Prediction of Physicochemical Properties of Alkanes Using Multilinear QSPR Models Based on the Eccentricity Zagreb Index and VL-Index

Abstract

Topological indices are important mathematical descriptors that facilitate the quantitative correlation between molecular structures and their physicochemical properties or chemical reactivity. In this study, quantitative structure–property relationship (QSPR) models are developed to predict selected physicochemical properties

of alkanes using the eccentricity-based first Zagreb index and the VL-index. The relationship between the molecular structures of alkanes and these eccentricity-based topological indices is systematically analyzed through multilinear regression techniques. The obtained results indicate that the eccentricity Zagreb index and the VL-index act as reliable molecular descriptors and provide effective predictive capability for the physicochemical properties of lower alkanes. These findings demonstrate the potential applicability of eccentricity-based topological indices in QSPR modeling and molecular property prediction.

Keywords: Topological indices; Zagreb index; VL -index; Eccentricity; Alkanes; Physical properties; Structure–property relationship.

1 Introduction

In theoretical and mathematical chemistry, *topological indices* are numerical invariants derived from the *molecular graph* $G = (V(G), E(G))$ (Trinajstić, 1992). In this representation, the vertex set $V(G)$ corresponds to carbon atoms, whereas the edge set $E(G)$ represents covalent C–C bonds. These graph-theoretical descriptors provide a rigorous mathematical framework for encoding molecular connectivity and structural complexity into quantitative parameters that can be correlated with experimentally measurable physicochemical properties, chemical reactivity, and biological activity.

Formally, the molecular graph G of an alkane is a simple, connected, undirected graph in which each vertex $v \in V(G)$ has degree $d(v)$, representing the number of carbon atoms directly bonded to v. The distance $d(u, v)$ between two vertices $u, v \in V(G)$ is defined as the length of the shortest path connecting them. The *eccentricity* $\varepsilon(v)$ of a vertex v is defined as

$$\varepsilon(v) = \max_{u \in V(G)} d(u, v),$$

which represents the maximum topological distance from v to any other vertex in the graph. By incorporating such local and global structural characteristics, topological indices serve as molecular descriptors in *quantitative structure–property relationship (QSPR)* and *quantitative structure–activity relationship (QSAR)* studies (Kier and Hall, 1986; Rasheed et al., 2024).

Among the various classes of topological descriptors, *degree-based indices* have received considerable attention due to their computational simplicity and strong predictive performance. One of the earliest and most widely studied examples is the *Zagreb index*, introduced by Gutman and Trinajstić (1972) in 1972. The first Zagreb index is defined as

$$M_1(G) = \sum_{v \in V(G)} d(v)^2,$$

which represents the second moment of the vertex degree distribution. This index has been extensively used for modeling physicochemical properties of organic molecules because of its sensitivity to molecular size and branching patterns.

Recent research has extended classical degree-based indices by incorporating additional graph-theoretic parameters such as vertex eccentricity. One such extension is the *eccentricity-based first Zagreb index*, defined as

$$M_1^{\varepsilon}(G) = \sum_{v \in V(G)} d(v)^2 \, \varepsilon(v),$$

which combines *local connectivity information* through the squared vertex degree with *global structural information* represented by vertex eccentricity. This combined representation enhances the ability to distinguish structural isomers and improves correlations with size- and shape-dependent molecular properties.

Another recently proposed descriptor is the VL*-index*, introduced in 2020 and inspired by the Zagreb indices. The index is attributed to the work of Veerabhadraiah Lokesha and later formulated by Deepika (2021). The VL-index of a graph G is defined as

$$VL(G) = \frac{1}{2} \sum_{uv \in E(G)} (d_e + d_f + 4),$$

where $d_e = d_u + d_v - 2$ and $d_f = d_u d_v - 2$, with d_u and d_v denoting the degrees of vertices u and v, respectively. An equivalent simplified expression is given by

$$VL(G) = \frac{1}{2} \sum_{uv \in E(G)} (d_u + d_v + d_u d_v).$$

Lower *alkanes* (C_nH_{2n+2}) Alsharafi et al. (2024); Alamotie et al. (2019) provide an ideal model system for QSPR investigations because of their structural simplicity, systematic variation through branching, and the availability of reliable experimental data. The molecular graphs of alkanes are *trees* (connected acyclic graphs), in which graph-theoretical characteristics directly reflect molecular branching patterns that significantly influence intermolecular interactions and thermodynamic behavior.

