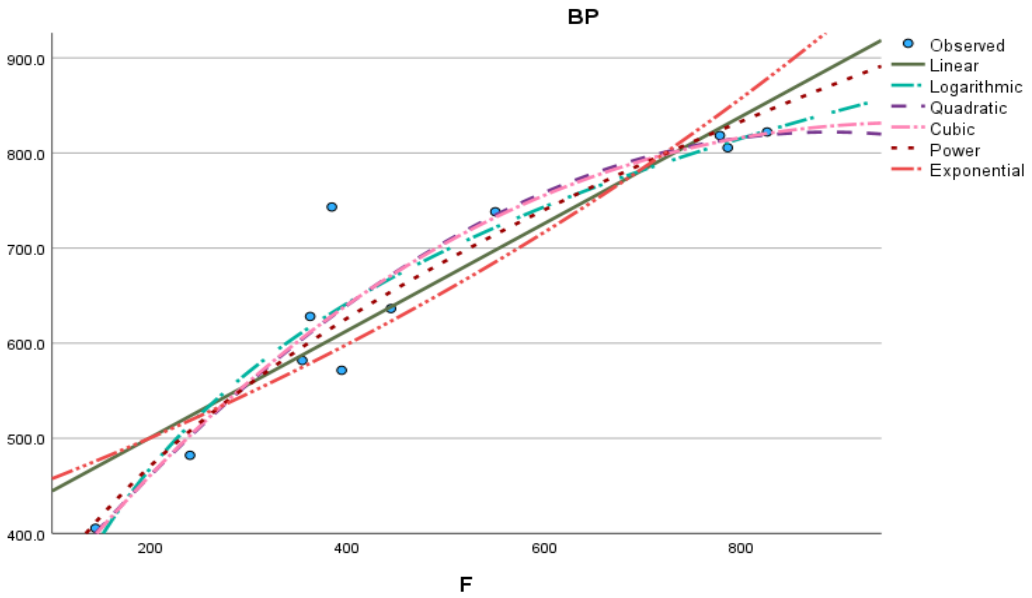

Fig. 5. Regression curves for BP against F

Table 12. Best predictor from exponential regression model

Property	R^2	Best predictor	P	F	SE
BP	-	-	-	-	-
EV	0.8521	F	0.001	51.8639	0.0935
FP	-	-	-	-	-
MR	0.9398	SS	0.001	156.2183	0.1194
C	0.8279	M_2	0.001	48.1189	0.2479
P	0.9391	SS	0.001	154.3161	0.1202
MW	0.9318	SS	0.001	136.6604	0.1211
MV	0.9462	ABC	0.001	175.9676	0.1272

Table 13. R^2 obtained by power regression model between topological indices and physicochemical properties of these drugs

Index/property	BP	EV	FP	MR	C	P	MW	MV
M_1	0.8861	0.8851	0.8867	0.9652	0.9514	0.9654	0.9658	0.9010
M_2	0.8819	0.8707	0.8833	0.9443	0.9609	0.9446	0.9464	0.8717
F	0.9033	0.8943	0.9034	0.9574	0.9522	0.9577	0.9587	0.8915
Y	0.9133	0.8987	0.9125	0.9450	0.9386	0.9453	0.9462	0.8817
S	0.9109	0.8916	0.9090	0.9229	0.9108	0.9232	0.9235	0.8650
ABC	0.8843	0.8973	0.8838	0.9806	0.9345	0.9806	0.9803	0.9253
H	0.8565	0.8872	0.8555	0.9830	0.9092	0.9829	0.9816	0.9376
SS	0.8710	0.8749	0.8718	0.9658	0.9468	0.9660	0.9659	0.9033

Table 14. Best predictor from power regression model

Property	R^2	Best predictor	P	F	SE
BP	0.9133	Y	0.001	94.8102	0.0714
EV	0.8987	Y	0.001	79.8616	0.0774
FP	0.9125	Y	0.001	93.8216	0.0826
MR	0.9830	H	0.001	579.5826	0.0634
C	0.9609	M_2	0.001	245.5654	0.1182
P	0.9829	H	0.001	575.1301	0.0637
MW	0.9816	H	0.001	532.1113	0.0630
MV	0.9376	H	0.001	150.3010	0.1370

4. M-POLYNOMIAL OF PNEUMONIA DRUGS

The definition of an M-polynomial is [35]:

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

where, $\mathbf{n_{ab}(G)}$ is the number of edges of $\mathbf{G}$, such that $\mathbf{ij} \in \mathbf{E(G)}$ and $\{\boldsymbol{\chi_i}, \boldsymbol{\chi_j}\} = \{\mathbf{a}, \mathbf{b}\}$. In this section, we expressed the M-polynomial of molecular graphs of pneumonia drugs such as Azithromycin, Amoxicillin, Ciprofloxacin, Erythromycin, Clarithromycin, Clindamycin, Levofloxacin, Sulfamethoxazole, Metronidazole, Moxifloxacin, Tetracycline, Cefotaxime. In Fis. 6 and 7 depicts the 3d surface plot for the M-polynomial of these drugs.

