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QSPR Study of Anti-Hepatitis Drugs using Degree-Based Topological Indices

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Abstract

Topological indices provide an effective approach to relate molecular structure with the physicochemical properties of pharmaceutical compounds. In this study, selected anti-hepatitis drugs are modelled as molecular graphs, where atoms and bonds are characterized as vertices and edges, respectively. Anti-hepatitis drugs are widely used in the treatment and management of viral hepatitis, and understanding their structural behaviour is important for predicting their physicochemical characteristics. Five degree-based topological descriptors are computed and utilized for quantitative structure–property relationship (QSPR) analysis. The correlations between these indices and selected physicochemical properties, including boiling point (BP), surface tension (ST), index of refraction (IR), molar refractivity (MR), and polar surface area (PSA), are examined. The results indicate that three of the five descriptors exhibit strong positive correlations with BP, MR, and PSA, whereas the remaining two descriptors show comparatively weaker relationships with these physicochemical properties. These findings demonstrate the effectiveness of selected topological descriptors in predicting physicochemical behavior and highlight the applicability of graph-theoretical methods in pharmaceutical research.

Keywords: QSPR, Topological Indices, Anti-Hepatitis Drugs, Molecular Graphs, Physicochemical Properties.

Introduction

Viral hepatitis is a major global public health concern caused by a variety of factors, including viral infections, chemical exposure, drug-induced toxicity, and excessive alcohol consumption. The disease is primarily associated with hepatitis viruses A, B, C, D, and E, each differing in transmission mechanisms and clinical manifestations. Hepatitis A and E are generally transmitted through contaminated food and water, whereas Hepatitis B, C, and D are mainly spread through infected blood, unsafe injections, and other percutaneous exposures. Despite significant advances in medical science, viral hepatitis continues to affect millions of people worldwide and remains a serious healthcare challenge, particularly in developing countries[1].

Graph theory has emerged as an important branch of mathematics with extensive applications in chemistry, biology, computer science, communication networks, and pharmaceutical sciences[2]. The introduction of the Wiener index by Wiener in 1947 marked the beginning of the use of graph-theoretical descriptors in chemistry and laid the foundation for modern Chemical Graph Theory[3]. Subsequently, numerous mathematical and chemical concepts were developed to relate molecular structures with their physicochemical and biological properties[4,5].

With the rapid advancement of computational techniques, Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies have become indispensable tools in pharmaceutical research. These methods establish mathematical relationships between molecular structures and experimentally observed properties, thereby reducing the time, cost, and effort associated with laboratory investigations[6-10]. Numerous studies have demonstrated that the topological structure of a molecule is closely associated with its physical, chemical, and biological characteristics, such as boiling point, surface tension, molar refractivity, and biological activity.

Topological indices are numerical descriptors derived from molecular graphs and play a significant role in theoretical and computational chemistry. Depending on the structural information employed, these indices may be classified as degree-based, distance-based, eigenvalue-based, and neighborhood-based descriptors. Among these, degree-based topological indices have attracted considerable attention because of their computational simplicity and strong predictive capability. Classical descriptors such as the Wiener, Zagreb, Randić, Atom-Bond Connectivity (ABC), and Geometric-Arithmetic (GA) indices have been successfully applied to investigate a wide range of chemical compounds and pharmaceutical molecules.

Recent research has highlighted the effectiveness of topological indices in predicting the physicochemical properties of biologically active compounds and therapeutic drugs. Applications include antiviral agents, anti-hepatitis drugs, anticancer compounds, and other pharmaceutical molecules, where significant correlations have been observed between molecular descriptors and experimentally determined properties[11-17]. In particular, QSPR studies involving anti-

hepatitis drugs have demonstrated the usefulness of degree-based topological indices and regression techniques for estimating important physicochemical parameters[18-21].

In addition to pharmaceutical applications, several graph-theoretical descriptors have been investigated for various graph classes, including tensor products of graphs, ξ-graphs, graphene structures, and derived graphs of biologically important compounds[22-25]. These studies further demonstrate the versatility of topological methods and motivate the development of new descriptors for molecular characterization and property prediction.