In the present work, the predictive capability of the eccentricity-based first Zagreb index $M_1^{\varepsilon}(G)$ and the VL-index $\xi VL(G)$ is systematically investigated using a dataset of 72 lower alkanes, each represented by its corresponding molecular graph. QSPR analyses are performed to examine the correlations between these descriptors and seven important physicochemical properties, namely boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures, and surface tensions. The experimental data used in this study were obtained from reliable literature sources.

By integrating concepts from chemical graph theory with experimental thermophysical data, this study contributes to the development of reliable structure–property relationships. The results provide a useful framework for molecular property prediction, molecular design, and a deeper understanding of alkane behavior in chemical and chemical engineering applications (Aliannejadi and Alamoti, 2026).

2 Materials and Methods

Although numerous topological indices have been proposed in the literature, the present study focuses exclusively on those indices relevant to the proposed analysis.

Let $G = (V(G), E(G))$ be a simple connected graph representing the molecular structure of a compound, where $V(G)$ denotes the vertex set and $E(G)$ denotes the edge set. In the context of chemical graph theory, vertices correspond to atoms (typically carbon atoms in hydrocarbons), while edges represent covalent bonds. For a vertex $v \in V(G)$, the degree of v is denoted by $d(v)$.

Gutman and Trinajstić introduced the classical Zagreb indices in Gutman and Trinajstić (1972); Gutman et al. (1975), which are defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)\,,$$

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v,$$

where d_u and d_v denote the degrees of the end vertices u and v of the edge uv, respectively.

The redefined Zagreb index, denoted by $ReZG(G)$, is defined as

$$ReZG(G) = \sum_{uv \in E(G)} \frac{d(u) + d(v)}{d(u)\, d(v)},$$

where u and v are the end vertices of the edge uv, and $d(u)$ and $d(v)$ represent their respective vertex degrees.

The VL–index, introduced in 2020 and inspired by the Zagreb indices, is attributed to the work of Veerabhadraiah Lokesha and was later formulated by Deepika (2021). The VL–index of a graph G is defined as

$$VL(G) = \frac{1}{2} \sum_{uv \in E(G)} (d_u + d_v + d_u d_v)\,,$$

where d_u and d_v denote the degrees of the vertices u and v in G, respectively.

Eccentricity of a Graph: For a vertex $v \in V(G)$, the eccentricity of v, denoted by $\varepsilon(v)$, is defined as the maximum distance between v and any other vertex of the graph G, that is,

$$\varepsilon(v) = \max\{d(v,u) \mid u \in V(G)\},$$

where $d(v,u)$ denotes the length of the shortest path between the vertices v and u.

In chemical graph theory, vertex eccentricity plays an important role in characterizing the global structural properties of a molecular graph. It reflects the maximum separation of a vertex from the remaining vertices of the graph and therefore provides insight into the

overall topology and spatial extent of a molecule. By combining eccentricity with degree-based descriptors, hybrid topological indices can effectively encode both local connectivity and global structural information.

Definition 2.1. The *eccentricity-based first Zagreb index* of a graph G, denoted by $M_1^{\varepsilon}(G)$, is defined as

$$M_1^{\varepsilon}(G) = \sum_{v \in V(G)} d(v)^2 \, \varepsilon(v),$$

where $V(G)$ denotes the vertex set of G, $d(v)$ represents the degree of the vertex v, and $\varepsilon(v)$ denotes the eccentricity of v.

