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Topological descriptor-driven prediction of physicochemical properties of COVID-19 drugs

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Abstract

The rapid development of computational approaches has significantly enhanced the prediction of molecular properties, reducing the dependence on extensive experimental investigations in drug discovery and pharmaceutical research. In this study, the predictive capability of the Veerabhadraiah-Lokesha (VL) index and its variants is investigated for a dataset of selected COVID-19 drugs. Five important physicochemical properties, namely boiling point, enthalpy, polar surface area, molar refractivity, and polarizability, are analyzed using correlation and simple linear regression techniques. The correlation analysis reveals that the VL index exhibits excellent positive correlations with boiling point ($R = 0.9930$) and enthalpy ($R = 0.9893$), while strong correlations are also observed for polar surface area ($R = 0.9000$), molar refractivity ($R = 0.8690$), and polarizability ($R = 0.8691$). Among the transformed descriptors, $[VL(G)]^2$ provides the strongest correlations with boiling point ($R = 0.9973$) and enthalpy ($R = 0.9949$), demonstrating enhanced predictive capability. The corresponding regression models further validate the effectiveness of the proposed descriptors for estimating the selected physicochemical properties. These findings establish the VL index and its variants as reliable degree-based molecular descriptors for QSPR modeling and highlight their potential utility in the computational analysis of COVID-19 drugs.

Keywords: COVID-19 drugs, QSPR, topological indices, molecular descriptors, correlation analysis, linear regression, physicochemical properties

1. Introduction

The emergence of Coronavirus Disease 2019 (COVID-19), caused by Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2), created a major global health emergency and placed an enormous burden on healthcare systems worldwide. Since it was first identified in late 2019, the virus has spread rapidly across countries, leading to widespread illness, significant mortality, and substantial social and economic disruption. These challenges have stimulated extensive scientific efforts to identify, develop, and evaluate effective therapeutic agents for the prevention and treatment of COVID-19. Although vaccination has substantially reduced disease severity, antiviral drugs continue to play an essential role in the treatment of infected patients, particularly those at high risk of developing severe complications. Consequently, understanding the molecular characteristics and physicochemical properties of COVID-19 drugs has become an aspect of pharmaceutical and medicinal chemistry^[1].

Physicochemical properties, including boiling point, enthalpy, polar surface area, molar refractivity, and polarizability, significantly influence the pharmacokinetic and pharmacodynamic behaviour of drug molecules. These properties affect molecular stability, solubility, membrane permeability, and biological activity, thereby contributing to the overall therapeutic performance of pharmaceutical compounds. Experimental determination of these properties is often expensive, labor-intensive, and time-consuming, motivating the development of reliable computational methods for their prediction^[2].

Graph-theoretical techniques have become valuable computational tools in mathematical chemistry by representing chemical compounds as molecular graphs, where vertices

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correspond to atoms and edges represent chemical bonds. Numerical quantities derived from these molecular graphs, known as topological indices, effectively encode structural information and have found extensive applications in QSPR and QSAR investigations [3, 6]. Such descriptors enable the prediction of physicochemical and biological properties directly from molecular structures, thereby reducing the need for extensive experimental measurements.

Among the numerous degree-based topological descriptors proposed in the literature, the Veerabhadrarajah-Lokesha (VL) index has attracted attention because of its ability to characterize molecular connectivity through vertex degrees [9]. In addition to the original descriptor, several transformed forms of the VL index have been explored to investigate their predictive capabilities in QSPR studies. Recent investigations have demonstrated the usefulness of degree-based descriptors for studying graphene, anticancer drugs, triglycerides, and other molecular systems [7, 8, 12, 19]. Evaluating the effectiveness of these descriptors for different classes of pharmaceutical compounds therefore remains an active area of research.

Motivated by these considerations, the present study investigates the applicability of the VL index and its variants for predicting the physicochemical parameters of selected COVID-19 drugs. Correlation analysis is employed to examine the relationships among the considered topological descriptors and five important physicochemical properties. Furthermore, simple linear regression models are developed to evaluate the predictive performance of these descriptors. The obtained results provide further evidence that the VL index and its transformed variants can serve as effective molecular descriptors for QSPR modelling and may

contribute to the computational characterization of COVID-19 drugs [1, 13, 16, 19].

2. Materials and Methods

This section describes the dataset of COVID-19 drugs, the mathematical formulation of the Veerabhadrarajah-Lokesha (VL) index and its transformed variants, and the statistical procedures adopted to investigate their applicability in QSPR and QSAR analysis. The physicochemical data were collected from chemical databases and published literature, while the statistical analyses were performed using correlation and regression techniques [1, 10, 13, 16, 20].

