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Fourteen Degree-Based Topological Indices On Twelve Penicillin Class Of Drugs With Qspr Analysis

C.Tamilarasi[1], F. Simon Raj[2]

[1]Hindustan Institute of Technology and Science, Chennai, Tamilnadu, India;

Email: tamilbabu4864@gmail.com

[2]Hindustan Institute of Technology and Science, Chennai, Tamilnadu, India;

E mail: simon240906@gmail.com

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Abstract This research article aims to establish the values of fourteen notable topological indices that are defined on some chemical structures belonging to the Penicillin class of drugs, which are a type of antibiotic derived from Penicillin fungi. This is performed to predict the Physicochemical properties of these compounds through Quantitative Structure-Property Relationships (QSPR). Also, it is observed that these characteristics have a good correlation with the Physico-chemical characteristics of the selected chemical structures of the penicillin class of compounds. The chemical properties of the selected compounds that this paper discusses include Polarizability, Log Octanol-Water Partition Coefficient(Log K_{ow}), Molecular Volume, Molar Refractivity, Log P, Soil Absorption Coefficient (Koc), Log Koc.

MSC2010 codes 05C10, 05C30, 05C92, 05C90,05C09

Keywords Topological index, degree-based topological index, Quantitative Structure-Property Relationships, Penicillin, Physico-chemical properties.

1Introduction Chemical graph theory is one of the key branches of graph theory and plays a significant role in applied mathematics, which deals with chemical structures. Atoms represent vertices and chemical bonds represent edges of the chemical structures in chemical graph theory. The numeral value associated to the vertices as well as edges in the molecular graph is termed as topological index/molecular descriptor. One of the main qualities of the topological indices is to predict the Physicochemical Properties of the respected chemical compounds through QSPR study[2,9,10,12,13]. In this paper, some of the properties of the Penicillin class of drugs are taken for QSPR analysis with prominent fourteen degree-based topological indices which are given good correlation with them.

Penicillin was the first true antibiotic to be discovered, which helped to fight bacterial infections such as whooping cough, ear infection, Salmonella, and Tuberculosis. The Scottish bacteriologist Alexander Fleming first observed that colonies of the bacterium Staphylococcus aureus failed to grow in certain areas of its culture that had been accidentally contaminated by the mold Penicillium notatum which was green in color. This is the well-known Penicillium notatum, which was finally discovered in 1928.

Wiener index, the first topological index(distance-based) was introduced by Harold Wiener in 1947. It is defined as the summation of the shortest distance between every single vertex of graph *G*. The progress of degree-based topological indices[3,4] was started in 1975 by Milan Randic. Degree-based as well as distance-based topological indices are widely used in predicting the physicochemical properties[7,11] of a class of compounds. Based on that, this paper is established. Here, fourteen notable degree-based topological indices are taken with twelve penicillin classes of drugs in the prediction task of properties through QSPR analysis.

2 Preliminaries In this part, some supportive notions are mentioned here, like, molecular graph *G*, degree of a vertex, topological index, degree-based topological indices, and basic formulas of fourteen degree-based topological indices. Let the molecular graph be the two-dimensional model of the chemical compound and is denoted as graph *G* (*V*, *E*) holds two

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non-empty sets *V*(set of all atoms as vertices) & *E*(set of all chemical bonds as edges). The degree of vertex *v* is the number of vertices adjacent to the vertex *v*.

The basic definitions of the fourteen topological indices are as follows:

Definition 2.1 One of the important degree-based topological indices which have a highly predictive ability of Physico-chemical properties of chemical compounds is the Augmented Zagreb Index (*Az*(*G*)). It was introduced by Furtula *et al* and is denoted as follows:

