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Modeling the Physical Properties of Cholera Treatment Drugs via Neighborhood Sum Degree-Based Topological Indices

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Abstract. Cholera remains a global health challenge, which requires the optimization of treatment strategies, including the design of effective drugs. This study explores the utility of neighborhood sum degree-based topological indices (TIs) in predicting the physical properties of cholera treatment drugs through quantitative structure-property relationship (QSPR) modeling. Eight TIs, neighborhood first Zagreb, second Zagreb, hyper Zagreb, geometric-arithmetic, forgotten, harmonic, Randić and atom bond connectivity indices were evaluated using linear regression models across six physicochemical properties: boiling point, flash point, enthalpy of vaporization, molar refraction, polarization, and molar volume. Among all indices, neighborhood harmonic, sum connectivity, and atom bond connectivity indices stand out for their high R^2 values and low standard errors in modeling molar refraction and polarization. For boiling point and flash point, the neighborhood first and second Zagreb indices, and randic index provide moderate predictive power. Some indices such as neighborhood hyper, second Zagreb and forgotten indices showed moderate performance for all physical properties.

1. Introduction

According to the World Health Organization [13], cholera is an acute diarrheal infection caused by ingestion of food or water contaminated with the bacterium Vibrio cholerae. Cholera remains a global threat to public health and an indicator of inequality and lack of social development. Some of the symptoms associated with cholera includes vomiting, thirst, leg cramps, restlessness and irritability.

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The South African Department of Health [12] reported that in 2023, the country recorded a total cumulative number of 166 laboratory-confirmed cases and 202 suspected cases of cholera in five provinces between 1st of February and 6th of June 2023. Majority of cases were recorded in Hammanskraal region of Gauteng which accounts for at least 92% or 152 cases, while Free State Province accounts for 5% which translates into 9 cases. Other provinces which recorded positive cases include one in Limpopo, one in Mpumalanga, and three in North West. Cholera is a significant concern especially in areas with poor sanitation. Multifaceted approach is a key to control cholera, the prevention include clean water, proper hygiene and vaccination [13]. There are antimicrobial (drugs) used to treat cholera and they include; Tetracycline, Furazolidone, Erythromycin, Azithromycin, Ciprofloxacine, Norfloxacin, Doxycycline, Chloramphenicol etc. These drugs are produced via laboratory processes which requires rigorous testing and cost-effectiveness analysis before they obtain market authorization. Graph theoretical techniques such as quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) models plays a crucial role in drug design by aiding in the prediction and understanding of various properties and behavior of the chemical compounds inherent in drugs. These models establish quantitative relationships between the structural features of drugs or chemical compounds and their physicochemical properties, allowing researchers to make informed decisions during drug development process. A QSPR model is dependent on the type of regression analysis adopted, for example, a data that exhibit linear relationship is modeled via linear regression, a polynomial data is better modeled by polynomial regression. In many cases, dataset can exhibit nonlinear relationships, such dataset are better modeled via machine learning algorithms (see Abubakar et al. [1,2]). A simple QSPR model equation is given below;

$$y = f(x), \tag{1.1}$$

f establishes relationship between x and y, $y =$ physicochemical properties (dependent variable), and $x =$ topological index (independent variable). If the relationship is linear then y becomes,

$$y = c + sx, \tag{1.2}$$

where c is constant of regression, and s is regression coefficient. The molecular structure of drugs can be examined by topological indices to acquire vital information about the drug's molecular properties and connectivity. Topological indices (TI) are numerical descriptor derived from the molecular graph of a chemical compound, they encode structural information about the molecule, often used in QSAR and QSPR models. (See [1,4,10,11] for more details on QSPR models).
The first and the second Zagreb indices were proposed by Gutman and Trinajestic [8] in 1972, both indices are graph theoretical indices used to describe molecular structure in chemistry, they are calculated based on the vertices and edges of the graph representing a molecule size branching (see more on Zagreb indices [7,9]). It can be useful in predicting chemical and physical properties

of molecules. It is given by the equation below.

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v), \tag{1.3}$$

$$M_2(G) = \sum_{uv \in E(G)} (d_u d_v), \tag{1.4}$$

where d_u and d_v are degrees of vertices u and v.

A more general form of the Zagreb indices was also proposed by Gutman and Trinajestic [8] in the same article that introduced the Zagreb indices. Although, the forgotten index lacked practical applicability until Furtula and Gutman [6] investigated its chemical applicability. They showed that it can significantly enhance the physicochemical applicability of the first Zagreb index. The formula for computing the forgotten index is given in (1.5).

$$F(G) = \sum_{v \in V(G)} d_v^3 = \sum_{u,v \in E(G)} d_u^2 + d_v^2. \tag{1.5}$$

The Randić index was introduced by Milan Randić [15] in 1975 as one of the earliest degree-based index. It is used to determine the branching degree of a molecule by measuring the sum of the square roots of the vertex degree of each atom in the molecule and it is particularly useful in prediction of physical and chemical properties of a molecule (see [14,17,19] for details). It is given by the the equation below,

$$R(G) = \sum_{uv \in E(G)} \sqrt{\frac{1}{d_u d_v}}. \tag{1.6}$$

Several indices have been proposed to date with varying applications to modelling the physicochemical properties of compounds. Among them are Atom Bond Connectivity (ABC) [5], sum connectivity index (SCI) [19], third redefined Zagreb index [16] etc.

A new variant of the degree-based index was introduced by Mondal et al. [10] in 2019. Four topological indices named as neighborhood version of forgotten topological index (F_N), modified neighborhood version of forgotten topological index (F_N^*)*, neighborhood version of second Zagreb index (M_2^*) and the last one was the neighborhood version of of hyper Zagreb index (HM_N) were introduced. Based on the efficiency of the neighborhood sum degree-based TIs [1–3, 10, 11], this study aims to utilize neighborhood degree topological indices in modelling the physical properties of cholera treatment drugs.

This article is organized into four sections: (i) Introduction, which provides the background of the study; (ii) Preliminary, where we discuss relevant past results that will be used; (iii) Result, in which we present our study's findings; and (iv) Conclusion, where we summarize our conclusions based on those findings.

2. Preliminaries

A Graph $G = (V, E)$ is a mathematical structure consisting of two sets V and E. The elements of V are called vertices and the elements of E are called edges. Each edge has a set of one or two vertices

associated to it, which are called its endpoints (See [18]). Adjacent vertices are two vertices that are joined by an edge. The degree of a vertex v in a graph G, denoted by d_v is the number of edges incident to a vertex v. A graph is connected if for every pair of vertices u and v, there is a path from u to v. A graph is simple if it does not contains self-loops and multiple edges. A chemical graph is a simple graph representation of molecular structure of a compound where atoms are represented as vertices and bonds are represented as edges. The neighbors degree of a vertex v denoted as δ_v is defined as the sum of degree of vertices adjacent to v. Let G be a chemical graph, δ_u and δ_v be the neighbor degree sum of vertices u and v. Then the neighborhood version of some TIs are defined as (see [3, 10, 11] for details):

(i) Neighborhood first Zagreb index [10] is given by

$$NM1(G) = \sum_{u,v \in E(G)} [\delta_u + \delta_v]. \tag{2.1}$$

(ii) Neighborhood second zagreb index [10]

$$NM_2 = \sum_{uv \in E(G)} [\delta_u \delta_v]. \tag{2.2}$$

(iii) Neighborhood forgotten index [10]

$$NF(G) = \sum_{v \in V(G)} \delta_v^3 = \sum_{uv \in E(G)} \delta_u^2 + \delta_v^2. \tag{2.3}$$

(iv) Neighborhood hyper Zagreb index [10] is given by

$$NHP(G) = \sum_{u,v \in E(G)} [\delta_u + \delta_v]^2. \tag{2.4}$$

(v) Neighborhood harmonic index [11] is given by

$$NHM(G) = \sum_{uv \in E(G)} \frac{2}{\delta_u + \delta_v}. \tag{2.5}$$

(vi) Neighborhood Randić index [11] is given by

$$NR(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\delta_u \delta_v}}. \tag{2.6}$$

(vii) Neighborhood inverse Randić index [11] is given by

$$NGA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\delta_u \delta_v}}{\delta_u + \delta_v}. \tag{2.7}$$

(viii) Neighborhood atom bond connectivity index [11] is given by

$$NABC(G) = \sum_{uv \in E(G)} \frac{\sqrt{\delta_u + \delta_v - 2}}{\delta_u \delta_v}. \tag{2.8}$$

(ix) Neighborhood sum connectivity index [11] is given by

$$NSCI(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\delta_u + \delta_v}}. \tag{2.9}$$

3. **Main Result**

In this section, we display the molecular structures of ten selected drugs used to treat cholera and we compute their TI.