2.1 Dataset of COVID-19 Drugs

A dataset comprising eight clinically relevant COVID-19 drugs was selected to investigate the predictive capability of the Veerabhadrarajah-Lokesha (VL) index and its variants. The selected drugs include Lopinavir, Ritonavir, Arbidol, Thalidomide, Chloroquine, Hydroxychloroquine, Theaflavin, and Remdesivir. The corresponding physicochemical data were compiled from the ChemSpider database and published literature to ensure the accuracy and consistency of the analysis [1, 10].

Five physicochemical properties were considered in this investigation, namely boiling point (Bp), enthalpy (E), polar surface area (PSA), molar refractivity (MR), and polarizability (P). These properties are widely employed in Quantitative Structure-Property Relationship studies because of their importance in describing the physicochemical behaviour and molecular characteristics of pharmaceutical compounds [1, 13, 16, 19].

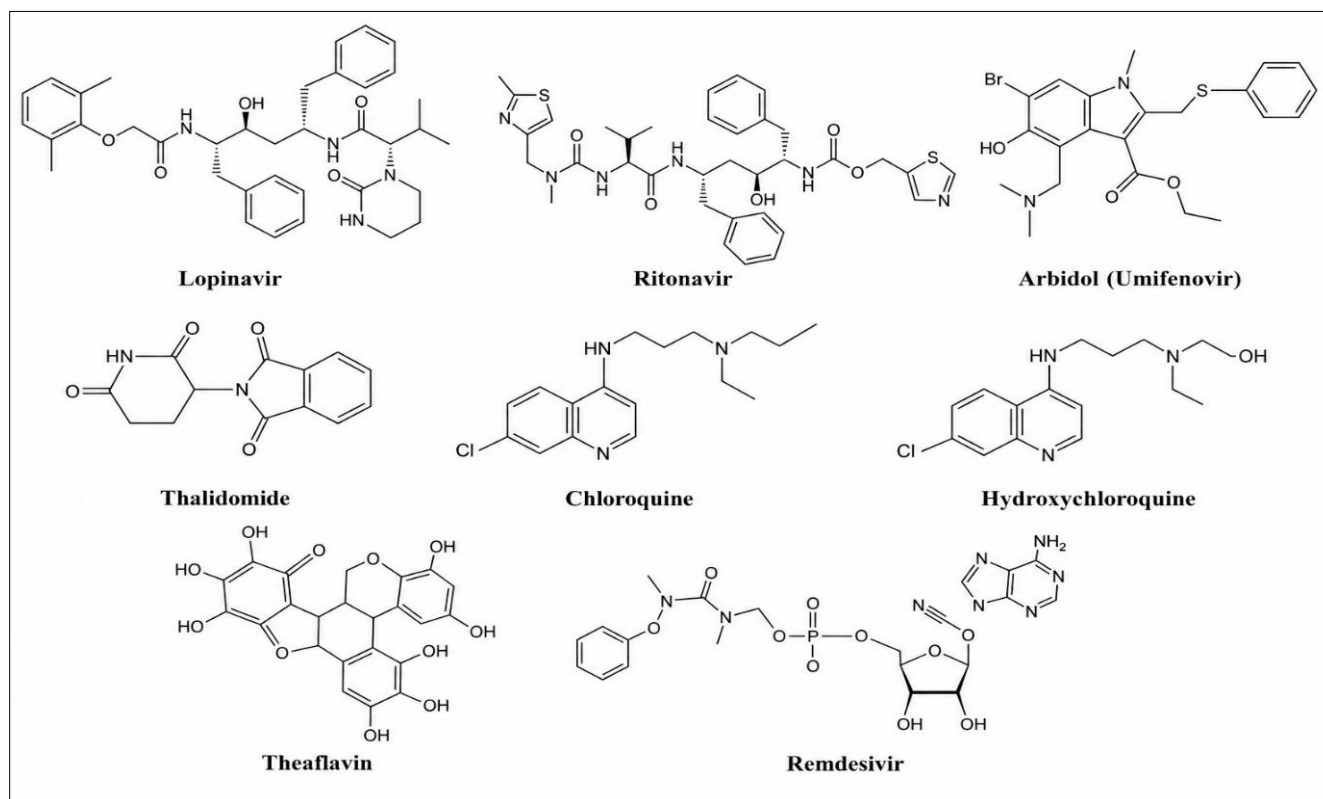


Fig 1: Molecular structures of the selected COVID-19 drugs.