Theorem 4.1: Let A be the graph of Azithromycin. Then M-polynomial of A is $M(A;x,y)=7xy^2+10xy^3+3xy^4+20x^2y^3+5x^2y^4+10x^3y^3+4x^3y^4$.

Proof: The edge partitions of azithromycin as follows: $|E_{2,3}|=20, |E_{3,3}|=10, |E_{1,3}|=10, |E_{1,2}|=7, |E_{3,4}|=4, |E_{2,4}|=5, |E_{1,4}|=3$. From defintion of M-polynomial

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

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

We get the entire result.

Theorem 4.2: Let Am be the graph of Amoxicillin. Then M-polynomial of Am is $M(Am;x,y) = 7xy^3 + 3xy^4 + 2x^2y^2 + 6x^2y^3 + 8x^3y^3 + x^3y^4$.

Proof: The edge partitions of amoxicillin as follows: $|E_{2,3}| = 6, |E_{3,3}| = 8, |E_{1,3}| = 7, |E_{2,2}| = 2, |E_{3,4}| = 1, |E_{1,4}| = 3$. From defintion of M-polynomial

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

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

We get the entire result.

Theorem 4.3: Let C be the graph of Ciprofloxacin. Then M-polynomial of C is $M(C;x,y) = 4xy^3 + 5x^2y^2 + 10x^2y^3 + 8x^3y^3$.

Proof: The edge partitions of ciprofloxacin as follows: $|E_{2,3}| = 10, |E_{3,3}| = 8, |E_{1,3}| = 4, |E_{2,2}| = 5$. From defintion of M-polynomial:

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

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

We get the entire result.

Theorem 4.4: Let E be the graph of Erythromycin. Then M-polynomial of E is $M(E;x,y) = 2xy^2 + 13xy^3 + 5xy^4 + 15x^2y^3 + 3x^2y^4 + 11x^3y^3 + 4x^3y^4$.

Proof: The edge partitions of erythromycin as follows: $|E_{2,3}| = 15, |E_{3,3}| = 11, |E_{1,3}| = 13, |E_{1,2}| = 2, |E_{3,4}| = 4, |E_{2,4}| = 3, |E_{1,4}| = 5$. From defintion of M-polynomial

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

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

We get the entire result.

Theorem 4.5: Let Cl be the graph of Clarithromycin. Then M-polynomial of Cl is $M(Cl;x,y) = 3xy^2 + 13xy^3 + 4xy^4 + 15x^2y^3 + 4x^2y^4 + 11x^3y^3 + 4x^3y^4$.

Proof: The edge partitions of erythromycin as follows: $|E_{2,3}| = 15, |E_{3,3}| = 11, |E_{1,3}| = 13, |E_{1,2}| = 3, |E_{3,4}| = 4, |E_{2,4}| = 4, |E_{1,4}| = 4$. From defintion of M-polynomial

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

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

We get the entire result.

Theorem 4.6: Let Cli be the graph of Clindamycin. Then M-polynomial of Cli is $M(Cli;x,y)=2xy^2+7xy^3+x^2y^2+10x^2y^3+8x^3y^3$.

Proof: The edge partitions of clindamycin as follows: $|E_{2,3}|=10, |E_{3,3}|=8, |E_{1,3}|=7, |E_{1,2}|=2, |E_{2,2}|=1$. From defintion of M-polynomial

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

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

We get the entire result.

Theorem 4.7: Let L be the graph of Levofloxacin. Then M-polynomial of L is $M(L;x,y)=6xy^3+3x^2y^2+10x^2y^3+10x^3y^3$.

Proof: The edge partitions of levofloxacin as follows: $|E_{2,3}|=10, |E_{3,3}|=10, |E_{1,3}|=6, |E_{2,2}|=3$. From defintion of M-polynomial

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

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

We get the entire result.

Theorem 4.8: Let S be the graph of Sulfamethoxazole. Then M-polynomial of S is $M(S;x,y)=2xy^3+2xy^4+3x^2y^2+9x^2y^3+x^2y^4+x^3y^4$.