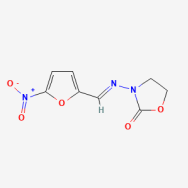


FIGURE 1. Furazolidone

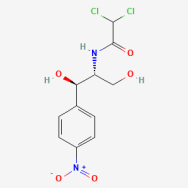


FIGURE 2. Chloramphenicol

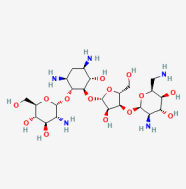


FIGURE 3. Paromomycine

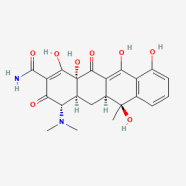


FIGURE 4. Tetracycline

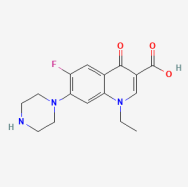


FIGURE 5. Norfloxacine

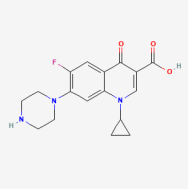


FIGURE 6. Ciprofloxacine

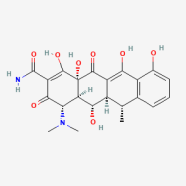


FIGURE 7. Doxycycline

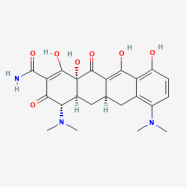


FIGURE 8. Minocycline

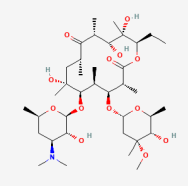


FIGURE 9. Erythromycin

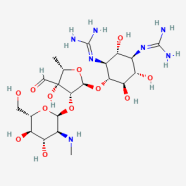


FIGURE 10. Streptomycin

The neighborhood degree sum topological indices of the ten cholera drugs are computed beginning with furazolidone in Theorem 3.1.

Theorem 3.1. *Let G_1 be a chemical graph of furazolidone, the neighborhood sum degree-based TI are given as follows:*

(i) $NM_1(G_1) = 182$
(ii) $NM_2(G_1) = 488$
(iii) $NHP(G_1) = 1992$
(iv) $NHM(G_1) = 3.25$
(v) $NR(G_1) = 5.24$
(vi) $NGA(G_1) = 16.79$
(vii) $NABC(G_1) = 9.53$
(viii) $NF(G_1) = 1016$
(ix) $NSCI(G_1) = 3.18$.

Proof. We partition the edge set of G_1 of the furazolidone chemical graph via the sum of degrees of neighbors of vertices as follow:

Edge label	$\delta(u,v)$	Number of edges (m)
m_1	(3,5)	2
m_2	(5,7)	4
m_3	(7,6)	2
m_4	(5,5)	2
m_5	(5,6)	3
m_6	(6,6)	1
m_7	(6,3)	1
m_8	(5,4)	2

(i) Using (2.1), the neighborhood first Zagreb index is:

$$\begin{aligned} NM_1(G_1) &= m_1(\delta_3+\delta_5) + m_2(\delta_5+\delta_7) + m_3(\delta_7+\delta_6) + m_4(\delta_5+\delta_5) + m_5(\delta_5+\delta_6) \\ &\quad + m_6(\delta_6+\delta_6) + m_7(\delta_6+\delta_3) + m_8(\delta_5+\delta_4) \\ &= 182. \end{aligned}$$

(ii) For neighborhood second Zagreb index, from (2.2),

$$\begin{aligned} NM_2(G_1) &= m_1(\delta_3\cdot\delta_5) + m_2(\delta_5\cdot\delta_7) + m_3(\delta_7\cdot\delta_6) + m_4(\delta_5\cdot\delta_5) \\ &\quad + m_5(\delta_5\cdot\delta_6) + m_6(\delta_6\cdot\delta_6) + m_7(\delta_6\cdot\delta_3) + m_8(\delta_5\cdot\delta_4) \\ &= 488. \end{aligned}$$

(iii) We use (2.4) to compute neighborhood hyper Zagreb index of G_1,

$$\begin{aligned} NHP(G_1) &= m_1(\delta_3+\delta_5)^2 + m_2(\delta_5+\delta_7)^2 + m_3(\delta_7+\delta_6)^2 + m_4(\delta_5+\delta_5)^2 \\ &\quad + m_5(\delta_5+\delta_6)^2 + m_6(\delta_6+\delta_6)^2 + m_7(\delta_6+\delta_3)^2 + m_8(\delta_5+\delta_4)^2 \\ &= 1992. \end{aligned}$$

(iv) We use (2.5) to compute the neighborhood harmonic index of G_1,

$$\begin{aligned} NHM(G_1) &= m_1\left(\frac{2}{\delta_3+\delta_5}\right)+m_2\left(\frac{2}{\delta_5+\delta_7}\right)+m_3\left(\frac{2}{\delta_7+\delta_6}\right)+m_4\left(\frac{2}{\delta_5+\delta_5}\right)+m_5\left(\frac{2}{\delta_5+\delta_6}\right) \\ &\quad + m_6\left(\frac{2}{\delta_6+\delta_6}\right)+m_7\left(\frac{2}{\delta_6+\delta_3}\right)+m_8\left(\frac{2}{\delta_5+\delta_4}\right), \\ &= 3.25. \end{aligned}$$

(v) We utilize (2.6) to compute neighborhood Randić Index of G_1,

$$\begin{aligned} NR(G_1) &= m_1\left(\frac{1}{\sqrt{\delta_3+\delta_5}}\right)+m_2\left(\frac{1}{\sqrt{\delta_5+\delta_7}}\right)+m_3\left(\frac{1}{\sqrt{\delta_7+\delta_6}}\right)+m_4\left(\frac{1}{\sqrt{\delta_5+\delta_5}}\right) \\ &\quad + m_5\left(\frac{1}{\sqrt{\delta_5+\delta_6}}\right)+m_6\left(\frac{1}{\sqrt{\delta_6+\delta_6}}\right)+m_7\left(\frac{1}{\sqrt{\delta_6+\delta_3}}\right)+m_8\left(\frac{1}{\sqrt{\delta_5+\delta_4}}\right), \\ &= 5.24. \end{aligned}$$

(vi) We utilize (2.7) to compute neighborhood geometric arithmetic index of G_1:

$$\begin{aligned} NGA(G_1) &= m_1\left(\frac{2\sqrt{\delta_3\cdot\delta_5}}{\delta_3+\delta_5}\right)+m_2\left(\frac{2\sqrt{\delta_5\cdot\delta_7}}{\delta_5+\delta_7}\right)+m_3\left(\frac{2\sqrt{\delta_7\cdot\delta_6}}{\delta_7+\delta_6}\right)+m_4\left(\frac{2\sqrt{\delta_5\cdot\delta_5}}{\delta_5+\delta_5}\right) \\ &\quad + m_5\left(\frac{2\sqrt{\delta_5\cdot\delta_6}}{\delta_5+\delta_6}\right)+m_6\left(\frac{2\sqrt{\delta_6\cdot\delta_6}}{\delta_6+\delta_6}\right)+m_7\left(\frac{2\sqrt{\delta_6\cdot\delta_3}}{\delta_6+\delta_3}\right)+m_8\left(\frac{2\sqrt{\delta_5\cdot\delta_4}}{\delta_5+\delta_4}\right) \\ &= \frac{4\sqrt{15}}{8}+\frac{8\sqrt{35}}{12}+\frac{4\sqrt{42}}{13}+2+\frac{6\sqrt{30}}{11}+1+\frac{2\sqrt{18}}{9}+\frac{4\sqrt{20}}{9}, \\ &= 16.79. \end{aligned}$$