Motivated by these developments, the present work focuses on the QSPR analysis of a collection of anti-hepatitis drugs using the Veerabhadraiah-Lokesha (VL) index and its derived forms[26]. The molecular structures of the selected anti-hepatitis drugs are converted into graph representations, and their corresponding topological descriptors are computed.

Correlation and regression analyses are then employed to investigate the relationships between the computed indices and selected physicochemical properties. The findings provide valuable insights into the structural behavior of anti-hepatitis drugs and further demonstrate the effectiveness of graph-theoretical descriptors in QSPR modelling.

Materials and Methods

A set of sixteen anti-hepatitis drugs, namely Baraclude, Acetaminophen, Glecaprevir, Daclatasvir, Adefovir Dipivoxil, Epivir-HBV, Morphothiadin, Sofosbuvir, Pibrentasvir, Ritonavir, Ombitasvir, Ribavirin, Telbivudine, Tenofovir alafenamide, Voxilaprevir, and Velpatasvir, is considered for the present study. The molecular structures of these drugs are represented as molecular graphs, where atoms correspond to vertices and chemical bonds correspond to edges. Five physicochemical properties, namely boiling point (BP), surface tension (ST), index of refraction (IR), molar refractivity (MR), and polar surface area (PSA), are selected for analysis because of their significance in understanding the physical and pharmacological behavior of drug molecules.

In the present study, the Veerabhadraiah-Lokesha (VL) index and its associated variants $VL(G)$, $\sqrt{VL(G)}$, $[VL(G)]^2$, $\frac{1}{VL(G)}$, and $\frac{1}{\sqrt{VL(G)}}$ are employed as molecular descriptors. Initially introduced by Deepika[26], the VL index has shown promising applicability in the structural characterization of graphs.

Similar graph-theoretical approaches have also been utilized in the study of ξ-graphs, graphene structures, anticancer drugs, and triglyceride-derived molecular graphs. Owing to its enhanced discriminatory capability, the VL index serves as a useful complement to classical descriptors such as the Wiener index and related topological measures.

A QSPR analysis is performed to investigate the relationship between the computed topological descriptors and the selected physicochemical properties.

For a simple graph G with vertex set V(G) and edge set E(G), the VL index is defined by

$$\mathrm{VL(G)} = \frac{1}{2}\sum[\mathrm{d_m} + \mathrm{d_n} + 4] \quad (1)$$

where $\mathrm{d_m} = \mathrm{d_u} + \mathrm{d_v} - 2$ and $\mathrm{d_n} = (\mathrm{d_u} * \mathrm{d_v}) - 2$.

Correlation analysis is performed to examine the strength and direction of the relationship among the variables. Further, linear regression models are developed to study the dependence of physicochemical properties on the selected topological indices and to evaluate their predictive capability.

All statistical computations, including correlation coefficients and regression analysis, are carried out using Google Sheets.

Results and Discussion

In this section, the dataset and computed topological indices are first presented, followed by an analysis of their correlations with selected physicochemical properties. Subsequently, the predictive performance of the proposed models is evaluated through a comparison of observed and estimated values.

Dataset Description and Correlation Analysis of $VL(G)$and Its Derived Forms: Table-1 summarizes the physicochemical properties of the selected drugs, which were extracted from published literature sources, including the study by Mahboob et al[1]. and supplemented with data retrieved from ChemSpider. Table-2 presents the computed values of $VL(G)$and its transformed forms used as structural descriptors. Based on these, Table-3 examines the correlation between the indices and the properties. The analysis reveals that $VL(G)$, $\sqrt{VL(G)}$, and $[VL(G)]^2$ show strong positive correlations with BP, MR, and PSA, whereas the inverse forms exhibit negative correlations. These results confirm the effectiveness of the proposed indices in describing and predicting the physicochemical behavior of the compounds.

The computed correlation coefficients between the selected topological indices and physicochemical properties of anti-hepatitis drugs are presented in Table-3. The analysis reveals that the indices VL(G), $\sqrt{\mathrm{VL(G)}}$, and $[\mathrm{VL(G)}]^2$exhibit strong positive correlations with boiling point (BP), molar refractivity (MR), and polar surface area (PSA).