$Az(G) = \sum_{u,v \in E} \left(\frac{du\ dv}{du+\ dv-2}\right)^3$

Definition 2.2 Estrada *et al.* introduced the degree-based topological index named Atom Bond connectivity index(*ABC*(*G*)) which is a good predictor for the stability of alkanes and strain energy and is denoted as follows:

$$ABC(G) = \sum_{u,v\epsilon E} \sqrt{\frac{du+\ dv-2}{du\ dv}}$$

Definition 2.3 The GeometricArithmetic Index(*GA*(*G*))[1] is the well-studied degree-based topological index and is denoted as follows:

$$GA(G) = \sum_{u,v\epsilon E} \frac{2\sqrt{du\ dv}\,)}{du+\ dv}$$

Definition 2.4 Harmonic Index(*H*(*G*))[15]

$$H(G) = \sum_{u,v\epsilon E} \frac{2}{du+\ dv}$$

Definition 2.5 Forgotten Index(*F*(*G*))[14] was defined to be used in the analysis of drug molecular structures which was introduced by B. Furtula *et al.* and is denoted as follows:

$$F(G) = \sum_{u,v\epsilon E} du^2 + dv^2$$

Definition 2.6 The Zagreb indices $M_1(G)$, $M_2(G)$, and $M_3(G)$ are the numerical measures to pronounce the structure-property relationships. $M_1(G)$ is the oldest degree-based topological index that was initiated in 1972 and the related versions were developed later.

$$M_1(G) = \sum_{u,v\epsilon E}(du + dv)$$

$$M_2(G) = \sum_{u,v\epsilon E}(du\ dv)$$

$$M_3(G) = \sum_{u,v\epsilon E} |du - dv\ |$$

Definition 2.7 The Randic Index[5] is one of the most powerful degree-based topological indices to study the structure-property relationships of graphs and is denoted as follows:

$$R(G) = \sum_{u,v\epsilon E} \frac{1}{\sqrt{du\ dv}}$$

Definition 2.8 Sum Connectivity Index[16] is denoted as follows:

$$S(G) = \sum_{u,v\epsilon E} \frac{1}{\sqrt{du+\ dv}}$$

Definition 2.9 In 2013, Shirdel *et al*. proposed novel indices such as the First Hyper-Zagreb index($H_1(G)$), Second Hyper-Zagreb index($H_2(G)$) and are denoted as follows:

$$H_1(G) = \sum_{u,v\epsilon E}(du + dv)^2$$

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$$H_2(G) = \sum_{u,v\epsilon E}(dudv)^2$$

Definition 2.10 FORAN index($FR(G)$) holds the properties of the Forgotten index as well as the Randic index, and it is suitable for predicting the relationship between molecular structures of drugs and their physicochemical properties. It is denoted as follows:

$$FR(G) = \sum_{u,v\epsilon E} du\sqrt{\frac{du}{dv}} + dv\sqrt{\frac{dv}{du}}$$

Definition 2.11 Symmetric Division Deg Index($SDD(G)$)[6] was defined as D.Vukicevic in 2010 by the order of its vertex degrees with the maximum degree and the minimum degree and is denoted as follows:

$$SDD(G) = \sum_{u,v\epsilon E}\frac{\max(du,dv)}{\min(du,dv)} + \frac{\min(du,dv)}{\max(du,dv)}$$

Based on the above fourteen degree-based topological indices, we computed twelve penicillin classes of drugs. Table 1 and its continuation show the values of fourteen topological indices with the chemical structures of the penicillin class of compounds. Table 2 shows the results of the properties.