Definition 2.2. The *eccentricity-based* VL*–index* of a graph G is defined as Narendra and Mahalakshmi (2023)

$$\xi VL(G) = \frac{1}{2} \sum_{uv \in E(G)} \left(\varepsilon(u) + \varepsilon(v) + \varepsilon(u)\varepsilon(v)\right),$$

where $\varepsilon(u)$ and $\varepsilon(v)$ denote the eccentricities of the end vertices u and v of the edge uv in the graph G.

Example 2.1 (Illustration of Definition 2.1). Let G be the molecular graph of $2,3$–dimethylbutane, which consists of six vertices corresponding to the carbon atoms of the molecule. The associated molecular graph is illustrated below.

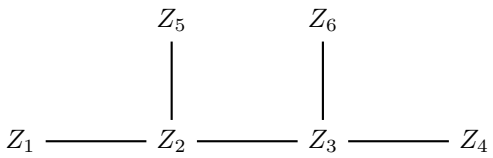

Fig. 1. Molecular structure of 2,3-dimethyl butane

The degree, eccentricity, and corresponding contributions to $M_1^{\varepsilon}(G)$ for each vertex are summarized in Table 1.

Table 1. Degree, eccentricity, and contributions to $M_{\varepsilon}^{1}(G)$ for each vertex

Vertex	$d(v)$	$\varepsilon(v)$	$d(v)^2\varepsilon(v)$
Z_1	1	3	3
Z_2	3	2	18
Z_3	3	2	18
Z_4	1	3	3
Z_5	1	3	3
Z_6	1	3	3

Using Definition 2.1, we obtain

$$\begin{aligned} M_1^{\varepsilon}(G) &= 1^2(3) + 3^2(2) + 3^2(2) + 1^2(3) + 1^2(3) + 1^2(3) \\ &= 3 + 18 + 18 + 3 + 3 + 3 \\ &= 48. \end{aligned}$$

$$\boxed{M_1^{\varepsilon}(G) = 48}$$

Example 2.2 (Illustration of Definition 2.2). Let $G = (V(G), E(G))$ be the molecular graph of $2,3,3,4$–tetramethylpentane consisting of $|V(G)| = 9$ vertices corresponding to the carbon atoms in the molecular formula $\mathrm{C_9H_{20}}$. The corresponding molecular graph is shown Fig. 2.

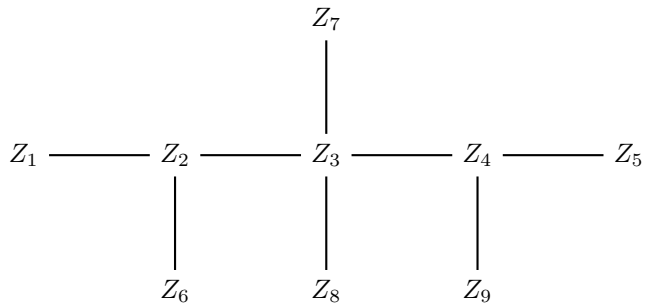

Fig. 2. Molecular structure of 2, 3, 3, 4–tetramethyl pentane

The eccentricities of the vertices are given by

$\varepsilon(Z_1) = 4$, $\varepsilon(Z_2) = 3$, $\varepsilon(Z_3) = 2$, $\varepsilon(Z_4) = 3$, $\varepsilon(Z_5) = 4$, $\varepsilon(Z_6) = 4$, $\varepsilon(Z_7) = 3$, $\varepsilon(Z_8) = 3$, and $\varepsilon(Z_9) = 4$.

Using Definition 2.2, the eccentricity–based VL–index of G is computed as

$$\xi VL(G) = \frac{1}{2}(19 + 19 + 11 + 11 + 11 + 11 + 19 + 19) = 60.$$

$$\boxed{\xi VL(G) = 60}$$

3 Preliminary Results

Let G denote the molecular graph of an alkane, where the vertex set represents carbon atoms and the edge set corresponds to carbon–carbon bonds. The *eccentricity–based first Zagreb index* of a graph G, denoted by $M_1^{\varepsilon}(G)$, is defined as introduced in Dankelmann et al. (2012). Similarly, the *eccentricity–based VL–index* of a graph G, denoted by $\xi VL(G)$, is defined in Narendra and Mahalakshmi (2023).