In particular, VL(G) shows a strong correlation with BP (r=0.858), MR (r=0.9573), and PSA (r=0.843), indicating its effectiveness in predicting these properties. Similarly, $\sqrt{\mathrm{VL(G)}}$ shows strong positive correlations with BP (r=0.8482), MR (r=0.9528), and PSA (r=0.8705), indicating its reliability in predicting these physicochemical properties.

Likewise, $[VL(G)]^2$ also exhibits notable positive correlations with BP ($r = 0.8538$), MR ($r = 0.9263$), and PSA ($r = 0.7729$), demonstrating that this derived form consistently captures the structural influence on these properties.

On the other hand, surface tension (ST) and index of Refraction (IR) properties show weak to moderate negative correlations with these indices, suggesting that these properties are less dependent on the selected topological descriptors. The reciprocal indices $\frac{1}{VL(G)}$ and $\frac{1}{\sqrt{VL(G)}}$ exhibit negative correlations with BP, MR, and PSA, indicating an inverse relationship.

Regression Analysis and Comparison of Observed and Predicted Values: Table-4 to 6 present the observed, predicted, and residual values based on VL(G), $\sqrt{VL(G)}$, and $[VL(G)]^2$, respectively. Among these, Table-5 shows the strong consistency with minimal residuals, indicating superior predictive accuracy, followed by Table-4, while Table-6 exhibits comparatively larger deviations. Overall, the $\sqrt{VL(G)}$ model demonstrates the highest consistency and reliability.

Regression Model Interpretation of [VL(G)]

BP = 327.6576 + 1.8992 [VL(G)] (2)

MR = 8.7050 + 0.5724 [VL(G)] (3)

PSA = 83.4309 + 0.2894 [VL(G)] (4)

Figure-1 presents the correlations between $VL(G)$ and the selected physicochemical properties of anti-hepatitis drugs. The statistical results indicate that $VL(G)$ has a strong positive influence on BP, MR, and PSA, as reflected by high correlation coefficients (r>0.84). The model explains a substantial portion of variance, with $R^2 = 0.7364$ for BP and $R^2 = 0.7109$ for PSA, indicating good predictive capability, while MR shows an excellent fit R^2=0.9165. The slope coefficients further confirm that each unit increase in $VL(G)$ leads to a consistent rise in these properties. Although some residual deviations exist, the overall statistical evidence supports the suitability of $VL(G)$ as a reliable descriptor, particularly for MR.

Table-1: Physicochemical properties of anti-hepatitis medications.

Drugname	IR	BP	Surface Tension	MR	PSA (Å²)
Baraclude	1.837	-	84.2±7	67.6±0.5	126
Acetaminophen	1.619	387.8±25	52.8±3	42.4±0.3	49
Glecaprevir	1.610	-	64.6±5	198.2±0.4	204
Daclatasvir	1.595	1071.2±65	55.4±3	200.8±0.3	175
Adifovir Dipivoxil	1.569	641.0±65	51.2±7	121.0±0.5	-
Epivir-HBV	1.755	475.4±55	79.3±7	54.1±0.5	113
Morphothiadin	1.678	577.2±60	54.0±7	120.9±0.5	104
Sofosbuvir	1.573	-	58.7±5	123.5±0.4	163
Pibrentasvir	1.614	-	57.6±3	284.5±0.3	200
Ritonavir	1.600	947.0±65	53.7±3	198.9±0.3	202
Ombitasvir	1.595	1065.6±65	54.3±3	248.1±0.3	179
Ribavirin	1.837	639.8±65	106.8±7	51.1±0.5	144
Telbivudine	1.619	-	62.3±3	55.8±0.3	99
Tenofovir alafenamide	1.610	640.4±65	55.1±7	121.8±0.5	153
Voxilaprevir	1.595	-	61.5±5	207.5±0.4	204
Velpatasvir	1.569	-	60.1±3	-	193

Table-2: TI Values of *VL(G)* and its transformed forms.