Figure 1 Molecular structures of Penicillin class of drugs

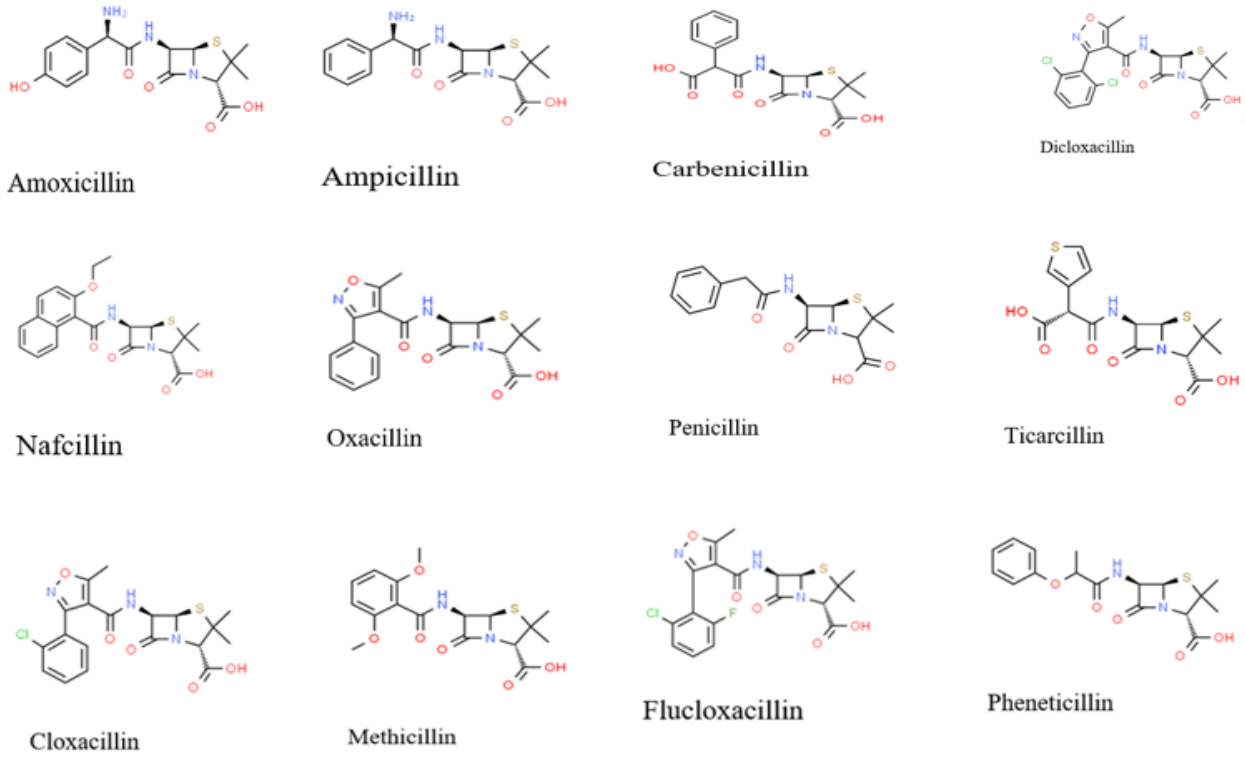

Table 1. It shows the calculated values of twelve Penicillin class of drugs with fourteen degree-based topological indices.

Penicillin class of drugs	$Az\ (G)$	$ABC(G)$	$GA(G)$	$H(G)$	$F(G)$	$M_1(G)$	$M_2(G)$

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Amoxicillin	209.9397	19.6809	25.5873	10.8857	390	138	168
Ampicillin	206.5647	18.8644	24.7615	10.5857	370	132	161
Carbenicillin	221.3303	20.3475	26.6277	11.4191	398	142	173
Dicloxacillin	276.1237	24.5956	32.3278	13.6571	504	176	221
Nafcillin	274.1024	22.8761	30.7981	13.0524	453	163	203
Oxacillin	239.522	22.3192	29.7213	12.5525	440	158	195
Penicillin	195.6454	18.2454	18.0254	10.0571	375	129	158
Ticarcillin	230.7237	21.1999	27.2766	11.5237	448	158	190
Cloxacillin	267.3487	23.9189	31.3298	13.1237	498	172	215
Methicillin	230.5803	21.5430	26.7407	11.5525	398	142	175
Flucloxacillin	266.8772	23.8715	31.4533	13.2190	480	170	211
Phenethicillin	267.1741	19.4049	25.7213	11.0523	378	136	164

Table 1 continuation

Penicillin class of drugs	$M_3(G)$	$R(G)$	$S(G)$	$HM_1(G)$	$HM_2(G)$	$FR(G)$	$SDD(G)$
Amoxicillin	28	11.6308	11.9878	774	1326	159.0796	68.2500
Ampicillin	24	11.2370	11.6827	692	1177	150.0692	64.5822
Carbenicillin	26	12.1475	12.5909	744	1267	162.4651	69.9166
Dicloxacillin	34	14.5521	15.1634	946	1731	200.0976	84.5000
Nafcillin	25	13.6832	14.3792	859	1503	181.0681	76.0833
Oxacillin	26	13.2201	13.8936	830	1427	177.3061	74.9167
Penicillin	29	10.7570	11.1611	691	1212	150.9228	64.1666
Ticarcillin	32	12.4311	12.8607	828	1520	178.3217	75.6666
Cloxacillin	34	13.9867	14.6495	928	1671	197.7770	86.9998
Methicillin	26	12.2236	12.6400	748	1297	226.3317	68.5833
Flucloxacillin	30	14.0415	14.7101	902	1575	192.8531	81.5833
Phenethicillin	26	11.7201	12.1690	706	1168	126.4385	66.9167