(vii) We utilize (2.8) to compute the neighborhood Atom Bond Connectivity Index:

$$\begin{aligned} NABC(G_1) &= m_1\left(\sqrt{\frac{\delta_3+\delta_5-2}{\delta_3\delta_5}}\right)+m_2\left(\sqrt{\frac{\delta_5+\delta_7-2}{\delta_5\delta_7}}\right)+m_3\left(\sqrt{\frac{\delta_7+\delta_6-2}{\delta_7\delta_6}}\right) \\ &\quad + m_4\left(\sqrt{\frac{\delta_5+\delta_5-2}{\delta_5\delta_5}}\right)+m_5\left(\sqrt{\frac{\delta_5+\delta_6-2}{\delta_5\delta_6}}\right) \\ &\quad + m_6\left(\sqrt{\frac{\delta_6+\delta_6-2}{\delta_6\delta_6}}\right)+m_7\left(\sqrt{\frac{\delta_6+\delta_3-2}{\delta_6\delta_3}}\right)+m_8\left(\sqrt{\frac{\delta_5+\delta_4-2}{\delta_5\cdot\delta_4}}\right) \\ &= 2\cdot\sqrt{\frac{6}{15}}+4\cdot\sqrt{\frac{10}{35}}+2\cdot\sqrt{\frac{11}{42}}+2\cdot\sqrt{\frac{8}{25}}+3\cdot\sqrt{\frac{9}{30}}+\frac{\sqrt{10}}{6}+\sqrt{\frac{7}{18}}+2\cdot\sqrt{\frac{7}{20}} \\ &= 9.53 \end{aligned}$$

(viii) From (2.3), we compute the neighborhood forgotten index of G_1,

$$\begin{aligned} NF(G_1) &= m_1\left[(\delta_3)^2+(\delta_5)^2\right]+m_2\left[(\delta_5)^2+(\delta_7)^2\right]+m_3\left[(\delta_7)^2+(\delta_6)^2\right]+m_4\left[(\delta_5)^2+(\delta_5)^2\right] \\ &\quad + m_5\left[(\delta_6)^2+(\delta_6)^2\right]+m_6\left[(\delta_6)^2+(\delta_6)^2\right]+m_7\left[(\delta_6)^2+(\delta_3)^2\right]+m_8\left[(\delta_5)^2+(\delta_4)^2\right], \\ &= 1016. \end{aligned}$$

(xi) From (2.9) we compute the neighborhood sum connectivity index of G_1

$$\begin{aligned} NSCI(G_1) &= m_1\left(\frac{1}{\sqrt{\delta_3+\delta_5}}\right)+m_2\left(\frac{1}{\sqrt{\delta_5+\delta_7}}\right)+m_3\left(\frac{1}{\sqrt{\delta_7+\delta_6}}\right) \\ &+ m_4\left(\frac{1}{\sqrt{\delta_5+\delta_5}}\right)+m_5\left(\frac{1}{\sqrt{\delta_5+\delta_6}}\right)+m_6\left(\frac{1}{\sqrt{\delta_6+\delta_6}}\right) \\ &+ m_7\left(\frac{1}{\sqrt{\delta_6+\delta_3}}\right)+m_8\left(\frac{1}{\sqrt{\delta_5+\delta_4}}\right)=2\left(\frac{1}{\sqrt{15}}\right)+4\left(\frac{1}{\sqrt{35}}\right) \\ &+ 2\left(\frac{1}{\sqrt{42}}\right)+2\left(\frac{1}{5}\right)+3\left(\frac{1}{\sqrt{30}}\right)+\frac{1}{6}+\frac{1}{\sqrt{18}}+2\left(\frac{1}{\sqrt{20}}\right), \\ &= 3.18. \end{aligned}$$

□

Theorem 3.2. *Let G_2 be a chemical graph of chloramphenicol drug compound, the neighborhood degree sum TI for G_2 are given as follows:*

(i) $NM_1(G_2) = 212$
(ii) $NM_2(G_2) = 547$
(iii) $NHP(G_2) = 2340$
(iv) $NHM(G_2) = 3.95$
(v) $NR(G_2) = 4.06$
(vi) $NGA(G_2) = 9.56$
(vii) $NABC(G_2) = 11.42$
(viii) $NF(G_2) = 1208$
(ix) $NSCI(G_2) = 6.25$.

Proof. We partition the edge set of chloramphenicol chemical graph via the sum of degrees of neighbors of vertices as follows:

Edge Label	$\delta(u,v)$	Number of Edges (m)
m_1	(5,3)	4
m_2	(5,5)	2
m_3	(5,7)	5
m_4	(7,7)	2
m_5	(3,7)	1
m_6	(7,4)	1
m_7	(4,2)	1
m_8	(7,6)	1
m_9	(6,6)	1
m_{10}	(6,3)	1
m_{11}	(6,5)	1

(i) From (2.1), we have

$$\begin{aligned}NM_1(G_2) &= m_1(\delta_5+\delta_3)+m_2(\delta_5+\delta_5)+m_3(\delta_5+\delta_7)+m_4(\delta_7+\delta_7)+m_5(\delta_3+\delta_7)\\&\quad+m_6(\delta_7+\delta_4)+m_7(\delta_4+\delta_2)+m_8(\delta_7+\delta_6)+m_9(\delta_6+\delta_6)\\&\quad+m_{10}(\delta_6+\delta_3)+m_{11}(\delta_6+\delta_5).\\&=212.\end{aligned}$$

(ii) From (2.2), we have

$$\begin{aligned}NM_2(G_2) &= m_1(\delta_5\delta_3)+m_2(\delta_5\delta_5)+m_3(\delta_5\delta_7)+m_4(\delta_7\delta_7)+m_5(\delta_3\delta_7)+m_6(\delta_7\delta_4)\\&\quad+m_7(\delta_4\delta_2)+m_8(\delta_7\delta_6)+m_9(\delta_6\delta_6)+m_{10}(\delta_6\delta_3)+m_{11}(\delta_6\delta_5)\\&=547.\end{aligned}$$

(iii) From (2.4), we compute the neighborhood hyper Zagreb index,

$$\begin{aligned}NHM(G_2) &= m_1(\delta_5+\delta_3)^2+m_2(\delta_5+\delta_5)^2+m_3(\delta_5+\delta_7)^2+m_4(\delta_7+\delta_7)^2\\&\quad+m_5(\delta_3+\delta_7)^2+m_6(\delta_7+\delta_4)^2+m_7(\delta_4+\delta_2)^2+m_8(\delta_7+\delta_6)^2\\&\quad+m_9(\delta_6+\delta_6)^2+m_{10}(\delta_6+\delta_3)^2+m_{11}(\delta_6+\delta_5)^2\\&=2340.\end{aligned}$$

(iv) From (2.5), we compute the neighbourhood harmonic index,

$$\begin{aligned}NH(G_2) &= m_1\left(\frac{2}{\delta_5+\delta_7}\right)+m_2\left(\frac{2}{\delta_5+\delta_5}\right)+m_3\left(\frac{2}{\delta_5+\delta_7}\right)+m_4\left(\frac{2}{\delta_7+\delta_7}\right)+m_5\left(\frac{2}{\delta_3+\delta_7}\right)\\&\quad+m_6\left(\frac{2}{\delta_7+\delta_4}\right)+m_7\left(\frac{2}{\delta_4+\delta_2}\right)+m_8\left(\frac{2}{\delta_7+\delta_6}\right)+m_9\left(\frac{2}{\delta_6+\delta_6}\right)+m_{10}\left(\frac{2}{\delta_6+\delta_3}\right)\\&\quad+m_{11}\left(\frac{2}{\delta_6+\delta_5}\right)\\&=3.95.\end{aligned}$$