Name of Medicine	VL(G)	$\sqrt{VL(G)}$	$[VL(G)]^2$	$\frac{1}{VL(G)}$	$\frac{1}{\sqrt{VL(G)}}$
Baraclude	122.5	11.06797	15006.25	0.008163	0.090351
Acetaminophen	51.5	7.17635	2652.25	0.019417	0.139347
Glecaprevir	356	18.86796	126736	0.002809	0.053
Daclatasvir	313.5	17.70593	98282.25	0.00319	0.056478
Adifovir Dipivoxil	183	13.52775	33489	0.005464	0.073922
Epivir-HBV	82	9.055385	6724	0.012195	0.110432
Morphothiadin	180.5	13.43503	32580.25	0.00554	0.074432
Sofosbuvir	168.5	12.98075	28392.25	0.005935	0.077037
Pibrentasvir	484.5	22.01136	234740.3	0.002064	0.045431
Ritonavir	264	16.24808	69696	0.003788	0.061546
Ombitasvir	368.5	19.19635	135792.3	0.002714	0.052093
Ribavirin	96.5	9.823441	9312.25	0.010363	0.101797
Telbivudine	96	9.797959	9216	0.010417	0.102062
Tenofoviral afenamide	301.5	17.36376	90902.25	0.003317	0.057591
Voxilaprevir	365.5	19.11805	133590.3	0.002736	0.052307
Velpatasvir	399.5	19.9875	159600.3	0.002503	0.050031

Table-3: Correlation of various physicochemical parameters with *VL(G)* and its variants.

Drugs/TI	PSA	BP	Surface Tension	IR	MR
VL(G)	0.843	0.858	-0.4027	-0.5328	0.9573
$\sqrt{VL(G)}$	0.8705	0.8482	-0.4162	-0.5421	0.9528
$[VL(G)]^2$	0.7729	0.8538	-0.3458	-0.4765	0.9263
$\frac{1}{VL(G)}$	-0.8824	-0.7603	0.3120	0.4226	-0.8163
$\frac{1}{\sqrt{VL(G)}}$	-0.8936	-0.7978	0.3736	0.4883	-0.8824

Table-4: Observed, Predicted, and Residual Values of BP, MR, and PSA Based on $VL(G)$.

VL(G)	BP (observed)	BP (predicted)	BP Residual	MR (observed)	MR (predicted)	MR Residual	PSA (observed)	PSA (predicted)	PSA Residual
122.50	-	-	-	67.60	78.82	-11.22	126.00	118.89	7.11
51.50	387.80	425.47	-37.67	42.40	38.18	4.22	49.00	98.34	-49.34
356.00	-	-	-	198.20	212.48	-14.28	204.00	186.47	17.53
313.50	1071.20	923.07	148.13	200.80	188.15	12.65	175.00	174.16	0.84
183.00	641.00	675.22	-34.22	121.00	113.45	7.55	-	-	-
82.00	475.40	483.39	-7.99	54.10	55.64	-1.54	113.00	107.16	5.84
180.50	577.20	670.47	-93.27	120.90	112.02	8.88	104.00	135.67	-31.67
168.50	-	-	-	123.50	105.15	18.35	163.00	132.20	30.80
484.50	-	-	-	284.50	286.03	-1.53	200.00	223.66	-23.66
264.00	947.00	829.05	117.95	198.90	159.82	39.08	202.00	159.84	42.16
368.50	1065.60	1027.52	38.08	248.10	219.63	28.47	179.00	190.08	-11.08
96.50	639.80	510.93	128.87	51.10	63.94	-12.84	144.00	111.36	32.64
96.00	-	-	-	55.80	63.66	-7.86	99.00	111.22	-12.22
301.50	640.40	900.28	-259.88	121.80	181.28	-59.48	153.00	170.69	-17.69
365.50	-	-	-	207.50	217.92	-10.42	365.50	204.00	189.21
399.50	-	-	-	-	-	-	193.00	199.06	-6.06

Table-5: Observed, Predicted, and Residual Values of BP, MR, and PSA Based on $\sqrt{VL(G)}$.

