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STRUCTURAL MODELING OF PLANT REGULATORS BASED ON TOPOLOGICAL INDICES AND CURVE FITTING

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Abstract. Topological indices are important quantifiers of chemical graphs which are valuable tools to establish quantitative structure-property relationship (QSPR) modeling. This work derives topological indices of plant growth regulators and their QSPR models. Plant growth regulators (PGRs) are substances, either organic or inorganic, that influence the metabolic and developmental activities of plants. Investigating the physiochemical and biological properties of various regulators is crucial for elucidating their theoretical char-acteristics with greater precision. This study employs degree-based topological indices to achieve a comprehensive structural analysis of PGRs. Thirteen of the plant regulators' topological indices are used to construct a QSPR model after fifteen plant regulators are assessed for some of their physiochemical characteristics. Accord-ing to this QSPR model, properties including molar refractivity, complexity, flash point, molar volume of plant regulators are highly correlated to the indices. Moreover, we conducted a comparative analysis of curvilinear regression models and singled out best fit models of topological indices which give high prediction of phys-iochemical properties of the regulators. It gives an insight to the potential of topological indices (TIs) to better represent theoretical characteristics and exhibits effective computational approach to the structural analysis of PGRs.

Keywords: chemical graph, curvilinear regression, QSPR model, topological in-dices.

1. Introduction

Plant growth regulators (PGRs), also referred to as phytohormones, are naturally occurring organic compounds in higher plants. They are not nutrients but influence growth and other physiological processes at sites distant from their origin, even in very low concentrations [18]. PGRs, sometimes referred to as biostimulants or bio-inhibitors, function within plant cells to activate or suppress enzymes or enzyme systems, thereby regulating plant metabolism. They often only become active in plants at extremely low concentrations. Examples of plant growth regulators include auxins, cytokinins, ethylene, gibberellins, growth inhibitors, and growth retardants. The first hormones found in plants were auxins; later, gibberellins and cytokinins were also found. To distinguish plant hormones from animal hormones, Thimann [21], in 1963, gave them the name "phytohormones" (because these hormones are produced in plants). He defined a phytohormone as a naturally produced organic compound in higher plants that controls growth or other physiological processes at sites distant from its origin and is effective in minimal quantities. Van Overbeek et al. [16] defined plant hormones with an even broader reach. He describes plant hormones as organic substances that regulate plant physiological functions. These compounds can be either natural or synthetic and may either stimulate or inhibit processes. Additionally, they can act locally or at sites distant from where they are produced. Only naturally occurring plant compounds that fit into one of five categories are allowed. Gibberellins, ABA, ethylene, auxin, and cytokinin. Hor-mones that exist naturally as well as synthetic substances make up plant growth regulators. In the 1930s, the significance of PGRs was first appreciated. Since then, both natural and man-made substances that modify the size, shape, and function of agricultural plants have been found. Today, certain PGRs are employed to alter the growth pattern and pace of crops at various developmental phases, from germi-nation to harvest and post-harvest storage. It may be beneficial to use chemicals that regulate growth and have a good impact on important agronomic crops.

Topological Indices (TIs) are numerical descriptors obtained from chemical graphs that comprehensively characterize chemical systems. They are commonly em-ployed in the study of the physicochemical properties of various drugs. In chemical graph theory, polynomials and TIs are widely used to represent chemical structures [14, 4, 3]. Graph invariants, also known as Topological Indices (TIs), are utilized in diverse disciplines including bioinformatics, mathematics, informatics, and biology. Recently, they have gained significant attention in research involving quantitative structure-property relationships (QSPR) and quantitative structure-activity rela-tionships (QSAR). Bhatia [5] explored the physicochemical importance of Topological Indices (TIs) by examining their correlations with empirical parameters to explain physicochemical properties, as well as their use in developing predictive

QSAR models. Recently researchers [1, 2, 19, 15] investigated the physicochemical relevance of topological parameters using QSPR integrated with decision making and machine learning. For additional information on QSPR modeling for specific drugs, readers are encouraged to consult further studies [13, 12, 20].