Table 2. It shows the Penicillin class of drugs with their physicochemical properties

Penicillin class of drugs	Polarizability 10^{-24} cm^3	Log K_{ow}	Molar Volume	Molar Refractivity Cm^3	Log P	K_{oc}	Log k_{oc}

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Amoxicillin	36.3	0.97	236.2	91.5	0.61	865.5	115.7
Ampicillin	35.7	1.45	239.3	89.9	1.35	534.4	105.4
Carbenicillin	36.7	1.19	246.2	92.6	1.01	2169	113.0
Dicloxacillin	44	3.86	290.1	111.0	3.02	9004	106.5
Nafcillin	43.7	3.79	289.9	110.3	3.52	1448	109.6
Oxacillin	40.2	2.57	268.5	101.3	2.05	3294	105.8
Penicillin	34.2	1.85	235.2	86.3	1.67	421.4	102.5
Ticarcillin	36	1.01	236.4	90.7	0.69	1176	117.3
Cloxacillin	42.1	3.22	279.3	106.2	2.53	5446	106.2
Methicillin	37.4	2.20	262.6	94.4	1.27	50.31	99.3
Flucloxacillin	42.1	3.42	283.7	106.3	2.60	9004	104.4
Phenethicillin	36.7	2.29	258	92.7	2.22	292.3	104.0

3 Results and discussions

Part 1 Here, the indices are correlated with the penicillin class of drugs and are presented in table 3. High correlation coefficients are highlighted in the table and establish linear regression models for the highlighted values through QSPR analysis.

Table 3. It shows correlation coefficients between the physicochemical properties and indices.

Topological Index	Polarizability 10^{-24} cm^3	Log K_{ow}	Molar Volume	Molar Refractivity Cm^3	Log P	K_{oc}	Log K_{oc}
$A_Z(G)$	**0.8566**	**0.8404**	**0.8952**	**0.8593**	**0.8155**	0.6169	0.4897
$ABC(G)$	**0.9277**	0.7935	**0.8844**	**0.9271**	0.6491	**0.8135**	0.6709
$GA(G)$	**0.8885**	0.6753	**0.8268**	**0.8870**	0.5719	0.7057	0.6488
$H(G)$	**0.9694**	0.8373	**0.9242**	**0.9689**	0.7335	**0.8078**	0.7167
$F(G)$	**0.8664**	0.7263	0.7783	**0.8649**	0.6091	**0.8376**	0.7799
$M_1(G)$	**0.8959**	0.7408	**0.8129**	**0.8945**	0.6294	**0.8210**	0.7708
$M_2(G)$	**0.9201**	0.7798	**0.8430**	**0.9188**	0.6663	**0.8342**	0.7670
$M_3(G)$	0.3654	0.3021	0.2720	0.3646	0.1785	0.6449	0.5569
$R(G)$	**0.9558**	**0.8160**	**0.9023**	**0.9552**	0.7055	**0.8289**	0.7370
$S(G)$	**0.9623**	**0.8299**	**0.9110**	**0.9617**	0.7266	**0.8243**	0.7421

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$HM_1(G)$	**0.8841**	0.7133	0.7795	**0.8824**	0.5902	**0.8320**	0.7847
$HM_2(G)$	**0.8264**	0.6630	0.7121	**0.8243**	0.5353	**0.8024**	0.7524
$FR(G)$	0.5563	0.4655	0.5608	0.5557	0.2305	0.4579	0.1602
$SDD(G)$	**0.8508**	0.7016	0.7663	**0.8495**	0.5841	**0.8378**	0.7868

Part 2 In this section, suitable linear regression[8] models(based on the highlighted values of table 3) of fourteen topological indices, and physicochemical properties of twelve penicillin class of drugs are established.

Linear regression models(QSPR analysis)

Linear regression model N = n(Topological index) + n°

where N = physical property, *TI* = Topological index, n = slope & n° = intercept.

Using this, we obtained the following.