$\sqrt{VL(G)}$	BP (observed)	BP (predicted)	BP Residual	MR (observed)	MR (predicted)	MR Residual	PSA (observed)	PSA (predicted)	PSA Residual
11.07	-	-	-	67.60	82.92	-15.32	126.00	120.22	5.78
7.18	387.80	389.21	-1.41	42.40	18.32	24.08	49.00	86.26	-37.26
18.87	-	-	-	198.20	212.38	-14.18	204.00	188.31	15.69
17.71	1071.20	914.85	156.35	200.80	193.10	7.70	175.00	178.16	-3.16
13.53	641.00	706.27	-65.27	121.00	123.75	-2.75	-	-	-
9.06	475.40	483.01	-7.61	54.10	49.51	4.59	113.00	102.66	10.34
13.44	577.20	701.64	-124.44	120.90	122.21	-1.31	104.00	140.88	-36.88
12.98	-	-	-	123.50	114.67	8.83	163.00	136.92	26.08
22.01	-	-	-	284.50	264.56	19.94	200.00	215.74	-15.74
16.25	947.00	842.07	104.93	198.90	168.90	30.00	202.00	165.44	36.56
19.20	1065.60	989.25	76.35	248.10	217.83	30.27	179.00	191.17	-12.17
9.82	639.80	521.35	118.45	51.10	62.26	-11.16	144.00	109.36	34.64
9.80	-	-	-	55.80	61.84	-6.04	99.00	109.14	-10.14
17.36	640.40	897.76	-257.36	121.80	187.42	-65.62	153.00	175.18	-22.18
19.12	-	-	-	207.50	216.53	-9.03	204.00	190.49	13.51
19.99	-	-	-	-	-	-	193.00	198.08	-5.08

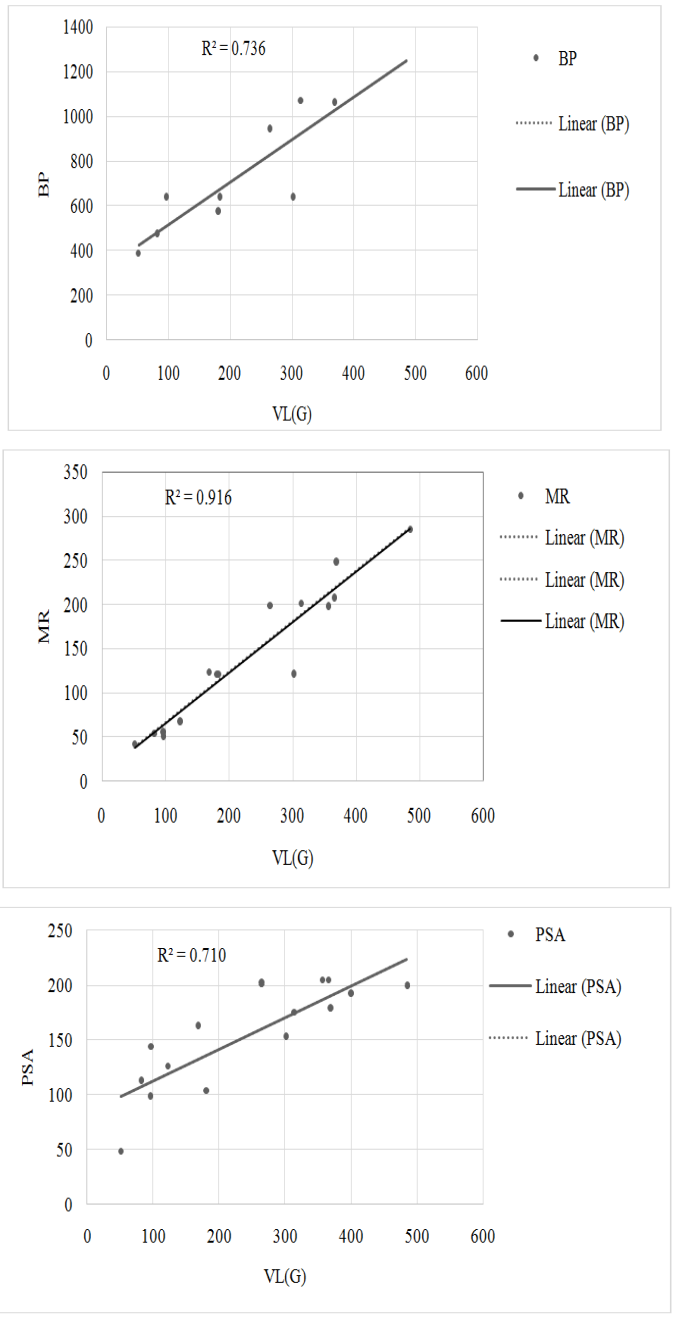


Figure-1: Linear Regression of VL(G) with physicochemical properties of anti-hepatitis drugs.