Based on these definitions, the values of $M_1^{\varepsilon}(G)$ and $\xi VL(G)$ are computed for a set of alkane molecules and their corresponding structural isomers. The calculated indices, together with the corresponding molecular graph representations, are presented in Table 2.

Table 2. Calculated $M_1^{\varepsilon}(G)$ and ξVL-indices values for alkanes

Sl. No.	**Name of the Chemical Compound**	$\boldsymbol{M_1^{\varepsilon}(G)}$	$\boldsymbol{\xi VL(G)}$
01	Ethane	2	1.5
02	Propane	8	5
03	Butane	22	15
04	2-Methylpropane(isobutane)	15	7.5
05	Pentane	40	30
06	2-Methylbutane	35	20.5
07	2,2-Dimethylpropane	24	10
08	Hexane	66	55.5
09	2-Methylpentane	39.5	89
10	3-Methylpentane	53	39.5
11	2,2-Dimethylbutane	47	35.5

Sl. No.	Name of the Chemical Compound	$M_1^e(G)$	$\xi VL(G)$
12	2,3-Dimethylbutane	48	26
13	Heptane	96	26
14	2-Methylhexane	117	70
15	3-Methylhexane	123	65
16	3-Ethylhexane	97	79.5
17	2,2-Dimethylpentane	93	49
18	2,3-Dimethylpentane	82	45
19	2,4-Dimethylpentane	56	49
20	3,3-Dimethylpentane	70	41
21	2,3,3-Trimethylbutane	65	31.5
22	Octane	134	55.5
23	2-Methylheptane	187	109.5
24	3-Methylheptane	193	103.5
25	4-Methylheptane	171	98.5
26	2,2-Dimethylhexane	194	84.5
27	2,3-Dimethylhexane	213	89
28	2,4-Dimethylhexane	227	79.5
29	2,5-Dimethylhexane	154	84.5
30	3,3-Dimethylhexane	121	74.5
31	3,4-Dimethylhexane	134	74.5
32	3-Ethyl-2-methylpentane	145	54.5
33	3-Ethyl-3-methylpentane	77	50.5
34	2,2,3-Dimethylpentane	131	54.5
35	2,2,4-Dimethylpentane	161	58.5
36	2,3,3-Trimethylpentane	112	50.5
37	2,3,4-Trimethylpentane	113	54.5
38	2,2,3,3-Tetramethylbutane	82	37
39	Nonane	176	196
40	2-Methyloctane	255	164.5
41	3-Methyloctane	250	157.5
42	4-Methyloctane	240	151.5
43	3-Ethylheptane	187	124
44	2,2-Dimethylheptane	307	130
45	2,3-Dimethylheptane	199	124
46	2,4-Dimethylheptane	222	119
47	2,5-Dimethylheptane	204	124
48	2,6-Dimethylheptane	224	130
49	3,3-Dimethylheptane	310	118
50	3,4-Dimethylheptane	191	113
51	3,5-Dimethylheptane	199	118
52	4,4-Dimethylheptane	212	108
53	3-Ethyl-2-methylhexane	196	94
54	4-Ethyl-2-methylhexane	170	94
55	3-Ethyl-3-methylhexane	190	89
56	3-Ethyl-4-methylhexane	169	87
57	2,2,3-Trimethylhexane	203	94
58	2,2,4-Trimethylhexane	197	94
59	2,2,5-Trimethylhexane	201	99