1. **Augmented Zagreb Index**
   Polarizability = 0.1021($Az(G)$) + 14. 212
   Log Kow = 0.0309 ($Az(G)$) – 5.1145
   Molar Volume = 0.6717 ($Az(G)$) + 98.9103
   Molar Refractivity = 0.2591($Az(G)$) + 35.4633
   Log P = 0.0263($Az(G)$) – 4.4479
2. **Atom Bond Index**
   Polarizability = 1.4956($ABC(G)$) + 6.7448
   Molar Volume = 8.9797 ($ABC(G)$) + 68.2343
   Molar Refractivity = 3.78171($ABC(G)$) + 16.8166
   Koc = 1244.774 ($ABC(G)$) – 23836.4
3. **Geometric-Arithmetic Index**
   Polarizability = 0.7673($GA(G)$) + 17.6341
   Molar Volume = 4.4964 ($GA(G)$) + 136.6615
   Molar Refractivity = 1.9381($GA(G)$) + 44.4099
4. **Harmonic Index**
   Polarizability = 0.7677($H(G)$) + 17.6341
   Molar Volume = 4.4964 ($H(G)$) + 136.6615
   Molar Refractivity = 7.1243($H(G)$) + 13.0583
   Koc = 2228.133 ($H(G)$) – 23683.4
5. **Forgotten Index**
   Polarizability = 0.0608($F(G)$) + 12.7484
   Molar Refractivity = 0.1536($F(G)$) + 32.0659
   Koc = 55.8028 ($F(G)$) – 21056.3
6. **First Zagreb Index**
   Polarizability = 0.1847($M_1(G)$) + 10.8079
   Molar Volume = 1.0553 ($M_1(G)$) + 100.7412
   Molar Refractivity = 0.4666($M_1(G)$) + 27.1598
   Koc = 160.6362 ($M_1(G)$) – 20500.9

7. **Second Zagreb Index**
   Polarizability = 0.1406($M_2(G)$) + 12.5793
   Molar Volume = 0.8114 ($M_2(G)$) + 109.4039
   Molar Refractivity = 0.3553($M_2(G)$) + 31.6220
   Koc = 120.9964 ($M_2(G)$) – 19716.7

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8. **Randic Index**
   Polarizability = 2.6713($R(G)$) + 5.0046
   Log Kow = 0.7039 ($R(G)$) – 6.5758
   Molar Volume = 15.8801 ($R(G)$) + 59.7903
   Molar Refractivity = 6.7561($R(G)$) + 12.4161
   Koc = 2198.565($R(G)$) – 24972.1
9. **Sum Connectivity Index**
   Polarizability = 2.6713($S(G)$) + 5.0046
   Log Kow = 0.6561 ($S(G)$) – 6.3137
   Molar Volume = 14.694 ($S(G)$) + 67.111
   Molar Refractivity = 6.2326($S(G)$) + 15.763
   Koc = 2003.8($S(G)$) – 23556
10. **First Hyper Zagreb Index**
    Polarizability = 0.0333($HM_1(G)$) + 11.9924
    Molar Refractivity = 0.0841($HM_1(G)$) + 30.1714
    Koc = 29.7338(HM_1(G)) – 21097.2
11. **Second Hyper Zagreb Index**
    Polarizability = 0.0147($HM_2(G)$) + 18.0735
    Molar Refractivity = 0.0371($HM_2(G)$) + 45.5608
    Koc = 13.5559($HM_2(G)$) – 16253.1
12. **Symmetric Division Deg Index**
    Polarizability = 0.0147($HM_2(G)$) + 18.0735
    Molar Refractivity = 0.0371($HM_2(G)$) + 45.5608
    Koc = 13.5559($HM_2(G)$) – 16253.1

The above twelve indices are highly correlated with some specific physicochemical properties of the Penicillin class of compounds (Polarizability, Log Octanol-Water Partition Coefficient (Log K_{ow}), Molecular Volume, Molar Refractivity, Log P, Soil Absorption Coefficient (Koc), Log Koc).

Hence, the QSPR analysis is done with the specific properties. The third Zagreb index and the FORAN index have moderately correlated properties. Geometric-Arithmetic index, Harmonic index, Randic index, and Sum Connectivity index have a very high correlation with the properties, especially with Polarizability and Molecular Refractivity that are underlined and highlighted in table 3. Figures 2 to 6 give a piece of solid information regarding this.