Regression Model Interpretation of $\sqrt{VL(G)}$.

$$PSA = 23.6177 + 8.7284\sqrt{VL(G)} \quad (5)$$

$$MR = -100.7891 + 16.5981\sqrt{VL(G)} \quad (6)$$

$$BP = 30.9607 + 49.9203\sqrt{VL(G)} \quad (7)$$

Figure-2 presents the correlations between $\sqrt{VL(G)}$ and the selected physicochemical properties of anti-hepatitis drugs. The regression analysis (Table-5) indicates that $\sqrt{VL(G)}$ exhibits a strong positive linear relationship with PSA ($r = 0.8705$, $R^2 = 0.7575$), MR ($r = 0.9528$, $R^2 = 0.9078$), and BP ($r = 0.8482$, $R^2 = 0.7196$). These results suggest that a significant proportion of the variation in the respective properties is explained by the descriptor. Among the three models, MR demonstrates the highest correlation and predictive accuracy, followed by PSA and BP. Overall, $\sqrt{VL(G)}$ serves as a reliable and effective topological descriptor for modeling these physicochemical properties in QSPR analysis.

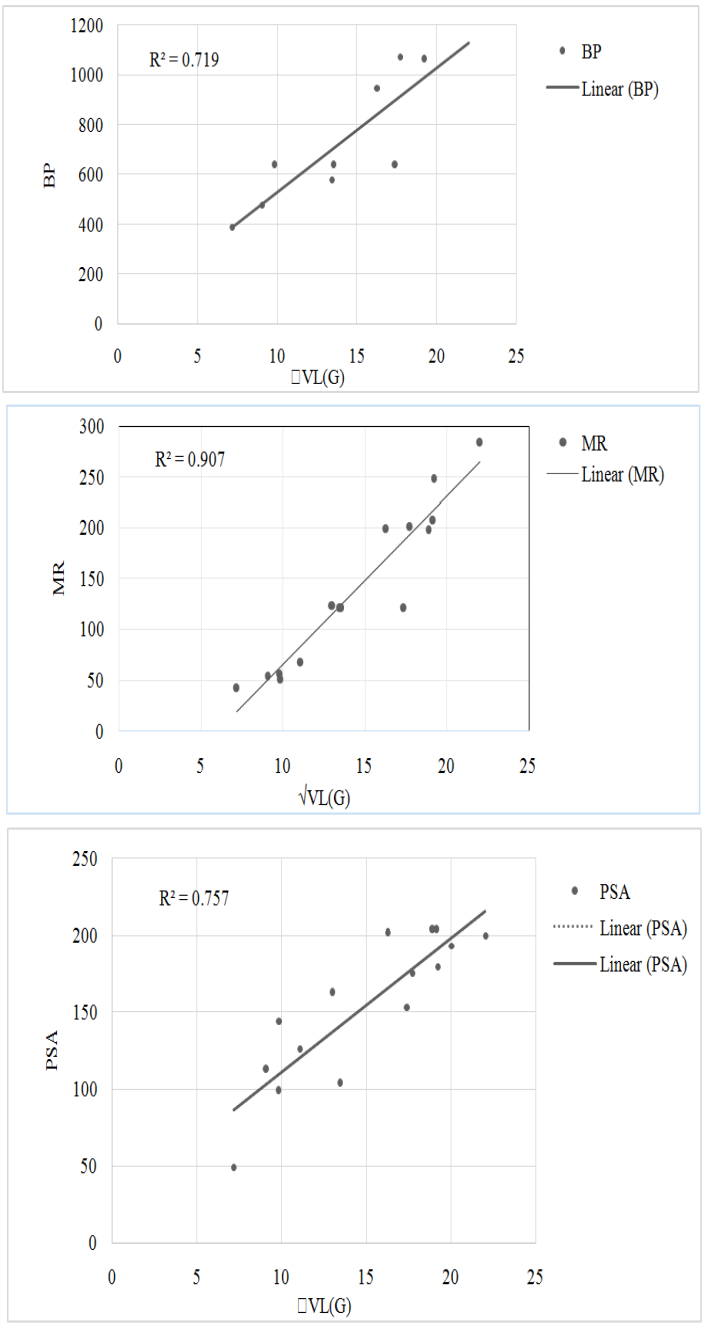


Figure-2: Linear Regression of $\sqrt{VL(G)}$ with physicochemical properties of anti-hepatitis drugs.