2.2 Veerabhadrarajah-Lokesha Index

For a simple graph G with vertex set $V(G)$ and edge set $E(G)$, the VL index is defined by [9],

$$VL(G) = \frac{1}{2} \sum_{uv \in E(G)} [d(u) + d(v) + d(u)d(v)]$$

Where $d(u)$ corresponds to the degree of a vertex u of vertex set $V(G)$.

The transformed variants of the VL index considered in this study are $\sqrt{VL(G)}$, $[VL(G)]^2$, $1/VL(G)$, and $1/\sqrt{VL(G)}$. These transformed forms were included to examine whether mathematical transformations of the original descriptor improve its capability to model the selected physicochemical characteristics of COVID-19 drug molecules. Similar transformations of topological descriptors have been successfully employed in recent QSPR investigations involving pharmaceutical compounds [12-19].

The values of the VL index and its transformed variants computed for the selected COVID-19 drugs are presented in Table 2 and were subsequently used for correlation and regression analyses.

2.3 Statistical Analysis

The association between the selected topological descriptors and the physicochemical properties of the COVID-19 drug molecules was examined through Pearson's correlation analysis. Pearson's correlation coefficient (R) was employed to measure the strength and direction of the linear relationship between each topological descriptor and the corresponding physicochemical property. The resulting correlation coefficients were used to assess the predictive relevance of the descriptors and to identify those exhibiting the strongest associations with the selected properties and the associated physicochemical property [15, 19].

To evaluate the predictive capability of the descriptors, simple linear regression analysis was performed. The regression model is expressed as

$$A = c + dB$$

where A represents the physicochemical property, B denotes the topological descriptor, c is the intercept, and d is the regression coefficient.

The goodness-of-fit of each regression model was assessed using the coefficient of determination (R^2), Correlation coefficient (R), residual standard deviation (S_{res}), the F-statistic, and the associated p -value. These statistical measures were used to evaluate the accuracy, significance, and predictive performance of the developed linear models [13, 15, 19].

The correlation coefficients and regression analyses were computed using Google Sheets, and the resulting statistical parameters were employed to assess the predictive performance of the VL index and its transformed variants.

3. Results and Discussion

The physicochemical parameters of the selected COVID-19 drugs considered in this investigation are presented in Table 1. Five important physicochemical properties, namely boiling point (Bp), enthalpy (E), polar surface area (PSA), molar refractivity (MR), and polarizability (P), were selected to evaluate the predictive capability of the VL index and its transformed variants. The corresponding values of the VL(G) index and its transformed variants are listed in Table 2. These descriptors were subsequently employed to investigate their relationships with the selected physicochemical properties through correlation and regression analyses [1, 13, 15, 19].

Table 1: Physicochemical Parameters and Antiviral Potency of COVID-19 Drugs

Drugs	Bp	E	MR	PSA	P
Lopinavir	924.2	140.8	179.2	120	71.0
Ritonavir	947.0	144.4	198.9	202	78.9
Arbidol	591.8	91.5	121.9	80	48.3
Thalidomide	487.8	79.4	65.2	87	25.9
Chloroquine	460.6	72.1	97.4	28	38.6
Hydroxy-chloroquine	516.7	83.0	99.0	48	39.2
Theaflavin	1003.9	153.5	137.3	218	54.4
Remdesivir	-	-	149.5	213	59.3

Table 2: VL(G) and Its Variants for COVID-19 Drugs

Drugs	VL(G)	$\sqrt{VL(G)}$	$[VL(G)]^2$	$\frac{1}{VL(G)}$	$\frac{1}{\sqrt{VL(G)}}$
Lopinavir	242.5	15.57241	58806.25	0.004124	0.064216
Ritonavir	251.5	15.85875	63252.25	0.003976	0.063057
Arbidol	164.5	12.82576	27060.25	0.006079	0.077968
Thalidomide	115.5	10.74709	13340.25	0.008658	0.093048
Chloroquine	113	10.63015	12769	0.00885	0.094072
Hydroxy-chloroquine	117	10.81665	13689	0.008547	0.09245
Theaflavin	261	16.15549	68121	0.003831	0.061898
Remdesivir	236.5	15.37856	55932.25	0.004228	0.065026

3.1 Correlation Analysis

The Pearson correlation coefficients between the considered topological descriptors and the selected physicochemical parameters are presented in Table 3.