We analysed some of the physiochemical traits of fifteen plant regulators and used thirteen topological indices to build a QSPR model. For this, we create models that connect each of the topological indices of the medications to the traits of plant regulators and computationally generate topological indices of the pharmaceuticals. According to this QSPR model, Molar Refractivity (MR), Molar volume (MV), Complexity (C) and Molar Weight (MW)of plant regulators are strongly connected.

2. Preliminaries

In the representation of drug structures, atoms serve as the vertices and the connections between them are known as edges. V and E denote the sets of vertices and edges in a chemical graph, respectively. The graph is considered to be simple, finite, and connected. The degree of a vertex in the graph Ω, the number of vertices adjacent to it, is denoted as d_u. The concepts of a compound's valence and a graph vertex's degree are closely related in chemistry [24, 7]. This article is inspired by the notion that distinct drugs (structures) can be identified and their properties can be predicted by analyzing them for their correlation with topological indices, by considering different statistical measures. Certain well-known topological indices which are employed in our computations are introduced as follows.

Definition 2.1. Atom Bond Connectivity index ($ABC(\Omega)$) was introduced by Estrada et al. in their work [6] where it is described as:

$$ABC(\Omega) = \sum_{uv\epsilon G} \sqrt{\frac{d_u + d_v + 2}{d_u d_v}}.$$

Definition 2.2. Randic index ($\chi(\Omega)$) was introduced by Milan Randic in their work [17] is formulated as:

$$RA(\Omega) = \sum_{uv\in E} \frac{1}{\sqrt{d_u d_v}}.$$

Definition 2.3. The first Zagreb index, denoted by $M_1(\Omega)$, was introduced by Gutman and Trinajestic in their research [10] stated as below:

$$M_1(\Omega) = \sum_{uv\in E} \left[d_u + d_v\right],$$

Definition 2.4. The Harmonic index $[H(\Omega)]$, proposed by Fajtlowicz in [8], is described as:

$$H(\Omega) = \sum_{uv\in E} \frac{2}{[d_u + d_v]}.$$

Definition 2.5. The sum-connectivity index, $SCI(\Omega)$, was introduced by Zhou and Trinjstic [26] is formulated as:

$$SCI(\Omega) = \sum_{uv \in E} \frac{1}{\sqrt{d_u + d_v}}.$$

Definition 2.6. The Geometric-Arithmetic index ($GA(\Omega)$) was introduced by Vukicevic et al. [22] and is stated as:

$$GA(\Omega) = \sum_{uv \in E} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

Definition 2.7. Vukicevic et al. [23] introduced inverse sum index, $IS(\Omega)$, which is described as:

$$IS(\Omega) = \sum_{uv \in E} \frac{d_u d_v}{d_u + d_v}.$$

Definition 2.8. Recently, Zhao et al. [25] formulated the Shilpa-Shanmukha index, $SS(\Omega)$, stated as:

$$SS(\Omega) = \sum_{uv \in E} \sqrt{\frac{d_u d_v}{d_u + d_v}}.$$

Definition 2.9. Gutman [11] formulated the Sombor index, $SO(\Omega)$, stated as:

$$SO(\Omega) = \sum_{uv \in E} \sqrt{d_u^2 + d_v^2}.$$

3. Quantitative Structure-Property Relations Using Curve Fitting

This section deals with curve-fitting models built with the help of Topological indices of regulators. We use linear, quadratic and cubic curves in quest of best fitting. We use a known dataset of PGRs to train our models and the same dataset is used for validation, comparison and finding standard error of estimate. The study examines thirteen plant regulators and presents their chemical structures in Figure 1. Regression analysis is applied to analyze these regulators. The computational analysis of drug structures focuses on thirteen topological indices for QSPR modeling. Table 1 lists the computed topological indices for the drugs. Additionally, Table 2 includes four physical properties: Molar Refractivity (MR), Molar Volume (MV), Complexity (C), and Molar Weight (MW). Linear, quadratic, and cubic models are implemented using the following equation:

$$P = a + b_1(TI) \quad n, R^2, SE, F, S_F \tag{1}$$

$$P = \alpha + b_1(TI) + b_2(TI)^2 \quad n, R^2, SE, F, S_F \tag{2}$$

$$P = a + b_1(TI) + b_2(TI)^2 + b_3(TI)^3 \quad n, R^2, SE, F, S_F \tag{3}$$

Equations 1, 2, and 3 represent curvilinear regression models with the following terms: n (number of samples), R^2 (coefficient of determination), SE (standard error of estimate), F (Fisher F-test value), and S_F (F-significance). Here, P represents

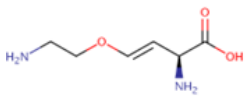
TABLE 1. Topological indices related to Plant regulators.

Drug's name	ABC(Ω)	RA(Ω)	M_1(Ω)	H(Ω)	SCI(Ω)	GA(Ω)	IS(Ω)	SS(Ω)	SO(Ω)
Aviglycine	7.358	5.181	42	4.9	4.933	9.521	9.617	9.735	30.885
Buminafos	16.327	11.139	104	10.816	11.074	22.342	24.467	23.531	75.618
Clofibric acid	10.484	6.415	68	5.919	6.416	13.029	14.897	14.328	50.889
Cloxyfonac	10.187	6.631	64	6.3	6.616	13.399	14.816	14.307	46.861
Dichlorprop	10.365	6.503	66	6.067	6.499	13.208	14.95	14.352	48.758
Etacelasil	12.727	9.243	76	9	8.942	17.542	18	17.885	55.117
Ethephon	4.7194	3.061	28	2.7	2.827	5.285	5.4	5.6545	21.905
Ethychlozate	12.159	7.703	80	7.434	7.918	16.493	18.967	17.857	57.981
Fenoprop	11.142	6.913	72	6.4	6.908	14.075	16.2	15.443	53.335
Glyoxime	3.535	2.914	18	2.834	2.655	4.885	4.334	4.6329	12.957
Kinetin	12.647	7.933	84	7.867	8.394	17.838	20.6	19.213	59.957
Metoxuron	10.963	7.041	70	6.634	7.024	14.265	16.067	15.398	51.437
Naphthaleneacetamide	10.745	6.771	70	6.567	6.999	14.611	16.7	15.754	50.585
Pentachlorophenol	8.898	5.464	60	5	5.449	11.196	13.5	12.545	44.429
Thidiazuron	11.423	7.343	72	7.2	7.577	15.704	17.35	16.629	51.805
Tribufos	11.473	8.182	68	7.9	7.904	15.456	15.8	15.808	49.704
Zeatin	12.049	7.808	78	7.634	8.024	16.667	18.816	17.800	56.093

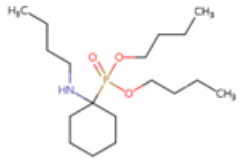
the dependent variable denoting the physicochemical property of the drug, while TI (topological index) serves as an independent variable. Constants are denoted by 'a', and regression coefficients 'b_1, b_2, b_3' quantify the relationship strength between the physicochemical property (P) and the topological index (TI) in the respective regression models (1). Analysis employed Microsoft Excel and SPSS software [9] for data processing. Curvilinear models were applied to analyze nine topological indices of plant regulators and their associated properties. The correlation explored between plant regulatory activity and topological indices suggests a link between the biological activity of plant regulators and molecular structural features represented by these indices. The information presented in Table 2 was obtained from ChemSpider and PubChem.

TABLE 2. Physical properties related to plant regulators.