(v) From (2.6), we have

$$\begin{aligned}NR(G_2) &= m_1\left(\frac{1}{\sqrt{\delta_5\delta_3}}\right)+m_2\left(\frac{1}{\sqrt{\delta_5\delta_5}}\right)+m_3\left(\frac{1}{\sqrt{\delta_5\delta_7}}\right)+m_4\left(\frac{1}{\sqrt{\delta_7\delta_7}}\right)+m_5\left(\frac{1}{\sqrt{\delta_3\delta_7}}\right)\\&\quad+m_6\left(\frac{1}{\sqrt{\delta_7\delta_4}}\right)+m_7\left(\frac{1}{\sqrt{\delta_4\delta_2}}\right)+m_8\left(\frac{1}{\sqrt{\delta_7\delta_6}}\right)+m_9\left(\frac{1}{\sqrt{\delta_6\delta_6}}\right)+m_{10}\left(\frac{1}{\sqrt{\delta_6\delta_3}}\right)\\&\quad+m_{11}\left(\frac{1}{\sqrt{\delta_6\delta_5}}\right)\\&=\frac{4}{\sqrt{15}}+\frac{2}{\sqrt{25}}+\frac{5}{\sqrt{35}}+\frac{2}{\sqrt{49}}+\frac{1}{\sqrt{27}}+\frac{1}{\sqrt{28}}+\frac{1}{\sqrt{8}}+\frac{1}{\sqrt{42}}+\frac{1}{\sqrt{36}}+\frac{1}{\sqrt{18}}+\frac{1}{\sqrt{30}},\\&=4.06.\end{aligned}$$

(vi) From (2.7) neighborhood geometric arithmetic index,

$$\begin{aligned}NGA(G_2) &= m_1\left(\frac{2\sqrt{\delta_5\cdot\delta_3}}{\delta_5+\delta_3}\right)+m_2\left(\frac{2\sqrt{\delta_5\cdot\delta_5}}{\delta_5+\delta_5}\right)+m_3\left(\frac{2\sqrt{\delta_5\cdot\delta_7}}{\delta_5+\delta_7}\right)+m_4\left(\frac{2\sqrt{\delta_7\cdot\delta_7}}{\delta_7+\delta_7}\right)\\ &+m_5\left(\frac{2\sqrt{\delta_3\cdot\delta_7}}{\delta_3+\delta_7}\right)+m_6\left(\frac{2\sqrt{\delta_7\cdot\delta_4}}{\delta_7+\delta_4}\right)+m_7\left(\frac{2\sqrt{\delta_4\cdot\delta_2}}{\delta_4+\delta_2}\right)+m_8\left(\frac{2\sqrt{\delta_7\cdot\delta_6}}{\delta_7\delta_6}\right)\\ &+m_9\left(\frac{2\sqrt{\delta_6\cdot\delta_6}}{\delta_6+\delta_6}\right)+m_{10}\left(\frac{2\sqrt{\delta_6\cdot\delta_3}}{\delta_6+\delta_3}\right)+m_{11}\left(\frac{2\sqrt{\delta_6\cdot\delta_5}}{\delta_6+\delta_5}\right)\\ &=2\left(\frac{\sqrt{15}}{8}\right)+2\left(\frac{\sqrt{25}}{10}\right)+5\left(\frac{\sqrt{35}}{12}\right)+2\left(\frac{\sqrt{49}}{14}\right)+2\left(\frac{\sqrt{37}}{10}\right)+\frac{2}{28}+\frac{2}{8}\\ &+\frac{2}{42}+\frac{2}{36}+\frac{2\sqrt{18}}{9}+\frac{2\cdot 30}{11}\\ &=19.56.\end{aligned}$$

(vii) From (2.8), the neighborhood atom bond connectivity index of G_2 is,

$$\begin{aligned}NABC(G_2) &= m_1\left(\sqrt{\frac{\delta_5+\delta_3-2}{\delta_5\delta_3}}\right)+m_2\left(\sqrt{\frac{\delta_5+\delta_5-2}{\delta_5\delta_5}}\right)+m_3\left(\sqrt{\frac{\delta_5+\delta_7-2}{\delta_5\delta_7}}\right)\\ &+m_4\left(\sqrt{\frac{\delta_7+\delta_7-2}{\delta_7\delta_7}}\right)+m_5\left(\sqrt{\frac{\delta_3+\delta_7-2}{\delta_3\delta_7}}\right)+m_6\left(\sqrt{\frac{\delta_7+\delta_4-2}{\delta_7\delta_4}}\right)\\ &+m_7\left(\sqrt{\frac{\delta_4+\delta_2-2}{\delta_4\delta_2}}\right)+m_8\left(\sqrt{\frac{\delta_7+\delta_6-2}{\delta_7\delta_6}}\right)+m_9\left(\sqrt{\frac{\delta_6+\delta_6-2}{\delta_6\delta_6}}\right)\\ &+m_{10}\left(\sqrt{\frac{\delta_6+\delta_3-2}{\delta_6\delta_3}}\right)+m_{11}\left(\sqrt{\frac{\delta_6+\delta_5-2}{\delta_6\delta_5}}\right)\\ &=4\left(\frac{6}{15}\right)+2\left(\frac{8}{35}\right)+5\left(\frac{10}{35}\right)+2\left(\frac{12}{49}\right)+8\left(\frac{21}{28}\right)+7\left(\frac{8}{9}\right)+\frac{9}{28}+\frac{11}{42}+\frac{10}{36}\\ &+\frac{7}{18}\\ &=11.42.\end{aligned}$$

(viii) From (2.3), the neighborhood forgotten index,

$$\begin{aligned}NF(G_2) &= m_1\left[(\delta_5)^2+(\delta_3)^2\right]+m_2\left[(\delta_5)^2+(\delta_5)^2\right]+m_3\left[(\delta_5)^2+(\delta_7)^2\right]+m_4\left[(\delta_7)^2+(\delta_7)^2\right]\\ &+m_5\left[(\delta_3)^2+(\delta_7)^2\right]+m_6\left[(\delta_7)^2+(\delta_4)^2\right]+m_7\left[(\delta_4)^2+(\delta_2)^2\right]\\ &+m_8\left[(\delta_7)^2+(\delta_6)^2\right]+m_9\left[(\delta_6)^2+(\delta_6)^2\right]+m_{10}\left[(\delta_6)^2+(\delta_3)^2\right]+m_{11}\left[(\delta_6)^2+(\delta_5^2\right]\\ &=1208.\end{aligned}$$

(ix) From (2.9), the neighborhood sum connectivity index for G_2 is,

$$\begin{aligned}NSCI(G_2) &= m_1\left(\frac{1}{\sqrt{\delta_5+\delta_3}}\right)+m_2\left(\frac{1}{\sqrt{\delta_5+\delta_5}}\right)+m_3\left(\frac{1}{\sqrt{\delta_5+\delta_7}}\right)+m_4\left(\frac{1}{\sqrt{\delta_7+\delta_7}}\right)\\ &+m_5\left(\frac{1}{\sqrt{\delta_3+\delta_7}}\right)+m_6\left(\frac{1}{\sqrt{\delta_7+\delta_4}}\right)+m_7\left(\frac{1}{\sqrt{\delta_4+\delta_2}}\right)+m_8\left(\frac{1}{\sqrt{\delta_7+\delta_6}}\right)\end{aligned}$$

$$+ m_9\left(\frac{1}{\sqrt{\delta_6+\delta_6}}\right) + m_{10}\left(\frac{1}{\sqrt{\delta_6+\delta_3}}\right) + m_{11}\left(\frac{1}{\sqrt{\delta_6+\delta_5}}\right)$$
$$= \frac{4}{\sqrt{8}} + \frac{2}{\sqrt{10}} + \frac{5}{\sqrt{12}} + \frac{2}{\sqrt{14}} + \frac{1}{\sqrt{9}} + \frac{1}{\sqrt{11}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{13}} + \frac{1}{\sqrt{12}} + \frac{1}{\sqrt{11}}$$
$$= 6.25.$$

□

We note that the computation for the remaining eight cholera drugs was performed using (2.1) -(2.9) as illustrated above. Furthermore, we present the numerical parameters obtained from the computation of TIs for ten drugs used in the treatment of cholera in Table 1.