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Figure 2 shows the correlation of $H(G)$

With Polarizability of Penicillin class of compounds.

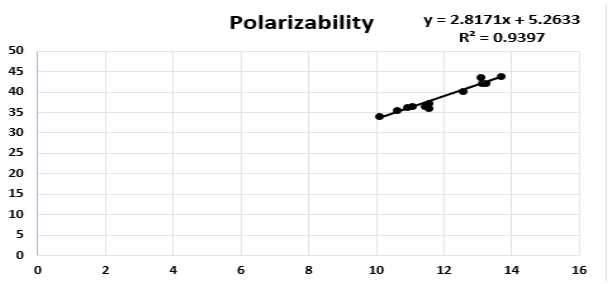


Figure 3 shows the correlation of $H(G)$

With Molar Refractivity of Penicillin class of compounds.

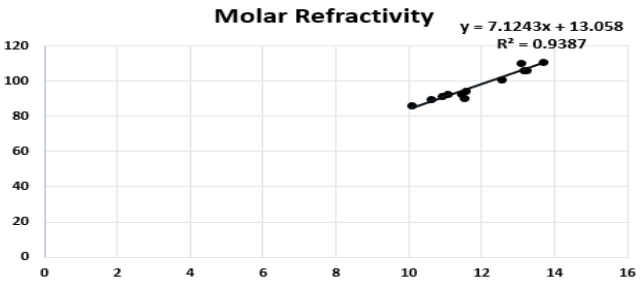


Figure 4 shows the correlation of $R(G)$

With Polarizability of Penicillin class of compounds.

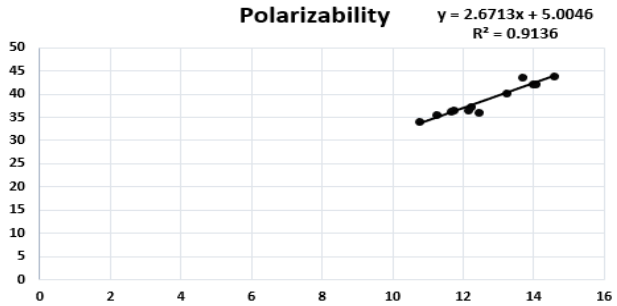


Figure 5 shows the correlation of $S(G)$

With Polarizability of Penicillin class of compounds.

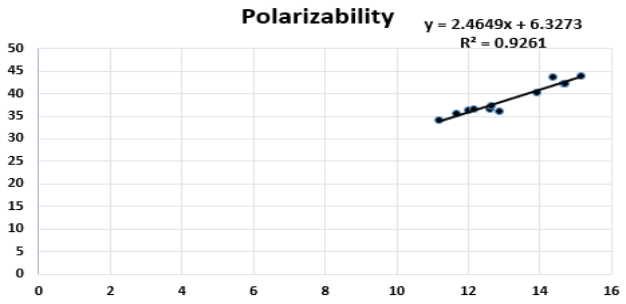
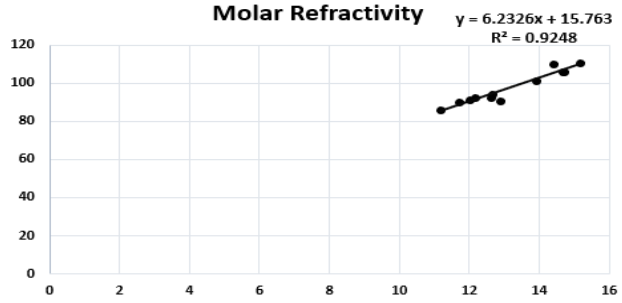


Figure 6 shows the correlation of $S(G)$

With Molar Refractivity of Penicillin class of compounds.



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Conclusion In this paper, a QSPR analysis was established between fourteen degree-based topological indices and twelve penicillin classes of drugs for the suitable pairs (topological index, property). In the field of pharmaceutical sciences, the properties of chemical compounds are very much required to establish new products. Instead of spending time, space for laboratory work, and the cost of research, topological indices are good alternators without these requirements. This theoretical approach obtained in this paper has promising aspects in designing new drugs.

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