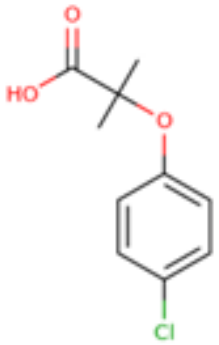
Drug's name	MR	MV	C	MW
Aviglycine	40.2	129.9	147	160.17
Buminafos	97.2	352.1	329	347.5
Clofibric acid	53.3	169.6	207	214.64
Cloxyfonac	50.5	150.3	197	216.62
Dichlorprop	53.5	165.4	210	235.06
Etacelasil	77.0	295.4	172	316.85
Ethephon	26.1	92.1	86.9	144.49
Ethychlozate	62.1	176.4	262	238.67
Fenoprop	58.4	177.3	237	269.5
Glyoxime	19.6	68.1	57.9	88.07
Kinetin	59.2	144.5	239	215.21
Metoxuron	60.5	182.2	224	228.67
Naphthaleneacetamide	57.2	157.2	214	185.22
Pentachlorophenol	52.6	147.6	150	266.3
Thidiazuron	-	-	220	220.25
Tribufos	88.5	292.7	179	314.5
Zeatin	59.5	156.6	258	219.24



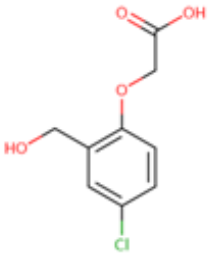
(A) Aviglycine



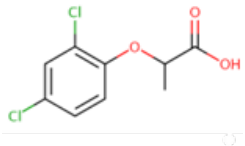
(B) Buminafos



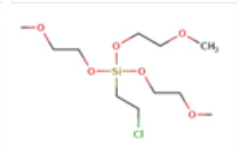
(C) Clofibric acid



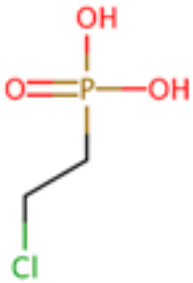
(D) Cloxyfonac



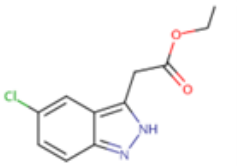
(E) Dichlorprop



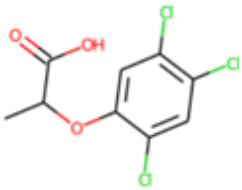
(F) Etacelasil



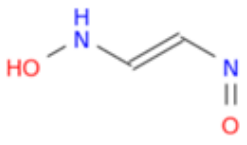
(G) Ethephon



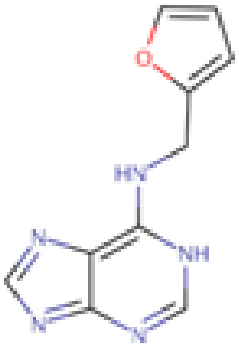
(H) Ethychlozate



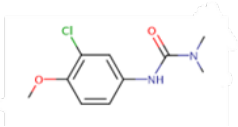
(I) Fenoprop



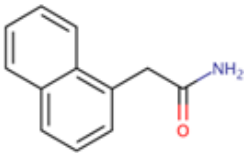
(J) Glyoxime



(K) Kinetin

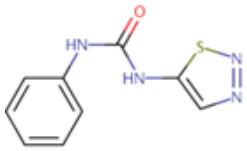


(L) Metoxuron

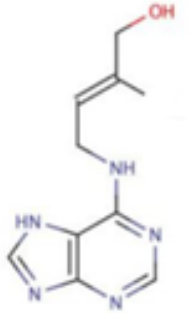


(M) Naphthaleneacetamide

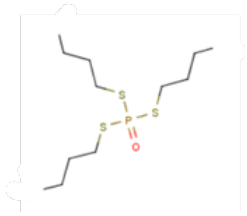
(N) Pentachlorophenol



(O) Thidiazuron



(P) Zeatin



(Q) Tribufos

FIGURE 1. Plant regulators with their chemical structure

The application of QSPR modeling has facilitated the analysis of the correlation between TIs and the physical properties of plant regulators. Analyses of this kind help understand the characteristics of recently developed regulators. The linear correlation coefficient (R), which was calculated using a linear regression model, is displayed in Table 3 between certain physicochemical parameters and degree-based topological indicators. Table 5 represents the correlation coefficient (R) among topological indices and various physicochemical characteristics using a quadratic regression model. In a similar way, Table 7 shows the cubic correlation coefficient (R) for topological indices and several physicochemical properties. The regression model with the highest R value for each physicochemical property is considered the most accurate predictor. The tables contain only values of R greater than 0.7 for convenience. Applying models of curvilinear regression model, the largest R becomes the most accurate predictor for a given physicochemical attribute. The ideal topological index for physicochemical property estimation is shown in Table 4. Figure 2 illustrates the cubic curve fitting through dataset.