Table-6: Observed, Predicted, and Residual Values of BP, MR, and PSA Based on$[VL(G)]^2$.

$[VL(G)]^2$	BP (observed)	BP (predicted)	BP Residual	MR (observed)	MR (predicted)	MR Residual	PSA (observed)	PSA (predicted)	PSA Residual
15006.25	-	-	-	67.60	81.99	-14.39	126.00	121.79	4.21
2652.25	387.80	487.55	-99.75	42.40	68.64	-26.24	49.00	115.38	-66.38
126736	-	-	-	198.20	202.69	-4.49	204.00	179.71	24.29
98282.25	1071.20	919.44	151.76	200.80	171.95	28.85	175.00	164.96	10.04
33489	641.00	626.82	14.18	121.00	101.95	19.05	-	-	-
6724	475.40	505.94	-30.54	54.10	73.04	-18.94	113.00	117.49	-4.49
32580.25	577.20	622.71	-45.51	120.90	100.97	19.93	104.00	130.90	-26.90
28392.25	-	-	-	123.50	96.45	27.05	163.00	128.73	34.27
234740.3	-	-	-	284.50	319.36	-34.86	200.00	235.71	-35.71
69696	947.00	790.34	156.66	198.90	141.07	57.83	202.00	150.14	51.86
135792.3	1065.60	1088.85	-23.25	248.10	212.47	35.63	179.00	184.41	-5.41
9312.25	639.80	517.63	122.17	51.10	75.83	-24.73	144.00	118.84	25.16
9216	-	-	-	55.80	75.73	-19.93	99.00	118.79	-19.79
90902.25	640.40	886.11	-245.71	121.80	163.98	-42.18	153.00	161.14	-8.14
133590.3	-	-	-	207.50	210.09	-2.59	204.00	183.27	20.73
159600.3	-	-	-	-	-	-	193.00	196.75	-3.75

Regression Model Interpretation of $[VL(G)]^2$

PSA = 114.0085 + 0.0005[VL(G)]² (8)

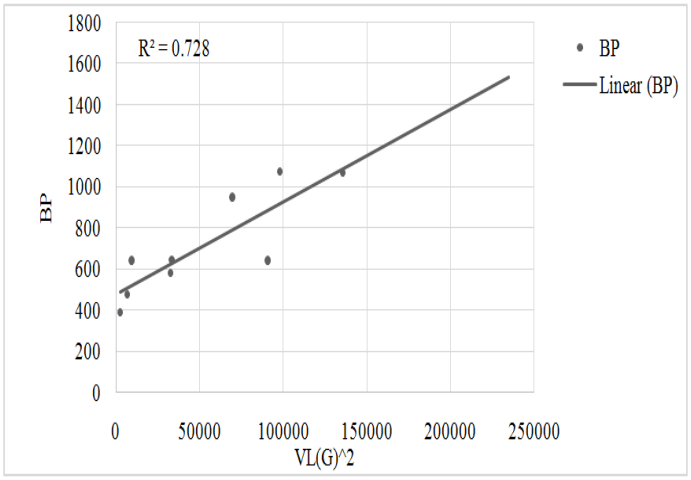
MR = 65.7737 + 0.0011 [VL(G)]² (9)

BP = 475.5716 + 0.0045[VL(G)]² (10)

Figure-3 illustrates the linear regression analysis of [VL(G)]² with the selected physicochemical properties of anti-hepatitis drugs. The regression analysis (Table-6) indicates that [VL(G)]² exhibits a positive linear relationship with PSA (r = 0.7729, R² = 0.5974), MR (r = 0.9263, R² = 0.8581), and BP (r = 0.8538, R² = 0.7289). These results suggest that a considerable proportion of the variation in the respective properties is explained by the descriptor. Among the three models, MR shows the highest correlation and predictive capability, followed by BP and PSA. The relatively small regression coefficients indicate that changes in the properties occur gradually with respect to [VL(G)]².