Sl. No.	Name of the Chemical Compound	$M_1^{\varepsilon}(G)$	$\xi VL(G)$
60	2,3,3-Trimethylhexane	166	89
61	2,3,4-Trimethylhexane	150	89
62	2,3,5-Trimethylhexane	154	94
63	2,4,4-Trimethylhexane	188	89
64	3,3,4-Trimethylhexane	190	84
65	3,3-Diethylpentane	136	60
66	2,3-Diethyl-3-ethylpentane	464	60
67	2,2-Diethyl-3-ethylpentane	264	64
68	2,2,3,3-Tetramethylpentane	108	60
69	2,2,3,4-Tetramethylpentane	132	64
70	2,2,4,4-Tetramethylpentane	100	68
71	2,3,3,4-Tetramethylpentane	132	60
72	4-Ethylpentane	160	113

4 Correlation Analysis of the Eccentricity–Based First Zagreb Index, VL–Index and Physicochemical Properties

Quantitative Structure–Property Relationship (QSPR) and Quantitative Structure–Activity Relationship (QSAR) methodologies provide a rigorous mathematical framework for establishing relationships between molecular structure and experimentally measurable physicochemical properties. In the present study, the eccentricity–based first Zagreb index $M_1^{\varepsilon}(G)$ and the VL–index $\xi VL(G)$ are employed as graph–theoretical descriptors to model several physicochemical properties of alkanes, including boiling point, molar volume, entropy, and enthalpy (Mahboob et al., 2024).

The computed values of $M_1^{\varepsilon}(G)$ and $\xi VL(G)$ for seventy–two alkane isomers are presented in Table 2. These topological indices encode important structural characteristics associated with vertex eccentricity, molecular size, and branching patterns, which are known to significantly influence thermodynamic and physicochemical properties (Hayat et al., 2025).

Let P denote a physicochemical property of interest. The linear relationship between P and a given topological index (TI) is initially evaluated using the Pearson correlation coefficient r, defined as

$$r = \frac{\sum_{i=1}^{n}(TI_i - \overline{TI})(P_i - \overline{P})}{\sqrt{\sum_{i=1}^{n}(TI_i - \overline{TI})^2 \sum_{i=1}^{n}(P_i - \overline{P})^2}},$$

where n denotes the number of molecules in the dataset, while $\overline{TI}$ and $\overline{P}$ represent the mean values of the corresponding variables.

4.1 Linear Regression Models

To assess the individual predictive capability of each molecular descriptor, simple linear regression (SLR) models are constructed. In these models, the relationship between a physicochemical property P and a given topological index is expressed through a linear function (Draper and Smith, 1998).

The regression model based on the eccentricity–based first Zagreb index is given by

$$P = a_1 + b_1\, M_1^{\varepsilon}(G),$$

whereas the model corresponding to the VL–index $\xi VL(G)$ is expressed as

$$P = a_2 + b_2\, \xi VL(G).$$

Here, a_1 and a_2 denote the intercepts of the respective regression equations, while b_1 and b_2 represent the regression coefficients associated with the descriptors $M_1^{\varepsilon}(G)$ and $\xi VL(G)$. These parameters are estimated using the least squares method.

4.2 Multilinear Regression Model

To further improve the predictive performance and account for the combined influence of both structural descriptors, a multilinear regression (MLR) model is also formulated Draper and Smith (1998). The corresponding regression equation is given by

$$P = a + b_1\, M_1^{\varepsilon}(G) + b_2\, \xi VL(G),$$

where a denotes the intercept of the model, and b_1 and b_2 are the regression coefficients corresponding to the eccentricity–based first Zagreb index $M_1^{\varepsilon}(G)$ and the VL–index $\xi VL(G)$, respectively. These coefficients quantify the relative contributions of the two descriptors in predicting the physicochemical property P.

4.3 Statistical Summary of Multilinear QSPR Models Using $M_1^{\varepsilon}(G)$ and $\xi VL(G)$ for the Prediction of Physicochemical Properties of Alkanes

Table 3 summarizes the statistical performance of the multilinear QSPR models developed using the eccentricity–based first Zagreb index $[M_1^{\varepsilon}(G)]$ and the VL–index $[\xi VL(G)]$ as molecular descriptors Hastie et al. (2009). The use of correlation–based validation measures is well established in quantitative structure–property relationship (QSPR) and quantitative structure–activity relationship (QSAR) studies (Kier and Hall, 1986; Trinajstić, 1992).