3.1. **Analysis of Curvilinear Regression Models.** Table 3 presents the correlation coefficients (R) derived from a linear regression analysis that connects the various degree-based topological indices with appropriate physicochemical characteristics of plant regulators. These coefficients differ depending on the indices and properties analyzed. A positive correlation implies that variables tend to change in tandem, whereas a negative correlation indicates opposite trends. Specifically,

TABLE 3. Linear correlation coefficient (R).

Physicochemical properties	Molar Refractivity	Molar Volume	Complexity	Molecular Weight
ABC(Ω)	0.909	0.794	0.922	0.828
RA(Ω)	**0.948**	**0.879**	0.849	**0.854**
$M_1(\Omega)$	0.865	0.723	**0.943**	0.793
H(Ω)	0.938	0.867	0.838	0.828
SCI(Ω)	0.927	0.832	0.882	0.823
GA(Ω)	0.903	0.785	0.905	0.793
IS(Ω)	0.856	0.707	0.936	0.762
SS(Ω)	0.883	0.749	0.927	0.785
SO(Ω)	0.866	0.729	**0.943**	0.805

TABLE 4. Optimal linear regression models for the physical characteristics of plant growth regulators.

Linear best regression model	R^2	F	SE
$\mathbf{MR = 9.034(RA) - 4.273}$	0.898	123.513	6.485
$\mathbf{MV = 31.733(RA) - 37.401}$	0.772	47.530	36.721
$\mathbf{C = 3.000(M_1) + 1.772}$	0.890	121.281	22.268
$\mathbf{C = 4.200(SO) - 2.775}$	0.890	121.587	22.244
$\mathbf{MW = 27.580(RA) + 39.702}$	0.730	40.545	34.627

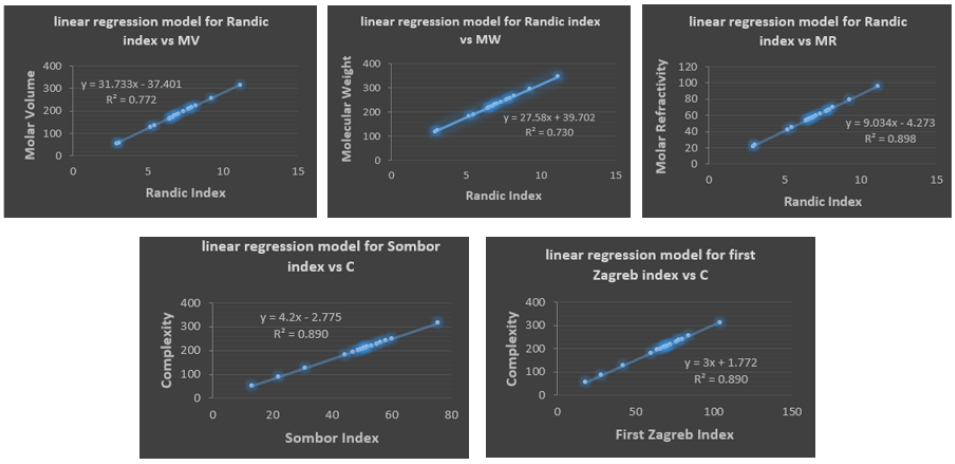


FIGURE 2. Linear curve fitting for predicting optimal physicochemical properties using degree-based topological indices.