Overall, [VL(G)]² can be considered a useful descriptor, although its predictive strength is comparatively lower than that observed for $\sqrt{\text{VL(G)}}$.

By observing Table-4,5,6 it is evident that the predicted values of BP, MR, and PSA are generally close to the observed values, indicating a reasonable agreement and supporting the validity of the regression models. The residual values for MR are relatively small in most cases, confirming high prediction accuracy, whereas BP and PSA show comparatively larger deviations for a few compounds. Despite these variations, the overall trend demonstrates that the model performs satisfactorily, with better predictive consistency for MR than for BP and PSA.



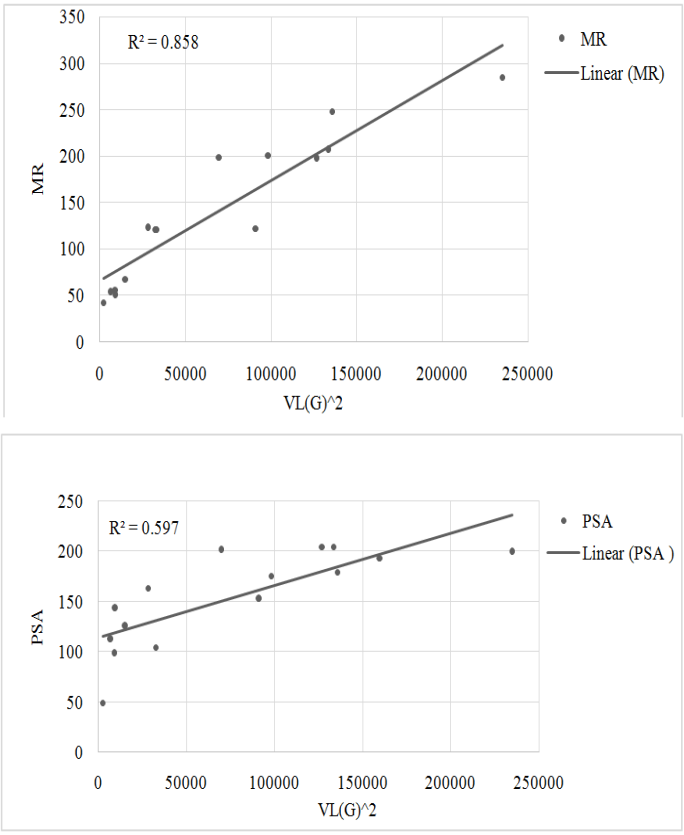


Figure-3: Linear Regression of $[VL(G)]^2$ with physicochemical properties of anti-hepatitis drugs.

Conclusion

In this study, a QSPR analysis of sixteen anti-hepatitis drugs was carried out using five degree-based topological descriptors: VL(G), $\sqrt{VL(G)}$, $[VL(G)]^2$, 1/VL(G), and $1/\sqrt{VL(G)}$. The correlation results presented in Table-3 indicate that VL(G), $\sqrt{VL(G)}$, and $[VL(G)]^2$ exhibit strong positive correlations with PSA, BP, and MR (r ranging from 0.7729 to 0.9573), whereas surface tension and IR show weak to moderate negative correlations. In contrast, the inverse descriptors 1/VL(G) and $1/\sqrt{VL(G)}$ display negative correlations with PSA, BP, and MR, and only weak positive correlations with surface tension and IR, highlighting their limited predictive relevance.

Comparative regression analysis further confirms that VL(G), $\sqrt{VL(G)}$, and $[VL(G)]^2$ are suitable for modelling PSA, BP, and MR. Among these, $\sqrt{VL(G)}$ demonstrates superior predictive performance with stronger correlations and improved agreement between observed and predicted values (Table-5), followed by VL(G) (Table-4). The $[VL(G)]^2$ model (Table-6), although statistically acceptable, shows comparatively lower predictive efficiency, particularly for PSA. Due to consistently weak and negative correlations, regression models were not developed for surface tension and IR.

Overall, the results establish $\sqrt{VL(G)}$ as the most effective descriptor for predicting the selected physicochemical properties, emphasizing the importance of appropriate descriptor transformation in enhancing QSPR model accuracy and reliability.

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