TABLE 1. Neighborhood Degree-sum Based TI of Cholera Drugs

Drug Name	**NM_1(G)**	**NM_2(G)**	**NHP(G)**	**NHM(G)**	**NR(G)**	**NGA(G)**	**NABC(G)**	**NF(G)**	NSCI(G)
Furazolidone	182	488	1992	3.25	5.24	16.79	9.53	1016	3.18
Streptomycine	510	1593	6604	7.54	7.51	40.89	23.04	3647	12.43
Paramomycine	546	1669	6890	7.84	8.11	43.85	24.54	3552	13.17
Tetracycline	478	1674	6974	5.55	5.74	33.70	18.51	3626	9.75
Erythromycine	648	1914	8037	9.25	9.44	24.13	28.35	4209	15.55
Norfloxacine	294	893	3662	4.56	4.56	24.57	13.72	1876	7.48
Ciprofloxacine	328	1022	4176	4.69	4.77	26.63	14.53	2132	7.90
Chloramphenicol	212	566	2340	3.96	4.06	19.56	11.42	1208	6.25
Doxycycline	474	1655	6906	5.63	5.83	33.92	18.52	3596	9.80
Minocycline	478	1629	6774	5.86	6.05	35.01	19.09	3516	10.27

3.1. **Implementation of Linear Regression Model.** To implement our QSPR model, we utilize linear regression to model the relationship between the TIs and physical properties of cholera treatment drugs. We note that the TI is represented as the independent or predictor variable while the physical properties of the cholera treatment drugs obtained from Chemspider and PubChem (National Library of Medicine) represent our depedent or response variable. We therefore present the dataset of the dependent variables variables in Table 2.

TABLE 2. Physicochemical properties of the selected cholera Drugs

Name of drugs	BP	MP	FP	EV	MR	P	MV	ST
Furazolidone	353.4	256	167.5	58.63	50.08	19.78	140	73.5
Streptomycin	872.9	230	481.7	156.55	149.47	55.87	401.1	92.7
Paramomycin	939.8	200	522.2	155.1	134.24	59.03	374.1	106.4
Tetracycline	738.2	172	400.2	113	106.9	42.4	266.3	73.0
Erythromycin	814.4	133	448.8	135.4	189.2	75	607.2	51.4
Norfloxacin	555.8	221	289.9	88.1	80.7	32	237.4	53.2
Ciprofloxacin	581.8	265	305.6	91.5	83.3	33	226.8	67.4
Chloramphenicol	644.9	148	348.8	100	72.6	28.8	208.8	66.1
Doxycycline	554.4	201	449.4	105.53	113.89	43.65	271.1	34.8
Minocycline	803.3	205	439.6	122.5	116.0	46	294.6	90

We employed the linear regression model in (1.2) to model the relationship between Table 1 and Table 2 and predict the physical properties of cholera drugs. Subsequently, the regression model ouput which consists of the statistical parameters are displayed in Table 3 to Table 11.

TABLE 3. Linear regression model parameters for $NM_1(G)$

Physical Property	c	s	R^2	F	p	Indicator	Standard Error
BP	300.8	0.928	0.623	13.219	0.007	significant	0.255
FP	134.58	0.604	0.74	22.65	0.001	significant	0.13
EV	42.898	0.168	0.694	18.176	0.002	significant	0.04
MR	4.28	0.2539	0.898	70.696	0.00	significant	0.03
P	1.0595	0.1024	0.9099	80..811	0.00	significant	0.011
MV	7.036	0.7464	0.752	24.32	0.001	significant	0.151

TABLE 4. Linear regression model parameters for $NM_2(G)$

Physical Property	c	s	R^2	F	p	Indicator	Standard Error
BP	348.72	0.2574	0.55	9.84	0.01	significant	0.08
FP	152.66	0.1776	0.7348	22.18	0.001	significant	0.04
EV	51.62	0.0466	0.6139	12.72	0.007	significant	0.01
MR	19.054	0.0691	0.7669	26.32	0.00089	significant	0.01
P	7.2787	0.0277	0.7657	26.15	0.0009	significant	0.005
MV	51.144	0.192	0.573	10.75	0.01	significant	0.058

TABLE 5. Linear regression model parameters for NHP(G)

Physical Property	c	s	R^2	F	p	Indicator	Standard Error
BP	355.18	0.0609	0.546	9.627	0.014	significant	0.19
FP	156.54	0.0421	0.7311	21.787	0.0016	significant	0.009
EV	52.754	0.011	0.608	12.43	0.007	significant	0.003
MR	20.096	0.0165	0.77	26.98	0.0008	significant	0.03
P	7.7326	0.0066	0.7685	26.569	0.00086	significant	0.001
MV	53.481	0.0459	0.579	11.00	0.01	significant	0.14

Table 6. Linear regression model parameters for NHM(G)

Physical Property	c	s	R^2	F	p	Indicator	Standard Error
BP	228.82	78.636	0.678	16.91	0.003	significant	19.119
FP	114.34	46.25	0.667	16.0821	0.003	significant	11.626
EV	28.957	14.394	0.77	27.31	0.000977	significant	2.7
MR	-14.449	21.346	0.964	214.36	0.00	significant	0.46
P	-6.8009	8.66	0.988	684.63	0.00	significant	0.33
MV	-87.003	67.046	0.9214	93. 87	0.00	significant	6.019

Table 7. Linear regression model parameters for NR(G)

Physical Property	c	s	R^2	F	p	Indicator	Standard Error
BP	239.99	72.74	0.48	7.4	0.02	significant	26.63
FP	127.25	42.103	0.45	6.606	0.03	significant	16.38
EV	28.472	13.727	0.584	11.24	0.01	significant	4.09
MR	-24.292	21.845	0.838	41.57	0.0001	significant	3.38
P	-11.236	8.9367	0.8738	55.4	0.00	significant	1.200
MV	-127.49	70.175	0.838	41.53	0.0001	significant	10.889.

Table 8. Linear regression model parameters for NGA(G)

Physical Property	c	s	R^2	F	p	Indicator	Standard Error
BP	233.49	15.13	0.57	10.66	0.01	significant	4.63
FP	87.839	9.9493	0.6913	17.91	0.0028	significant	2.35
EV	29.719	2.7725	0.6524	15.61	0.0047	significant	0.715
MR	36.662	2.4403	0.2864	3.211	0.11	insignificant	1.361
P	13.017	1.0211	0.3123	3.632	0.09	insignificant	0.535
MV	149.21	5.1338	0.1228	1.12	0.3	insignificant	4.85

Table 9. Linear regression model parameters for NABC(G)

Physical Property	c	s	R^2	F	p	Indicator	Standard Error
BP	234.72	24.895	0.6893	17.74	0.002	significant	5.909
FP	109.93	15.23	0.7218	20.76	0.001	significant	3.34
EV	30.473	4.533	0.777	27.87	0.0007	significant	0.858
MR	-11.63	6.6909	0.9594	189.25	0.00	significant	0,486
P	-5.6792	2.7163	0.9846	512.54	0.00	significant	0.11
MV	-68.964	20.508	0.8734	55.188	0.00	significant	2.76

TABLE 10. Linear regression model parameters for NF(G)

Physical Property	c	s	R^2	F	p	Indicator	Standard Error
BP	357.22	0.1158	0.5603	10.19	0.01	significant	0.036
FP	159.2	0.0797	0.742	23.01	0.001	significant	0.0166
EV	52.551	0.0212	0.6363	13.998	0.0056	significant	0.0056
MR	20.615	0.031	0.7918	30.42	0.0005	significant	0,005
P	8.1662	0.0125	0.779	28.202	0.000719	significant	0.002
MV	55.109	0.0873	0.5936	11.686	0.009	significant	0.02

TABLE 11. Linear regression model parameters for NSCI(G)

Physical Property	c	s	R^2	F	p	Indicator	Standard Error
BP	275.94	42.808	0.7363	22.34	0.001	significant	9.056
FP	134.59	26.184	0.7708	26.906	0.0008	significant	5.05
EV	39.139	7.6733	0.8044	32.09	0.0004	significant	1.34
MR	3.4559	11.087	0.9517	137.58	0.00	significant	0,88
P	0.5291	4.4921	0.9729	287.05	0.00	significant	0.26
MV	-22.437	33.952	0.8648	51.18	0.00	significant	4.74

3.2. **Comparison of Actual and Predicted Physical Properties of Cholera Drugs.** In tables 12-16, we present the tables of comparison between the actual and predicted values of the physical properties, showcasing the influence of each topological indices in predicting the physical properties of cholera drugs.