For each physicochemical property, two commonly used statistical indicators are reported:

- r **(Pearson correlation coefficient)**, which measures the strength and direction of the linear relationship between the descriptors $M_1^{\varepsilon}(G)$, $\xi VL(G)$ and the corresponding physicochemical property Rodgers and Nicewander (1988);
- **Correlation strength**, a qualitative interpretation of the magnitude of $|r|$ based on standard statistical classification criteria Cohen (1988).

The results presented in Table 3 demonstrate the strong predictive capability of the eccentricity–based first Zagreb index $M_1^{\varepsilon}(G)$ and the VL–index $\xi VL(G)$ for the considered physicochemical properties of alkanes. All seven properties exhibit *very strong* correlations, with correlation coefficients ranging from $|r| = 0.951$ to 0.984. Among these properties, the critical temperature shows the highest positive correlation ($r = 0.984$), indicating a particularly strong linear dependence on the proposed topological descriptors.

In contrast, the critical pressure exhibits a *very strong negative correlation* ($r = -0.902$). This behavior is chemically meaningful, since higher values of $M_1^{\varepsilon}(G)$ and $\xi VL(G)$ generally correspond to increased molecular branching and structural complexity. Such structural changes tend to weaken intermolecular van der Waals interactions, which may lead to lower critical pressure values.

Furthermore, boiling point, molar volume, molar refraction, heat of vaporization, and surface tension all display very strong positive correlations ($r > 0.95$). These results highlight the capability of the descriptors $M_1^{\varepsilon}(G)$ and $\xi VL(G)$ to effectively capture structural characteristics that influence the thermodynamic and physicochemical behavior of alkane molecular graphs.

Overall, the consistently high correlation strengths obtained in this study indicate that the eccentricity–based first Zagreb index $M_1^{\varepsilon}(G)$ together with the VL–index $\xi VL(G)$ provides reliable and efficient descriptors for QSPR modeling of alkane physicochemical properties. These findings are consistent with previous QSPR investigations employing Zagreb- and VL–type topological indices.

Table 3. Statistical performance of multilinear QSPR models based on the eccentricity–based first Zagreb index $M_1^{\varepsilon}(G)$ and the VL–index $\xi VL(G)$

Physicochemical Property	r	Correlation Strength
Boiling Point (bp)	0.982	Very Strong
Molar Volume (mv)	0.961	Very Strong
Molar Refraction (mr)	0.968	Very Strong
Heat of Vaporization (hv)	0.961	Very Strong
Critical Temperature (ct)	0.984	Very Strong
Critical Pressure (cp)	-0.902	Very Strong
Surface Tension (st)	0.951	Very Strong

5 Conclusion

Multilinear QSPR models were developed to evaluate the predictive ability of the eccentricity-based first Zagreb index $M_1^{\varepsilon}(G)$ and VL-index $\xi VL(G)$ for several physicochemical properties of alkanes. The results show that these descriptors exhibit very strong correlations with all seven properties, with Pearson correlation coefficients in the range $|r| = 0.951$–0.984.

A strong positive correlation is observed for critical temperature, while critical pressure shows a strong negative correlation, reflecting the influence of molecular branching and intermolecular interactions. These findings demonstrate a clear relationship between alkane molecular structure and physicochemical behavior.

Overall, $M_1^{\varepsilon}(G)$ and $\xi VL(G)$ effectively capture important topological features, providing a simple and reliable framework for predicting thermodynamic and physicochemical properties. The study highlights the usefulness of eccentricity-based descriptors in QSPR modeling and supports further research in chemical graph theory and computational chemistry (Kier and Hall, 1986; Sunil et al., 2017; Gutman and Trinajstić, 1972; Dankelmann et al., 2012).

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Competing Interests

Authors have declared that no competing interests exist.

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