Table 3: Correlation Coefficients of TIs with Physicochemical Properties of COVID-19 Drugs

Physio-chemical properties/TI's	VL(G)	$\sqrt{VL(G)}$	$[VL(G)]^2$	$\frac{1}{VL(G)}$	$\frac{1}{\sqrt{VL(G)}}$
Bp	0.993	0.9886	0.9973	-0.9669	-0.9755
E	0.9893	0.9844	0.9949	-0.961	-0.9701
MR	0.869	0.8724	0.8581	-0.8737	-0.8747
PSA	0.90	0.8953	0.9059	-0.8746	-0.8824
P	0.8691	0.8725	0.8581	-0.8737	-0.8748

As shown in Table 3, the original VL(G) exhibits excellent positive correlations with boiling point ($R = 0.9930$) and enthalpy ($R = 0.9893$). Strong positive correlations are also observed for polar surface area ($R = 0.9000$), while molar refractivity ($R = 0.8690$) and polarizability ($R = 0.8691$) show satisfactory linear relationships. Among the transformed descriptors, $[VL(G)]^2$ provides the highest correlations with boiling point ($R = 0.9973$), enthalpy ($R = 0.9949$), and polar surface area ($R = 0.9059$). The reciprocal descriptors exhibit negative correlations because they are inversely related to the original VL(G) values [13, 15, 19].

3.2 Regression Analysis

To further investigate the predictive performance of the proposed topological descriptors, simple linear regression analysis was carried out between each descriptor and the selected physicochemical parameters of the COVID-19 drugs. The resulting regression equations, together with the associated statistical parameters, provide a quantitative assessment of the predictive capability of the considered descriptors.

3.2.1 Regression Analysis of VL(G) for Predicting the Physicochemical characteristics of COVID-19 Drugs

The linear regression model describing the relationship between the boiling point and the VL(G) index is given by

$$\text{Bp} = 73.9956 + 3.4894 \text{VL(G)}.$$

The regression model exhibits an excellent fit with a coefficient of determination of $R^2 = 0.9860$, indicating that 98.6% of the variation in boiling point is explained by the VL(G) index. The corresponding correlation coefficient ($R = 0.9930$) confirms a very strong positive linear relationship between the two variables. Furthermore, the regression model is statistically highly significant ($F(1,5) = 351.46, p < 0.001$), demonstrating the effectiveness of VL(G) in predicting the boiling point of the selected COVID-19 drugs. The regression equation relating enthalpy to VL(G) is

$$E = 17.6437 + 0.5069 \text{VL(G)}.$$

This model explains 97.9% of the observed variation in enthalpy ($R^2 = 0.9787$) and exhibits a very strong positive correlation ($R = 0.9893$). The corresponding F -statistic ($F(1,5) = 229.89, p < 0.001$) further confirms the statistical significance of the developed regression model.

The relationship between molar refractivity and VL(G) is represented by

$$\text{MR} = 22.1862 + 0.5800 \text{VL(G)}.$$

The model yields $R^2 = 0.7552$, indicating that 75.5% of the variation in molar refractivity is explained by VL(G). The positive correlation coefficient ($R = 0.8690$) and the significant F -statistic ($F(1,6) = 18.51, p = 0.005$) indicate a statistically meaningful linear relationship.

For polar surface area, the regression equation is

$$\text{PSA} = -69.6317 + 1.0343 \text{VL(G)}.$$

The resulting regression model explains 81.0% of the variability in polar surface area ($R^2 = 0.8100$) and exhibits a strong positive correlation ($R = 0.9000$). The model is statistically significant with $F(1,6) = 25.58$ and $p = 0.002$. The regression equation for polarizability is given by

$$P = 8.7845 + 0.2300 \text{VL(G)}.$$

The corresponding model accounts for 75.5% of the observed variation in polarizability ($R^2 = 0.7553$). The correlation coefficient ($R = 0.8691$) together with the F -statistic ($F(1,6) = 18.52, p = 0.005$) confirms that the regression model is statistically significant.

The corresponding regression plots illustrating the relationships between VL(G) and the physicochemical parameters of COVID-19 drugs are presented in Figure 2.