Proof: The edge partitions of sulfamethoxazole as follows: $|E_{2,3}|=9, |E_{1,3}|=2, |E_{2,2}|=3, |E_{3,4}|=1, |E_{2,4}|=1, |E_{1,4}|=2$. From defintion of M-polynomial

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

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

We get the entire result.

Theorem 4.9: Let M be the graph of Metronidazole. Then M-polynomial of M is $M(M;x,y) = xy^2 + 3xy^3 + 2x^2y^2 + 3x^2y^3 + 3x^3y^3$.

Proof: The edge partitions of metronidazole as follows: $|E_{2,3}| = 3, |E_{3,3}| = 3, |E_{1,3}| = 3, |E_{1,2}| = 1, |E_{2,2}| = 2$. From defintion of M-polynomial

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

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

We get the entire result.

Theorem 4.10: Let Mo be the graph of Moxifloxacin. Then M-polynomial of Mo is $M(Mo;x,y) = xy^2 + 4xy^3 + 4x^2y^2 + 13x^2y^3 + 11x^3y^3$.

Proof: The edge partitions of moxifloxacin as follows: $|E_{2,3}| = 13, |E_{3,3}| = 11, |E_{1,3}| = 4, |E_{1,2}| = 1, |E_{2,2}| = 4$. From defintion of M-polynomial

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

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

We get the entire result.

Theorem 4.11: Let T be the graph of Tetracycline. Then M-polynomial of T is $M(T;x,y) = 9xy^3 + 3xy^4 + 2x^2y^2 + 4x^2y^3 + 12x^3y^3 + 5x^3y^4$.

Proof: The edge partitions of tetracycline as follows: $|E_{2,3}| = 4, |E_{3,3}| = 12, |E_{1,3}| = 9, |E_{2,2}| = 2, |E_{3,4}| = 5, |E_{1,4}| = 3$. From defintion of M-polynomial

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

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

We get the entire result.

Theorem 4.12: Let Ce be the graph of Cefotaxime. Then M-polynomial of Ce is $M(Ce;x,y) = xy^2 + 7xy^3 + 4x^2y^2 + 11x^2y^3 + 9x^3y^3$.

Proof: The edge partitions of cefotaxime as follows: $|E_{2,3}| = 11, |E_{3,3}| = 9, |E_{1,3}| = 7, |E_{1,2}| = 1, |E_{2,2}| = 4$. From defintion of M-polynomial

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

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

We get the entire result.

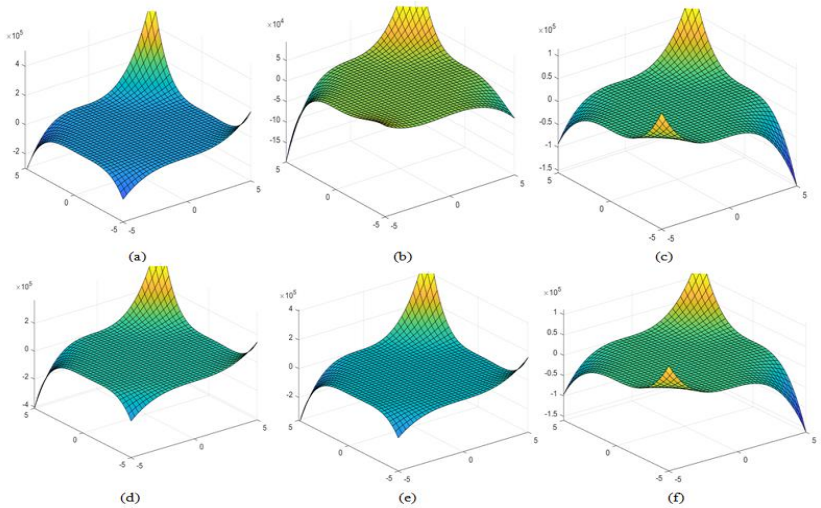

Fig . 6. 3D plots for M-polynomial of (a) Azithromycin (b)Amoxicillin (c) Ciprofloxacin (d) Erythromycin (e) Clarithromycin (f) Clindamycin