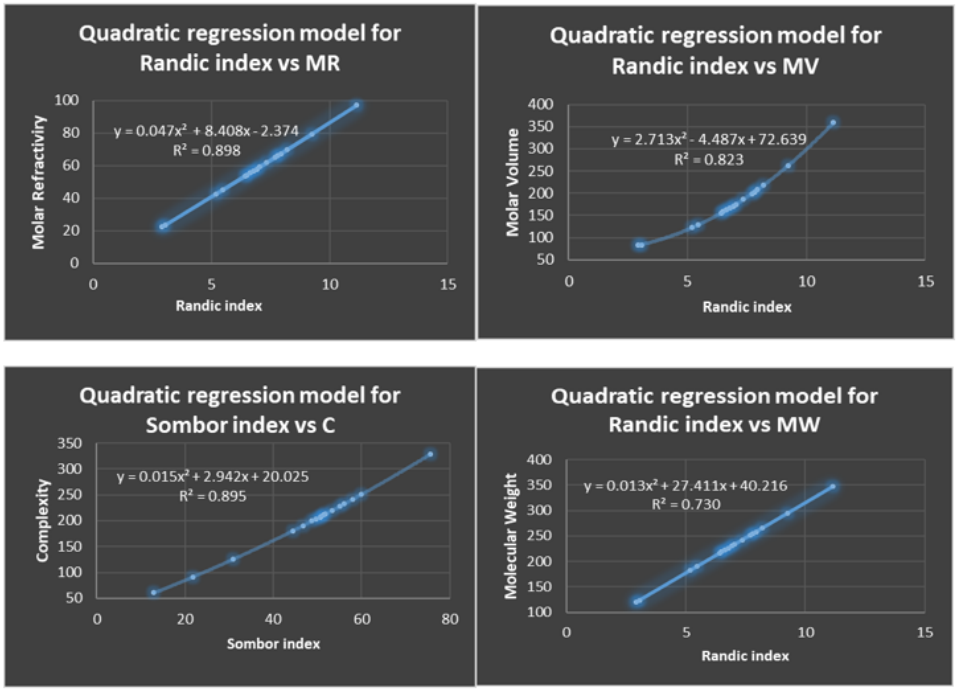


FIGURE 3. Quadratic curve fitting for predicting optimal physicochemical properties using degree-based topological indices.

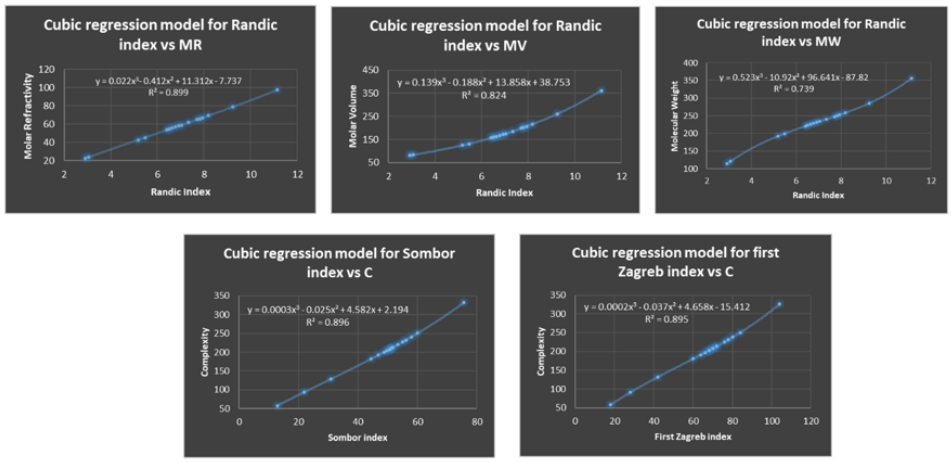


FIGURE 4. Cubic curve fitting for predicting optimal physicochemical properties using degree-based topological indices.

TABLE 5. Quadratic correlation coefficient(R).