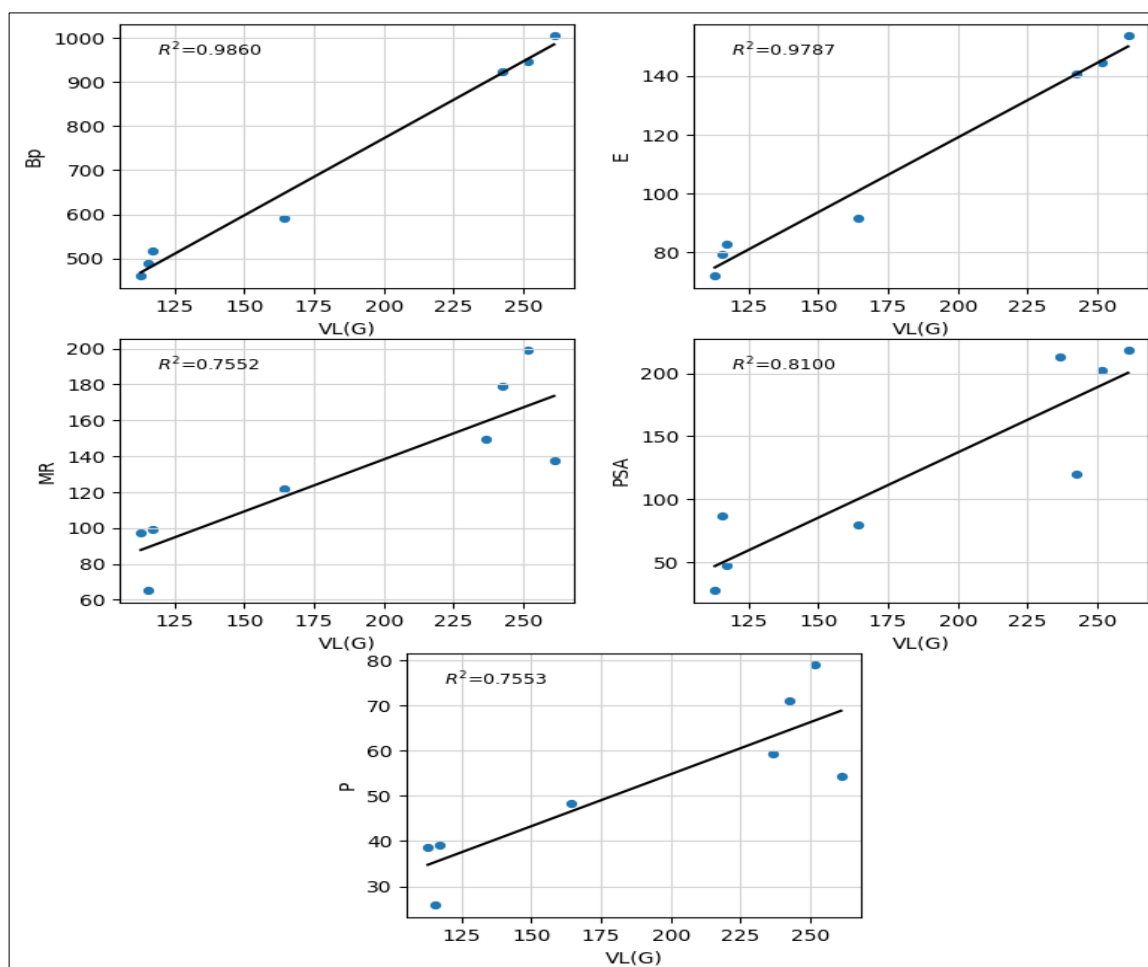


Fig 2: Regression plots of VL(G) and physicochemical parameters of COVID-19 drugs

Overall, the regression analysis demonstrates that the VL(G) index provides excellent predictive performance for boiling point and enthalpy, while yielding satisfactory predictive

accuracy for polar surface area, molar refractivity, and polarizability. These findings indicate that VL(G) is a reliable

degree-based molecular descriptor for QSPR analysis of the selected COVID-19 drugs.

3.2.2 Regression Analysis of $\sqrt{VL(G)}$ for COVID-19 Drugs

The linear regression model describing the relationship between the boiling point and $\sqrt{VL(G)}$ is given by

$$Bp = -522.8673 + 92.7806\sqrt{VL(G)}.$$

The model exhibits an excellent fit with $R^2 = 0.9774$, indicating that 97.7% of the variation in boiling point is explained by $\sqrt{VL(G)}$. The corresponding correlation coefficient ($R = 0.9886$) demonstrates a very strong positive linear relationship. Furthermore, the regression model is statistically highly significant ($F(1,5) = 216.06$, $p < 0.001$), confirming the effectiveness of the transformed descriptor in estimating the boiling point of the selected COVID-19 drugs.