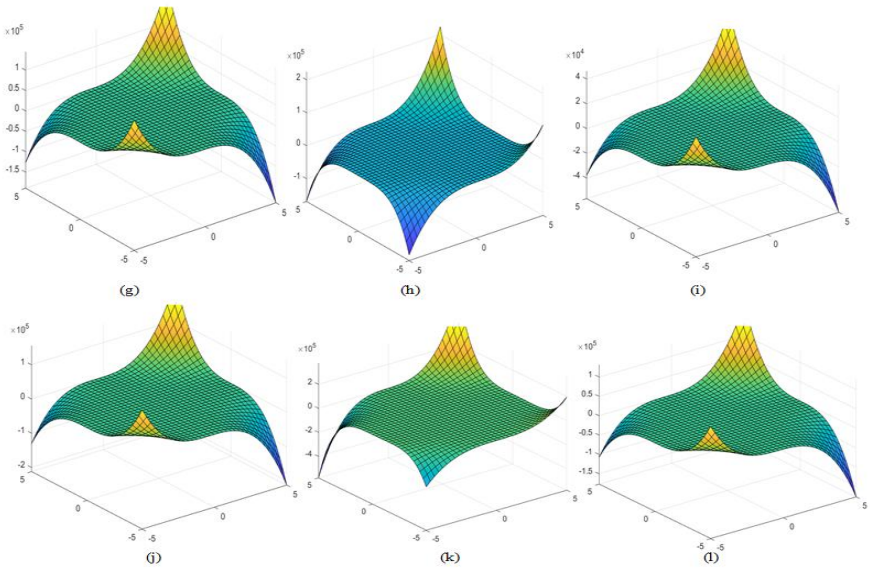

Fig . 7. 3D plots for M-polynomial of (g) Levofloxacin (h) Sulfamethoxazole (i) Metronidazole (j) Moxifloxacin (k) Tetracycline (l) Cefotaxime

5. CONCLUSION

In this paper, we proposed degree based topological indices for pneumonia drugs. Over all regressions, it is noticed that the H index is very best suited for predicting the property MW in cubic regression model. On comparing with the cubic and quadratic regression model, we observed that the cubic regression model have better predictive ability than quadratic regression model, because of, all physical properties gives the highest ($R^2 \geq 0.9$) value than quadratic model from Tables 6 and 8. We also derived the M-polynomial of these drugs. Topological indices are defined and used in many fields to investigate the properties of various objects such as atoms and molecules. Mathematicians and chemists have defined and studied a number of topological indices.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

REFERENCES

1. Gaynes R, Edwards JR. Overview of nosocomial infections caused by gram-negative bacilli. Clin Infect Dis. 2005; 41:848-854.
2. Aliberti S, Dela Cruz CS, Sotgiu G, Restrepo MI. Pneumonia is a neglected problem: it is now time to act. Lancet Respir. 2019;7:10-11.
3. Manuela Carugati, S. Aliberti, G. Sotgiu. Bacterial etiology of community-acquired pneumonia in immunocompetent hospitalized patients and appropriateness of empirical treatment recommendations: An international point-prevalence study. Euro. J. of Clinical Microbiology & Infectious Diseases. 2020;39:1513-1525.
4. Aliberti S, Di Pasquale M, Zanaboni AM, et al. Stratifying risk factors for multidrug-resistant pathogens in hospitalized patients coming from the community with pneumonia. Clin Infect Dis. 2012: 54: 470-8.
5. Aliberti S, Cilloniz C, Chalmers JD, et al. Multidrug-resistant pathogens in hospitalised patients coming from the community with pneumonia: A European perspective. Thorax. 2013;68:997-9.
6. Shindo Y, Ito R, Kobayashi D, et al. Risk factors for drug-resistant pathogens in community-acquired and healthcare-associated pneumonia. Am J Respir Crit Care Med. 2013;188:985-95.
7. Musher DM, Thorner AR. Community-acquired pneumonia. N Engl J Med. 2014;371(16):19-28.
8. Furman CD, Rayner AV, Tobin EP. Pneumonia in older residents of long-term care facilities. Am Fam Physician. 2004: 70: 1495-500.
9. Cillóniz C, Polverino E, Ewig S, et al. Impact of age and comorbidity on cause and outcome in community-acquired pneumonia. Chest. 2013;144:999-1007.
10. Marta Francesca Di Pasquale, Giovanni Sotgiu, Andrea Gramegna. Prevalence and Etiology of Community-acquired Pneumonia in Immunocompromised Patients. Clin Infect Dis. 2019;68: 1482-1493.
11. Madeddu G, Porqueddu EM, Cambosu F, et al. Bacterial community acquired pneumonia in HIV-infected inpatients in the highly active antiretroviral therapy era. Infection 2008: 36: 231-6.
12. Reid PT, Innes JA Respiratory Disease. In: Colledge NR, Walker BR and Ralston SH, ed, Davidson's principle and practice of Medicine, 21sted. Edinburgh: Elsevier Publications. 2010; 680-682.
13. Mandell LA, Bartlett JG, Dowell SF, File TM Jr, Musher DM, et al. Update of practice guidelines for the management of community-acquired pneumonia in immunocompetent adults. Clin Infect Dis. 2003;37:1405-1433.
14. Deutsch E, Rodriguez-Velzquez JA. The terminal Hosoya polynomial of some families of composite graphs, International Journal of Combinatorics. 2014;(1):1-4: Article ID 696507.
15. Ajmal M, Nazeer W, Khalid W, Kang SM. Forgotten polynomial and forgotten index for the line graphs of banana tree graph, firecracker graph and subdivision graphs. Global Journal of Pure and Applied Mathematics. 2017;13 (6):2673-2682.
16. Loghman A, Badakhshian L. Pi polynomial of zig-zag polyhex nanotubes. Digest Journal of Nanomaterials and Biostructures. 2008;3(4):299- 302.
17. Farahani MR. Schultz and modified Schultz polynomials of coronene polycyclic aromatic hydorcarbons, International Letters of Chemistry, Physics and Astronomy. 2014;32(1):1-10.