Physicochemical properties	Molar Refractivity	Molar Volume	Complexity	Molecular Weight
ABC(Ω)	0.912	0.829	0.922	0.828
RA(Ω)	**0.948**	**0.907**	0.865	**0.854**
$M_1(\Omega)$	0.866	0.745	0.945	0.794
H(Ω)	0.938	0.892	0.856	0.827
SCI(Ω)	0.928	0.860	0.887	0.822
GA(Ω)	0.903	0.807	0.905	0.793
IS(Ω)	0.856	0.718	0.936	0.765
SS(Ω)	0.883	0.768	0.927	0.786
SO(Ω)	0.868	0.754	**0.946**	0.805

TABLE 6. Best estimated Quadratic regression models for physical properties.

Quadratic best regression model	R^2	F	SE
$\mathbf{MR = 0.047(RA)^2 + 8.408(RA) - 2.374}$	**0.898**	57.482	6.722
$\mathbf{MV = 2.713(RA)^2 - 4.487(RA) + 72.639}$	0.823	30.297	33.577
$\mathbf{C = 0.015(SO)^2 + 2.942(SO) + 20.025}$	0.895	59.762	22.497
$\mathbf{MW = 0.013(RA)^2 + 27.411(RA) + 40.216}$	0.730	18.921	35.843

TABLE 7. Cubic correlation coefficient(R).

Physicochemical properties	Molar Refractivity	Molar Volume	Complexity	Molecular Weight
ABC(Ω)	0.913	0.834	0.925	0.839
RA(Ω)	**0.948**	**0.908**	0.887	**0.859**
$M_1(\Omega)$	0.873	0.770	**0.946**	0.816
H(Ω)	0.940	0.895	0.883	0.838
SCI(Ω)	0.929	0.865	0.902	0.822
GA(Ω)	0.907	0.820	0.917	0.818
IS(Ω)	0.870	0.754	0.942	0.802
SS(Ω)	0.890	0.788	0.932	0.814
SO(Ω)	0.873	0.774	**0.946**	0.821

for the Randic index, R ranges from 0.854 to 0.948, with best prediction for molar refractivity, Molar Volume and Molecular weight being 0.948, 0.879 and 0.854 respectively. For the first Zagreb index, the range is 0.793 to 0.943, indicating a high prediction accuracy for all physicochemical properties, with the optimal prediction of molar complexity at 0.943. Similarly, the Sombor index shows a range from 0.729 to 0.943 across all physicochemical properties, emphasizing high prediction accuracy, particularly for molar complexity at 0.943. Various other topological

TABLE 8. Best estimated Cubic regression models for physical properties.

Cubic best regression model	R^2	F	SE
$\mathbf{MR = 0.022(RA)^3 - 0.412(RA)^2 + 11.312(RA) - 7.737}$	0.899	35.442	6.991
$\mathbf{MV = 0.139(RA)^3 - 0.188(RA)^2 + 13.858(RA) + 38.753}$	0.824	18.707	34.899
$\mathbf{C = 0.000229(M_1)^3 - 0.037(M_1)^2 + 4.658(M_1) - 15.412}$	0.895	37.062	23.328
$\mathbf{C = 0.000293(SO)^3 - 0.025(SO)^2 + 4.582(SO) + 2.194}$	0.896	37.183	23.294
$\mathbf{MW = 0.523(RA)^3 - 10.920(RA)^2 + 96.641(RA) - 87.820}$	0.739	12.250	36.589

indices show less significant correlations with these properties. Table 4 presents five best linear regression models with their respective R^2, F, SE, and significance values S_F is zero for all TIs. The coefficient of determination (R^2), indicating the extent to which independent variables account for the variation in the dependent variable, spans from 0 to 0.898. A higher R^2 value indicates a better fit, with all models demonstrating relatively high values. The lowest R^2 among them is 0.730, still considered a robust fit. In summary the model for molar refractivity stands out best estimated property with an R^2 value of 0.898 and its corresponding regression equation $MR = 9.034(RA) - 4.273$.