TABLE 12. Actual values versus predicted values of boiling point (BP) under different neighborhood sum degree TI indices

Actual BP	$NM_1(G)$	$NM_2(G)$	NHP(G)	NHM(G)	NR(G)	NGA (G)	NABC(G)	NF (G)	NSCI(G)
353.4	469.7	474.31	476.397	484.39	621.14	487.57	471.976	474.91	412.07
872.8	774.1	758.696	757.045	821.74	786.62	852.74	808.31	779.67	808.05
939.8	807.5	778.256	774.448	845.33	829.91	896.928	845.65	768.669	839.72
738.8	744.4	779.54	779.56	665.25	657.51	743.36	695.51	777.24	693.32
814.4	902.2	841.309	844.25	955.969	926.65	598.53	940.51	844.77	941.43
555.8	573.6	578.54	578.01	581.938	571.68	605.22	576.16	574.52	596.14
581.8	605.2	611.74	609.29	597.938	586.81	636.39	596.48	604.18	614.13
644.9	497.5	494.385	497.57	540.06	535.31	529.42	519.03	497.15	543.5
554.4	740.7	774.65	775.42	671.54	664.05	746.689	695.786	773.79	695.46
803.3	744.4	767.96	767.38	689.628	680.06	763.40	709.98	764.499	715.6

TABLE 13. Actual values versus predicted values of FP under different neighborhood sum degree TI indices

Actual FP	$NM_1(G)$	$NM_2(G)$	NHP(G)	NHM(G)	NR(G)	NGA(G)	NABC(G)	NF(G)	NSCI(G)
167.5	244.57	239.33	240.40	265.87	347.86	254.89	254.47	240.18	217.85
481.7	442.78	435.58	434.56	465.89	443.44	494.66	460.24	449.86	460.05
522.2	464.53	449.07	446.60	479.87	468.60	524.11	483.08	442.29	479.43
400.2	423.44	449.96	450.14	373.10	368.92	423.13	391.23	448.19	389.88
448.8	526.17	492.58	494.89	545.48	524.60	327.80	541.11	494.65	541.65
289.9	312.25	311.26	310.71	327.04	319.24	332.29	318.21	308.72	330.45
305.6	332.80	334.17	332.35	333.19	327.99	352.79	330.64	329.12	341.44
348,8	262.70	253.18	255.05	298.88	298.18	282.45	283.26	255.48	298.24
449.4	421.02	446.59	447.28	376.83	372.71	425.32	391.39	445.70	391.19
439.6	423.44	441.97	441.72	387.56	381.97	436.16	400.07	439.42	403.5

TABLE 14. Actual values versus predicted values of EV under different neighborhood sum degree TI indices

Actual EV	$NM_1(G)$	$NM_2(G)$	NHP(G)	NHM(G)	NR(G)	NGA(G)	NABC(G)	NF(G)	NSCI(G)
58.63	73.47	74.34	74.697	75.74	100.40	76.27	73.67	74.06	63.54
156.55	128.59	125.79	125.503	137.488	131.56	143.088	134.91	129.76	134.51
155.1	134.64	129.33	128.65	141.81	139.79	151.29	141.71	127.75	140.1965
113	123.21	129.56	129.57	108.84	107.266	123.15	114.37	129.31	113.95
135.4	151.78	140.74	141.28	162.058	158.05	96.61	158.98	141.66	158.43
88.1	92.29	93.20	93.09	94.62	91.068	97.84	92.64	92.268	96.53
91.5	98.01	99.21	98.75	96.52	93.92	103.55	96.34	97.688	99.75
100	78.52	77.97	78.53	85.92	84.82	83.95	82.24	78.125	87.09
105.53	122.54	128.68	128.83	109.99	108.50	123.76	114.42	128.68	114.34
122.5	123.21	127.47	127.37	113.3	111.52	126.78	117	126.989	117.94

TABLE 15. Actual values vs predicted values of MR under different neighborhood sum degree TI indices

Actual MR	$NM_1(G)$	$NM_2(G)$	NHP(G)	NHM(G)	NR(G)	NGA(G)	NABC(G)	NF(G)	NSCI(G)
50.08	50.485	52.79	52.91	54.93	90.17	77.63	52.13	52.487	38.71
149.47	133.756	129.181	128.88	146.50	139.76	136.44	142.52	135.02	141.2611
134.24	142.895	134.43	133.598	152.9045	152.87	143.67	152.56	132.04	149.4651
106.9	125.632	134.78	134.98	104.0218	101.1008	118.899	112.21	134.36	111.55
189.2	168.791	151.37	152.49	182.94	181.9288	95.54	178.055	152.65	175.807
80.7	78.919	80.789	80.42	82.93	75.32	96.61	80.134	79.46	86.38
83.3	87.55	89.707	88.88	85.749	79.87	101.646	85.59	87.49	91.04
72.6	58.101	58.18	58.64	70.038	64.4	84.39	64.779	58.51	72.746
113.89	124.616	133.468	133.86	105.729	103.0669	119.44	112.28	133.42	112.10
116	125.632	131.67	131.68	110.6391	107.87	112.096	116.098	130.91	117.31

TABLE 16. Actual valies versus predicted values of P under different neighborhood sum degree TI indices

Actual P	$NM_1(G)$	$NM_2(G)$	NHP(G)	NHM(G)	NR(G)	NGA(G)	NABC(G)	NF(G)	NSCI(G)
19.78	19.69	20.788	20.86	21.35	35.59	30.16	20.21	20.83	14.81
55.87	53.28	51.379	51.138	58.511	55.87	54.79	56.91	53.64	56.36
59.03	56.966	53.483	53.138	61.11	61.24	57.79	60.97	52.46	59.69
42.4	50	53.62	53.691	41.27	40.06	47.428	44.59	53.38	44.33
75	67.41	60.26	60.697	73.297	73.126	36.65	71.33	60.65	70.36
32	31.16	32	31.865	32.715	29.515	38.105	31.57	31.56	34.13
33	34.64	35.57	35.25	33.85	31.37	40.21	33.79	34.75	36.02
28.8	22.76	22.948	23.15	27.48	25.046	32.98	25.34	23.23	28.60
43.65	49.59	53.095	53.24	41.966	40.86	47.65	44.63	53	44.55
46	50	52.37	52.37	43.95	42.83	48.76	46.17	52.01	46.66

TABLE 17. Actual values versus predicted values of MV under different neighborhood sum degree TI indices

Actual MV	$NM_1(G)$	$NM_2(G)$	NHP(G)	NHM(G)	NR(G)	NGA(G)	NABC(G)	NF(G)	NSCI(G)
140	128.817	144.847	144.83	130.89	240.2285	235.411	126.48	143.766	85.53
401.1	373.65	357.02	356.32	418.5	399.5247	359.136	403.549	373.35	399.58
374.1	400.524	371.61	369.44	438.63	441.6294	374.33	434.311	365.06	424.71
266.3	349.766	372.57	373.29	285.1	275.3158	322.22	310.62	371.51	308.59
607.2	476.662	418.6588	422.04	532.96	534.9615	273.083	512.45	422.39	505.38
237.4	212.419	222.6126	221.41	218.859	192.5099	273.35	212.31	218.81	231.52
226.8	237.798	247.38	244.98	227.709	207.1062	285.93	229.04	241.15	245.78
208.8	151.210	159.82	160.79	178.36	157.4226	249.63	165.24	160.52	189.76
271.1	346.780	368.93	370.17	290.46	281.6315	323.35	310.85	368.90	310.29
294.6	349.766	363.93	364.12	305.88	297.0699	328.94	322.55	361.92	326.248

3.3. **QSPR Models of Physical Properties.** In this subsection, we develop the QSPR model equations for each physical property. This models were developed using (1.2).