The regression equation relating enthalpy to $\sqrt{VL(G)}$ is

$$E = -68.9472 + 13.4692\sqrt{VL(G)}.$$

This model explains 96.9% of the observed variation in enthalpy ($R^2 = 0.9690$) and exhibits a very strong positive correlation ($R = 0.9844$). The corresponding F -statistic ($F(1,5) = 156.18$, $p < 0.001$) further confirms the statistical significance of the regression model.

The relationship between molar refractivity and $\sqrt{VL(G)}$ is represented by

$$MR = -78.3303 + 15.5118\sqrt{VL(G)}.$$

The regression model yields $R^2 = 0.7611$, indicating that 76.1% of the variation in molar refractivity is explained by the transformed descriptor. The positive correlation coefficient ($R = 0.8724$) and the significant F -statistic ($F(1,6) = 19.12$, $p = 0.005$) demonstrate a statistically meaningful linear relationship.

For polar surface area, the regression equation is

$$PSA = -245.4633 + 27.4085\sqrt{VL(G)}.$$

The resulting model explains 80.2% of the variability in polar surface area ($R^2 = 0.8016$) and exhibits a strong positive correlation ($R = 0.8953$). The model is statistically significant with $F(1,6) = 24.23$ and $p = 0.003$.

The regression equation for polarizability is

$$P = -31.0701 + 6.1505\sqrt{VL(G)}.$$

The corresponding model accounts for 76.1% of the observed variation in polarizability ($R^2 = 0.7613$). The correlation coefficient ($R = 0.8725$) together with the F -statistic ($F(1,6) = 19.13$, $p = 0.005$) confirms that the regression model is statistically significant.