18. Farrel E. An introduction to matching polynomials. Journal of Combinatorial Theory, Series B. 1979;27(1):75-86.
19. Merino C, Ramirez-Ibanez M, Rodriguez-Sanchez G. The tutte polynomial of some matroids, International Journal of Combinatorics. 2012;(1):1-40.
20. Vighesh Ravi, Natarajan Chidambaram, Ozge Colakoglu. QSPR Study and Distance Based New Topological Descriptors of Some Drugs Used in the COVID 19 Treatment. J. Math. 2023;1187415: 1-15.
21. Nagarajan S, Priyadharsini G, Pattabiraman K. QSPR modeling of status-based topological indices with COVID-19 drugs. Polycyclic Aromatic Compounds. 2022;30.
22. Jan Rashid, Normy Norfiza, Salah Boularras, Karthikeyan R. Fractional perspective evaluation of chikungunya infection with saturated incidence functions. Alexandra Eng. Jour. 2023; 11:35-42.
23. Jan Rashid, Normy Norfiza, Salah Boularras, Ziad Ur Rehman. Mathematical analysis of the transmission dynamics of viral infection with effective control policies via fractional derivative. Nonlinear Engineering. 2023;12 (20220342):1-19.
24. Tao-Qian Tang, Jan Rashid, Adil Khurshaid, Zahir Shah. Analysis of the dynamics of a vector-borne infection with the effect of imperfect vaccination from a fractional perspective. Scientific Reports. 2023;10(23):14398.
25. Jan Rashid, Salah Boularras, Sultan Alyobi, Muhammad Jawad. Transmission dynamics of Hand–Foot–Mouth Disease with partial immunity through non-integer derivative. Inter. Jour. of Biomath. 2022; 16(06): 2250115:
26. Asif Jan, Salah Boularras, Farah Aini Adbullah, Jan Rashid. Dynamical analysis, infections in plants, and preventive policies utilizing the theory of fractional calculus. Eur. Phys. J. Spec. Top; 2023.
27. Asif Jan, Hari Mohan Srivastava, Amin Khan, Pshtiwan Othman Mohammed, Jan Rashid YS. Hamed. *In vivo* HIV dynamics, modeling the interaction of HIV and Immune system via non-integer derivatives. Fractal and Fractional. 2023; 7(5):361.
28. Gutman I, Trinajstic N. Graph theory and molecular orbitals. Total ϕ-electron energy of alternant hydrocarbons, Chemical Physics Letters. 1972;17(4):535–538.
29. Furtula B, Gutman I. A forgotton topological index, Journal of Mathematical Chemistry. 2015;53:213–220.
30. Alameri A, AL-Naggar N, Al-Rumaima M, Alsharafi M. Y-index of some graph operations, Int. J. Appl. Eng. Res. 2020;15(2):173-179.
31. Nagarajan S, Kayalvizhi G, Priyadharsini G. S-index of different graph operations, Asian. Res. Jour. of Math. 2021;17(12):43-52.
32. Fajtlowicz S, On conjectures of grafitti II, Congr. Numerantium. 1987;60:189–197.
33. Estrada E, Torres L, Rodriguez L, Gutman I. An atom bond connectivity index: Modeling the enthalpy of formation of alkanes, Indian Journal of Chemistry. 1998;37:849–855.
34. Zhao W, Shanmukha MC, Usha A, Farahani MR, Shilpa KC. Computing SS index of certain dendrimers, Journal of Mathematics. 2021: Article ID 7483508 (2021):14.
35. Deutsch E, Klavžar S. M-polynomial and degree-based topological indices. Iranian Journal of Mathematical Chemistry. 2015; 6(2):93-102.

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