(i) Model equations for $NM_1(G)$ index

$$\begin{aligned}
\text{BP} &= 0.981\,(\text{NM}_1(G)) + 3008\\
\text{FP} &= 0.604\,(\text{NM}_1(G)) + 134.68\\
\text{EV} &= 0.168\,(\text{NM}_1(G)) + 42.898\\
\text{MR} &= 0.254\,(\text{NM}_1(G)) + 4.28\\
\text{P} &= 0.1024\,(\text{NM}_1(G)) + 1.0595\\
\text{MV} &= 0.7464\,(\text{NM}_1(G)) + 7.0364
\end{aligned}$$

(ii) Model Equations for the $NM_2(G)$ Index

$$\begin{aligned}
\text{BP} &= 0.2574\,(\text{NM}_2(G)) + 348.72\\
\text{FP} &= 0.1776\,(\text{NM}_2(G)) + 152.66\\
\text{EV} &= 0.0466\,(\text{NM}_2(G)) + 51.62\\
\text{MR} &= 0.0691\,(\text{NM}_2(G)) + 19.054\\
\text{P} &= 0.0277\,(\text{NM}_2(G)) + 7.279\\
\text{MV} &= 0.192\,(\text{NM}_2(G)) + 51.44
\end{aligned}$$

(iii) Model Equations for the NHP(G) Index

$$\begin{aligned}
\text{BP} &= 0.0609\,(\text{NHP}(G)) + 355.18\\
\text{FP} &= 0.0421\,(\text{NHP}(G)) + 156.54\\
\text{EV} &= 0.011\,(\text{NHP}(G)) + 52.74\\
\text{MR} &= 0.0165\,(\text{NHP}(G)) + 20.096\\
\text{P} &= 0.0066\,(\text{NHP}(G)) + 7.7326\\
\text{MV} &= 0.0459\,(\text{NHP}(G)) + 53.481
\end{aligned}$$

(iv) Model Equations for NHM(G) Index

$$\begin{aligned}
\text{BP} &= 78.636\,(\text{NHM}(G)) + 228.82\\
\text{FP} &= 46.625\,(\text{NHM}(G)) + 114.34\\
\text{EV} &= 14.394\,(\text{NHM}(G)) + 28.957\\
\text{MR} &= 21.346\,(\text{NHM}(G)) - 14.449\\
\text{P} &= 8.662\,(\text{NHM}(G)) - 6.8009\\
\text{MV} &= 67.046\,(\text{NHM}(G)) - 87.003
\end{aligned}$$

(v) Model Equations for NR(G) Index

$$\begin{aligned}
\text{BP} &= 72.74\,(\text{NR}(G)) + 239.99\\
\text{FP} &= 42.103\,(\text{NR}(G)) + 127.103\\
\text{EV} &= 13.727\,(\text{NR}(G)) + 28.472\\
\text{P} &= 8.9367\,(\text{NR}(G)) - 11.236\\
\text{MR} &= 21.845\,(\text{NR}(G)) - 24.292\\
\text{MV} &= 70.175\,(\text{NR}(G)) - 127.49
\end{aligned}$$

(vi) Model Equations for NGA(G) Index

$$\begin{aligned}
\text{BP} &= 15.13\,(\text{NGA}(G)) + 233.49\\
\text{FP} &= 9.9493\,(\text{NGA}(G)) + 87.839\\
\text{EV} &= 2.7725\,(\text{NGA}(G)) + 29.719\\
\text{MR} &= 2.4403\,(\text{NGA}(G)) + 36.662\\
\text{P} &= 1.0211\,(\text{NGA}(G)) + 13.017\\
\text{MV} &= 5.1338\,(\text{NGA}(G)) + 149.21
\end{aligned}$$

(vii) Model Equations for NABC(G) Index

$$\begin{aligned}
\text{BP} &= 24.895\,(\text{NABC}(G)) + 234.72\\
\text{FP} &= 15.23\,(\text{NABC}(G)) + 109.33\\
\text{EV} &= 4.533\,(\text{NABC}(G)) + 30.473\\
\text{MR} &= 6.6909\,(\text{NABC}(G)) - 11.63\\
\text{P} &= 2.7163\,(\text{NABC}(G)) - 5.6792\\
\text{MV} &= 20.508\,(\text{NABC}(G)) - 68.964
\end{aligned}$$

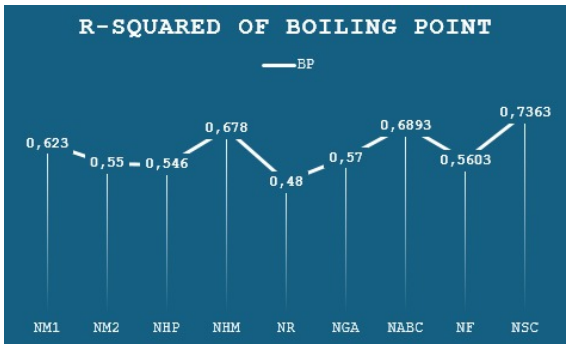
(viii) Model Equations for NF(G) Index

$$\begin{aligned}
\text{BP} &= 0.1158\,(\text{NF}(G)) + 357.22\\
\text{FP} &= 0.0797\,(\text{NF}(G)) + 159.2\\
\text{EV} &= 0.0212\,(\text{NF}(G)) + 52.551\\
\text{MR} &= 0.0314\,(\text{NF}(G)) + 20.615\\
\text{P} &= 0.0125\,(\text{NF}(G)) + 8.1662\\
\text{MV} &= 0.0873\,(\text{NF}(G)) + 55.109
\end{aligned}$$

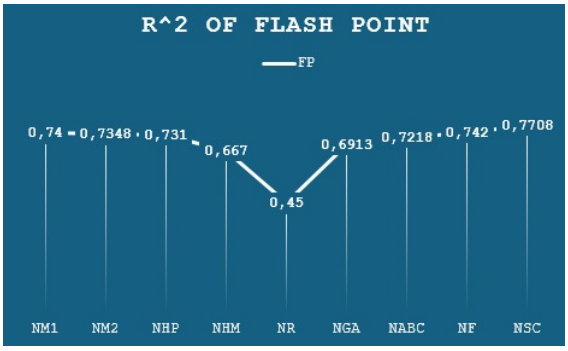
(ix) Model Equation for NSC(G) Index

$$\begin{aligned}
\text{BP} &= 42.808\,(\text{NSC}(G)) + 275\\
\text{FP} &= 26.148\,(\text{NSC}(G)) + 134.59\\
\text{EV} &= 7.6733\,(\text{NSC}(G)) + 39.139\\
\text{MR} &= 11.087\,(\text{NSC}(G)) + 3.4559\\
\text{P} &= 4.4921\,(\text{NSC}(G)) + 0.5291\\
\text{MV} &= 33.952\,(\text{NSC}(G)) - 22.437
\end{aligned}$$

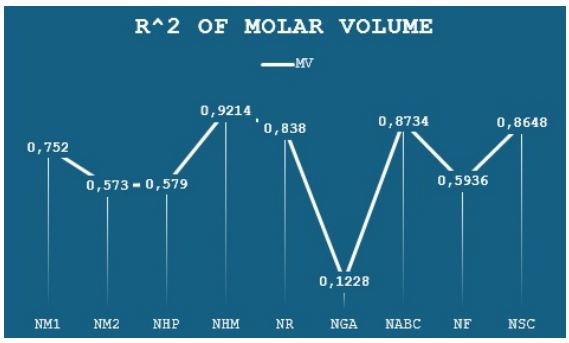
Next, we visualize the R^2 values for various physical properties of cholera drugs. This visualization allows us to identify the properties that exhibited a perfect or nearly perfect fit within the model, helping us assess their impact on the overall model.