Table 5 displays 'R' obtained from quadratic regression models linking various topological indices among their physicochemical properties of plant regulators. These coefficients vary across indices and properties. For instance, the Randic index shows 'R' ranging from 0.854 to 0.948, with highest predictions observed for molar refractivity, molar volume, and molecular weight at 0.948, 0.907, and 0.854, respectively. The Sombor index exhibits a range of 0.754 to 0.946, indicating strong prediction accuracy across all properties, particularly for molar complexity at 0.946. Other topological indices demonstrate weaker correlations with these properties. Table 6 presents four quadratic regression models along with their corresponding R^2, F, SE, and significance value is null throughout. R^2, the coefficient of determination, indicating the extent to which independent variables account for the variation in the dependent variable, spans from 0 to 0.898, with higher values 0.898 indicating better fit. All models exhibit relatively high R^2 values, with the lowest at 0.730, still indicating a robust fit. In summary, the model for molar refractivity stands out best estimated property with an R^2 of 0.898 and its corresponding regression equation $MR = 0.047(RA)^2 + 8.408(RA) - 2.374$.

Table 7 displays 'R' derived from a cubic regression model that examines topological indices and their relationships with the physicochemical properties of plant regulators. These coefficients vary across indices and properties. For example, the Randic index shows 'R' ranging from 0.859 to 0.948, with the highest predictions observed for molar refractivity, molar volume, and molecular weight at 0.948, 0.908, and 0.859, respectively. The first Zagreb index exhibits a range of 0.770 to 0.946, indicating strong prediction accuracy across all properties, particularly for molar complexity at 0.946. Similarly, the Sombor index ranges from 0.774 to 0.946, showing high prediction accuracy for molar complexity at 0.946 as well. Other topological

indices demonstrate weaker correlations with these properties. Table 8 presents five cubic regression models alongside their respective R^2, F, SE, and significance values. The coefficient of determination, R^2, measures how much of the variation in the dependent variable is explained by the independent variables. It ranges from 0 to 0.899, with higher values representing a better fit. All models show relatively high R^2 values, with the lowest at 0.739, still indicating a robust fit. In summary, molar refractivity stands out best estimated property with an R^2 of 0.899 and its corresponding regression equation $MR = 0.022(RA)^3 - 0.412(RA)^2 + 11.312(RA) - 7.737$. These models represent the best fitting and most accurate predictors for the data.

4. Conclusion

Our comprehensive study indicates that curvilinear regression models significantly improve the evaluation of plant regulators activity when using molecular descriptors. These models show superior predictive capabilities over linear regression models, especially when addressing non-linear data patterns. By incorporating molecular descriptors as independent variables, the accuracy and reliability of these models are significantly enhanced. This has major implications for drug discovery and development. The use of curvilinear regression models combined with molecular descriptors helps in identifying and optimizing more effective and selective drugs. This approach reduces the time and costs involved in the drug development process. The study highlights the importance of recognizing non-linear relationships between molecular descriptors and drug activity, which are often overlooked in traditional linear regression analyses.

Statistical metrics R^2 and SE indicate that quadratic regression models outperformed linear and cubic regression models. Cubic models are more prone to overfitting along with relatively higher SE value. Randic index showed the highest predictions observed for molar refractivity, molar volume, and molecular weight with R values 0.948, 0.908, and 0.859, respectively. The first Zagreb index exhibits a correlation range of 0.770 to 0.946, indicating strong prediction accuracy particularly for molar complexity at 0.946. Moreover, the Sombor index has R value ranging from 0.774 to 0.946, showing high prediction accuracy for molar complexity at 0.946 as well. Other topological indices demonstrate weaker correlations with these properties. In summary, our study emphasizes the power of curvilinear regression models, particularly when used with molecular descriptors, as a robust tool for analyzing drug activity. These findings pave the way for advancements in drug discovery and provide valuable insights into the molecular mechanisms that influence drug activity.

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Data Availability

The authors declare that the data supporting the findings of this study are available within the paper.

Conflict of Interest

The authors declare that there is no conflict of interest in publication of this paper.

Author Contribution

Fatima Saeed carried out computational investigation, analysis, methodology and wrote the manuscript and Nazeran Idrees worked on conceptualisations, figures, analysis and editing.

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