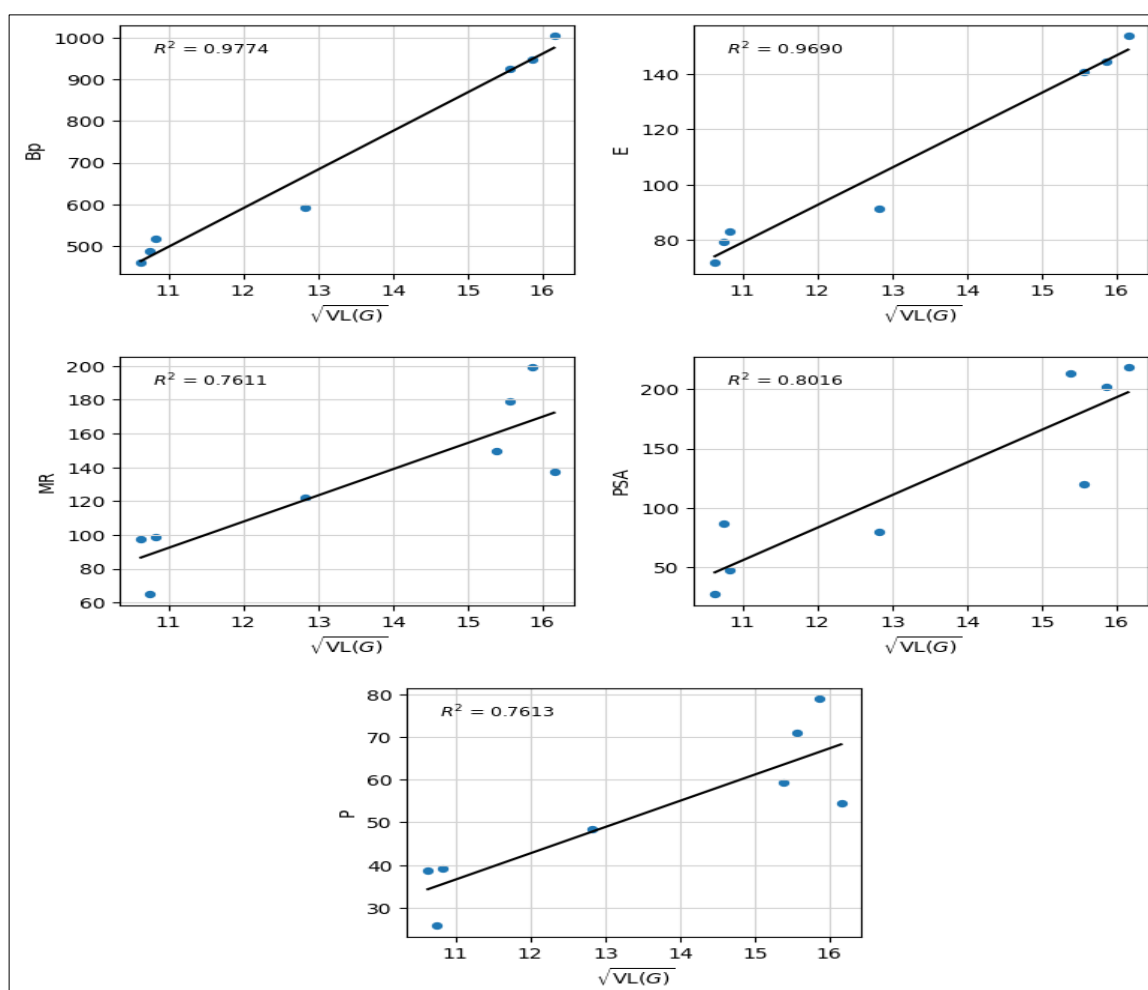


Fig 3: Regression plots of $\sqrt{VL(G)}$ and physicochemical parameters of COVID-19 drugs.

Overall, the regression analysis demonstrates that $\sqrt{VL(G)}$ exhibits excellent predictive performance for boiling point and enthalpy, while providing satisfactory prediction of polar surface area, molar refractivity, and polarizability. These findings indicate that the square-root transformation of the VL index is an effective molecular descriptor for QSPR modeling of the selected COVID-19 drugs.

3.2.3 Regression Analysis of $[VL(G)]^2$ for Predicting the Physicochemical Parameters of COVID-19 Drugs

The linear regression model describing the relationship between the boiling point and $[VL(G)]^2$ is given by

$$Bp = 358.0484 + 0.009437[VL(G)]^2.$$

The regression model exhibits an excellent fit with $R^2 = 0.9947$, demonstrating that 99.5% of the variation in boiling point is explained by the squared VL descriptor. The corresponding correlation coefficient ($R = 0.9973$) demonstrates an exceptionally strong positive linear relationship. Moreover, the model is statistically highly significant ($F(1,5) = 933.64, p < 0.001$), confirming the remarkable predictive capability of $[VL(G)]^2$ for estimating the boiling point of the selected COVID-19 drugs.

The regression equation relating enthalpy to $[VL(G)]^2$ is

$$E = 58.8454 + 0.001372[VL(G)]^2.$$

This model explains 99.0% of the observed variation in enthalpy ($R^2 = 0.9897$) and exhibits an excellent positive correlation ($R = 0.9949$). The corresponding F -statistic ($F(1,5) = 481.76, p < 0.001$) further confirms the statistical

significance of the regression model.

The relationship between molar refractivity and $[VL(G)]^2$ is represented by

$$MR = 70.3472 + 0.001552[VL(G)]^2.$$

The regression model yields $R^2 = 0.7363$, revealing that 73.6% of the variation in molar refractivity is explained by the squared descriptor. The positive correlation coefficient ($R = 0.8581$) and the significant F -statistic ($F(1,6) = 16.75, p = 0.006$) demonstrate a statistically meaningful linear relationship.

For polar surface area, the regression equation is

$$PSA = 14.1537 + 0.002821[VL(G)]^2.$$

The resulting model explains 82.1% of the variability in polar surface area ($R^2 = 0.8206$) and exhibits a strong positive correlation ($R = 0.9059$). The model is statistically significant with $F(1,6) = 27.45$ and $p = 0.002$.

The regression equation for polarizability is given by

$$P = 27.8804 + 0.0006153[VL(G)]^2.$$

The corresponding model accounts for 73.6% of the observed variation in polarizability ($R^2 = 0.7364$). The correlation coefficient ($R = 0.8581$), together with the F -statistic ($F(1,6) = 16.76, p = 0.006$), confirms that the regression model is statistically significant.

The regression plots depicting the relationships between $[VL(G)]^2$ and the selected molecular parameters of the selected COVID-19 drugs are shown in Figure 4.