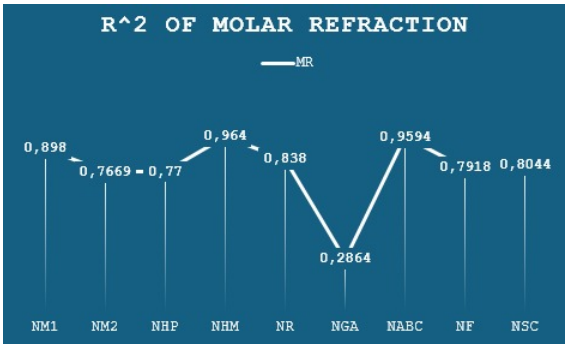
(A) Boiling Point



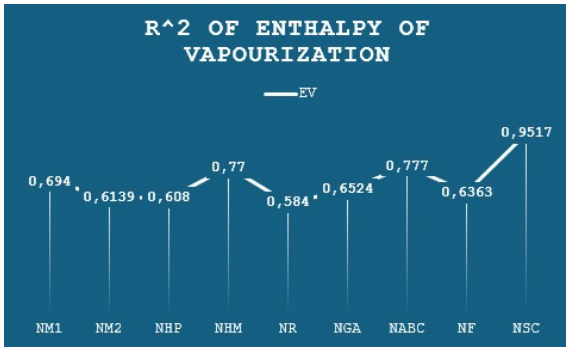
(B) Flash Point



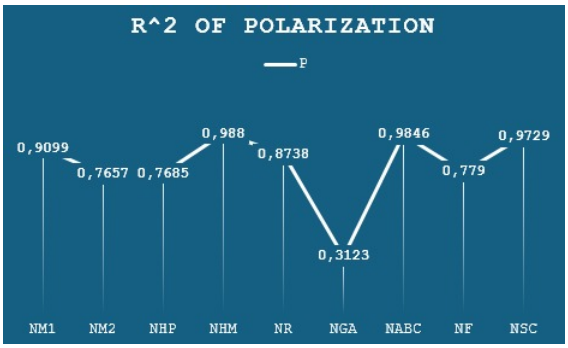
(C) Molar Volume



(D) Molar Refraction



(E) Enthalpy of Vaporization



(F) Polarization

FIGURE 11. Coefficient of Determination (R^2) for various properties

3.4. **Discussion of Results.** The performance of the neighborhood sum degree TI in predicting the physical properties of cholera drugs via linear regression models demonstrates varying levels of effectiveness. The majority of models have significant p-values (< 0.05), indicating a strong relationship between the TI and the physical properties of the drugs. The R^2 values vary across models and physical properties, providing insight into the effectiveness of each index.

3.4.1. *Performance of Topological Indices.*

(i) The neighborhood First Zagreb Index $NM_1(G)$ demonstrates strong R^2 values for molar refraction (0.898) and polarization (0.9099), highlighting its excellent predictive ability for these properties. For boiling point and enthalpy of vaporization, it achieved moderate R^2 values of 0.623 and 0.694, while flash point and molar volume yielded R^2 values of 0.74 and 0.752, respectively, showcasing the index's reliability in predicting these properties. Additionally, $NM_1(G)$ consistently produced significant p-values across the model. Overall, $NM_1(G)$ proves to be most effective for polarization and molar refraction.

(ii) The neighborhood second Zagreb index $(NM_2(G))$ achieved R^2 values ranging from $(0.55 \leq R^2 \leq 0.77)$ across the physical properties. The significant p-values across all properties affirm its utility in modeling the physical physical properties of the drugs.

(iii) The neighborhood hyper Zagreb index NHP(G) achieved R^2 values ranging from $(0.54 \leq R^2 \leq 0.77)$ across the physical properties. It further demonstrates strong predictive power, particularly for molar refraction $R^2 = 0.77$ and polarization $R^2 = 0.7685$. It also recorded significant p-values throughout the model.

(iv) The neighborhood harmonic index NHM(G) achieved its highest fit for molar refraction $(R^2 = 0.964)$, polarization $(R^2 = 0.988)$ and molar volume (0.924) making NHM(G) highly effective for these properties. For boiling point and flash point, moderate R^2 values (0.678 and 0.667) were recorded. All the p-values of NHM (G)are significant throughout the model.

(v) The neighborhood Randić Index (NR(G)) is effective in predicting molar refraction $(R^2 = 0.838)$, polarization (0.874) and molar volume (0.838), it obtained lower R^2 values for boiling points, flash points and enthalpy of vaporization. All the p-values were significant.

(vi) The neighborhood geometric arithmetic index (NGA(G)) shows moderate performance overall, with R^2 values peaking for flash point (0.6913), boiling point (0.57) and enthalpy of vaporization (0.6524). It recorded very low R^2 values for molar refraction and polarization, and molar volume (0.2864, 0.3123 and 0.1228 respectively) which suggested limited effectiveness or lack of relationship between the physical properties and neighborhood sum degree TI. It also recorded insignificant p-values for these properties.

(vii) The neighborhood atom bond connectivity index (NABC(G)) is highly predictive for molar refraction $((R^2 = 0.9594))$, polarization $(R^2 = 0.9846)$ and molar volume (0.8734). It achieved moderate R^2 values for boiling point,flash point and enthalpy of vaporization indicating its utility across diverse properties. All the p-values of NABC(G) were significant in the model.

(viii) The neighborhood forgotten index $(NF(G))$ obtained moderate performance with an R^2 of 0.742 for flash point, 0.7918 for molar refraction and $R^2 = 0.779$ for polarization. Other physical properties obtained slightly lower values. Its consistent R^2 values and significant p-values across the physical properties affirm its utility as a reliable descriptor.

(ix) The neighborhood sum connectivity index $NSCI(G)$ exhibits exceptional predictive power for the enthalpy of vaporization, molar refraction and polarization with values of $R^2 = 0.8044, 0.9517, 0.9729, 0.8648$). Other physical properties of boiling points and flash points obtained slightly lower R^2 values. The p-values across properties reinforce the robustness of NSCI(G) in property modeling.

4. Conclusions

This study explored the efficacy of neighborhood sum degree TIs in predicting the physical properties of cholera drugs through linear regression models. The results demonstrated that the indices provide varying levels of effectiveness and most models exhibit significant p-values (< 0.05), which indicate strong correlations between the topological indices and the physical properties. The results demonstrate that neighborhood sum degree TIs are effective in QSPR modeling of cholera drugs. The high R^2 values for several indices indicate their potential to accurately predict key physical properties, particularly molar refraction and polarization. Among all indices, NHM(G), NSCI(G), and NABC(G) stand out for their high R^2 values and low standard errors in predicting molar refraction and polarization. For boiling point and flash point, $NM_1(G)$, $NM_2(G)$, and NR(G) provide moderate predictive power. Some indices such as NHP(G), NM_2(G) and NF(G) show moderate performance for all physical properties, while the NGA(G) recorded the lowest performance while failing to model molar refraction, polarization, and molar volume, this is evident in the very low R^2 and insignificant p-values recorded. In contrast, indices such as NHM(G), NSCI(G), and NABC(G) excel in both predictive accuracy and consistency across diverse physical properties. This highlights the versatility and importance of neighborhood sum degree TI in QSPR modeling of cholera drugs. Overall, the study confirms the utility of neighborhood sum degree-based indices in modeling the physical properties of cholera drugs. The findings highlight their potential for broader applications in QSPR modeling, with specific indices such as NHM(G), NABC(G), and NSCI(G) demonstrating exceptional predictive accuracy. Future research could focus on applying these indices to other chemical compounds and exploring their integration with advanced machine learning models to enhance predictive performance.

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