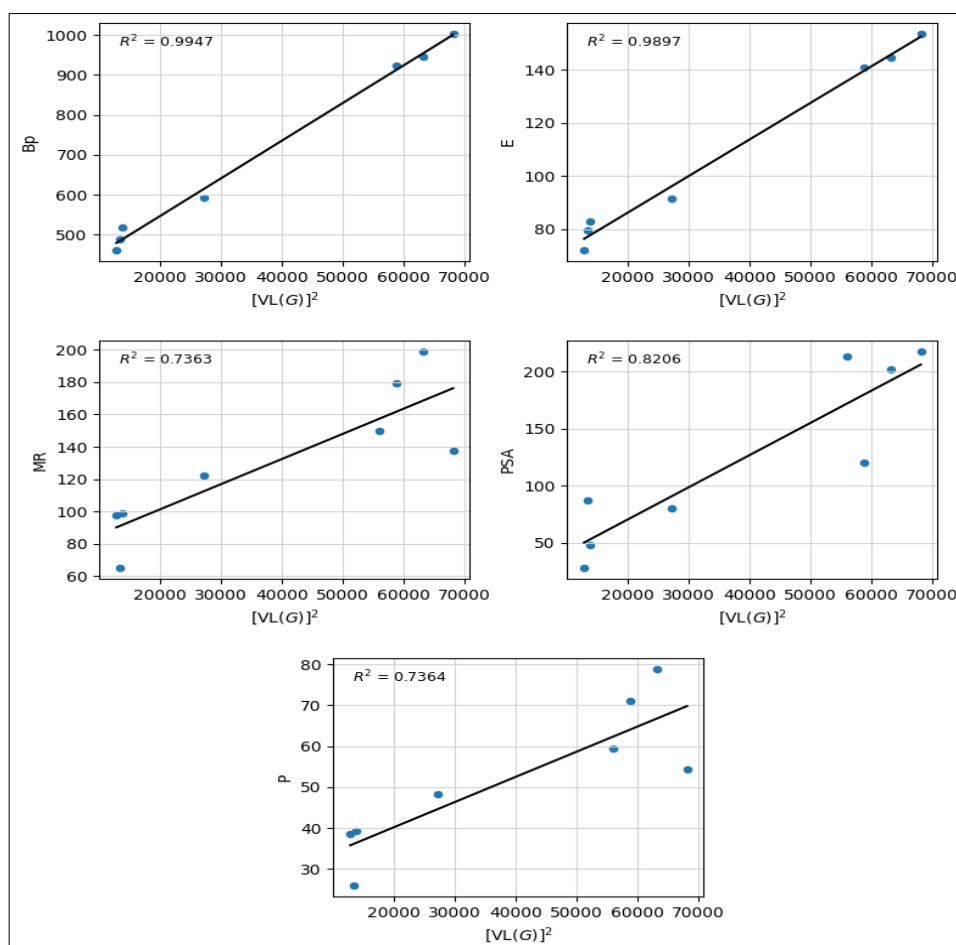


Fig 4: Regression plots of $[VL(G)]^2$ and physicochemical characteristics of COVID-19 drugs

Overall, the regression analysis demonstrates that the squared transformation of the VL index provides the strongest predictive performance among the considered descriptors. In particular, the regression models for boiling point and enthalpy exhibit outstanding goodness-of-fit, while satisfactory predictive accuracy is also achieved for polar surface area, molar refractivity, and polarizability. These findings suggest that $[VL(G)]^2$ is a highly effective transformed descriptor for QSPR studies of the selected COVID-19 drugs.

4. Conclusion

This study investigated the applicability of the Veerabhadraiah-Lokesha (VL) index and its transformed variants for predicting the physicochemical properties of selected COVID-19 drugs through QSPR analysis. Correlation analysis revealed that all the considered descriptors exhibited positive associations with boiling point, enthalpy, polar surface area, molar refractivity, and polarizability, with the squared transformation of the VL index showing the strongest correlations for most of the investigated properties.

The developed linear regression models further confirmed the predictive capability of the selected descriptors. Among the investigated transformations, $[VL(G)]^2$ produced the highest predictive accuracy, particularly for boiling point and enthalpy, achieving coefficients of determination of $R^2 = 0.9947$ and $R^2 = 0.9897$, respectively. The original $VL(G)$ and $\sqrt{VL(G)}$ also demonstrated excellent predictive performance for these properties while providing satisfactory models for polar surface area, molar refractivity, and polarizability. The statistical significance of all regression models indicates that the selected descriptors effectively capture structural information governing the physicochemical characteristics of the studied compounds.

Overall, the findings demonstrate that the VL index and its transformed variants constitute reliable molecular descriptors for QSPR investigations of COVID-19 drugs. The proposed approach offers a simple and computationally efficient framework for estimating physicochemical properties and may facilitate the preliminary screening and characterization of pharmaceutical compounds. Future studies may extend this methodology to larger datasets and explore the predictive performance of these descriptors using multiple linear regression and machine learning techniques.

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