QSPR Analysis of Molecular Biocontrol Agents for Fusarium Wilt Disease Using Degree-Based Spectral Topological Descriptors and Polynomial Regression Models

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Abstract

This study investigates ten molecular biocontrol agents associated with Fusarium wilt disease using degree-based spectral topological descriptors and QSPR analysis. Spectral energies derived from different degree-based matrices are used as molecular descriptors. Linear, quadratic, and cubic regression models are employed to examine their relationships with selected physicochemical properties. Model performance is evaluated using R, R^2, RMSE, F-statistic, and p-value. The results reveal strong predictive relationships, particularly for molecular weight and molar volume, while polynomial models effectively capture nonlinear structure–property relationships. The findings demonstrate the usefulness of degree-based spectral descriptors for QSPR analysis of molecular biocontrol agents.

MSC : 05C12, 05C76

Keywords: Biocontrol agents; Topological indices; Spectral energy; QSPR; Polynomial regression; Physicochemical properties.

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1 Introduction

Chemical graph theory provides a mathematical framework for representing and analyzing molecular structures, where atoms are modeled as vertices and chemical bonds as edges. This representation enables structural characteristics of chemical compounds to be expressed through numerical graph invariants known as topological indices. Such descriptors provide useful information about molecular connectivity, branching and other structural features, and have become important tools for relating molecular architecture to physicochemical and biological properties [1–3, 17-21].

Among the different classes of molecular descriptors, degree-based topological indices have received considerable attention because of their mathematical simplicity and chemical applicability. Classical descriptors such as the Zagreb and Randić indices, together with later developments including the sum-connectivity, atom–bond connectivity (ABC), geometric–arithmetic (GA), harmonic, inverse sum indeg (ISI), forgotten (F), symmetric division degree (SDD), and Sombor indices, provide different numerical characterizations of molecular structure [4–11]. In addition to their conventional forms, matrix representations and the corresponding eigenvalue-based energies provide a spectral perspective for examining molecular graphs.

Topological descriptors are particularly useful in quantitative structure–property relationship (QSPR) studies, where mathematical relationships are established between molecular structure and experimentally observed physicochemical properties. Recent investigations have demonstrated the usefulness of degree-based descriptors and regression techniques for predicting molecular properties across different classes of chemical and pharmaceutical compounds [12–15]. QSPR modeling can therefore provide a theoretical and computational approach for identifying significant structure–property relationships and reducing dependence on extensive experimental evaluation. Recent studies have successfully combined degree-based descriptors with linear and nonlinear regression models for molecular property prediction.

Fusarium wilt is an important plant disease that can considerably affect crop growth and productivity. Chemical and biological agents used for disease

management possess different molecular structures and physicochemical characteristics, and understanding these differences can assist in their comparative evaluation. In the present study, ten molecular agents associated with the management of Fusarium wilt are considered, including fungicides, soil fumigants and molecular biocontrol agents. Their molecular structures are characterized using degree-based spectral topological descriptors, and selected physicochemical properties are investigated through QSPR modeling. The original material considers these ten agents together with properties such as boiling point, molecular weight, solubility, density, molar volume and Log P.

The principal objective of this study is to investigate the predictive ability of degree-based spectral descriptors for the selected molecular agents using linear, quadratic and cubic regression models. The performance of these models is examined through appropriate statistical measures to identify significant relationships between molecular topology and physicochemical properties. The study thus provides a graph-theoretical and regression-based framework for understanding the structural behavior of molecular agents relevant to Fusarium wilt management.

2 Degree-Based Topological Indices of Graphs

Let $G = (V(G), E(G))$be a simple connected graph, where $d(x)$denotes the degree of a vertex $x \in V(G)$. The degree-based topological indices employed in this study are summarized in Table 1.

Table 1. Degree-based topological indices considered in this study

Topological index	Notation	Mathematical definition
First Zagreb index	$FZI(G)$	$\sum_{xy\in E(G)}[d(x)+d(y)]$
Second Zagreb index	$SZI(G)$	$\sum_{xy\in E(G)}d(x)d(y)$
Forgotten index	$FI(G)$	$\sum_{xy\in E(G)}[d^2(x)+d^2(y)]$
Randić index	$RI(G)$	$\sum_{xy\in E(G)}\frac{1}{\sqrt{d(x)d(y)}}$
Sum-connectivity index	$SCI(G)$	$\sum_{xy\in E(G)}\frac{1}{\sqrt{d(x)+d(y)}}$
Atom-bond connectivity index	$ABCI(G)$	$\sum_{xy\in E(G)}\sqrt{\frac{d(x)+d(y)-2}{d(x)d(y)}}$
Geometric-arithmetic index	$GAI(G)$	$\sum_{xy\in E(G)}\frac{2\sqrt{d(x)d(y)}}{d(x)+d(y)}$
Harmonic index	$HI(G)$	$\sum_{xy\in E(G)}\frac{2}{d(x)+d(y)}$
Symmetric division degree index	$SDD(G)$	$\sum_{xy\in E(G)}\frac{d^2(x)+d^2(y)}{d(x)d(y)}$
Inverse sum indeg index	$ISI(G)$	$\sum_{xy\in E(G)}\frac{d(x)d(y)}{d(x)+d(y)}$
Sombor index	$SOI(G)$	$\sum_{xy\in E(G)}\sqrt{d^2(x)+d^2(y)}$

These descriptors quantify different degree-dependent structural characteristics of molecular graphs and form the basis for constructing the corresponding spectral matrices and energies used in the present QSPR analysis.

3 Eigenvalue -based topological indices of graphs

In 2005, Das et al. [10] Presented Randic matrix of a graph *G* in Conjunction with Randic index [3]. A Randic Matrix *R* is *n*×*n* symmetric matrix of a graph *G* is defined as $(R)_{xy}=\begin{cases}\frac{1}{\sqrt{d(x)d(y)}} & if\ xy\in E(G)\\ 0 & otherwise\end{cases}$. Let $\lambda_1^r, \lambda_2^r, \ldots\ldots \lambda_n^r$, be the eigen values of *R*. Then the energy of *G* with respect to the matrix *R* is defined as $E_{rs} = E_{rs}(G)=\sum_{i=1}^{n}|\lambda_i^r|$. Zhou and Trinajstic [11] introduced the sum connectivity matrix *S* of *G* in 2010, is defined as$(S)_{xy}=\begin{cases}\frac{1}{\sqrt{d(x)+d(y)}} & if\ xy\in E(G)\\ 0 & otherwise\end{cases}$. Let $\lambda_1^s, \lambda_2^s, \ldots, \lambda_n^s$ be the eigen values of S. Then the energy of *S* is defined as $E_{ss} = E_{ss}(G)=\sum_{i=1}^{n}|\lambda_i^s|$. Estrada [12] studied that the *ABC* matrix of graph in the conjugative with *ABC* index and defined as $(ABC)_{xy}=\begin{cases}\sqrt{\frac{d(x)+d(y)-2}{d(x)d(y)}} & if\ xy\in E(G)\\ 0 & otherwise\end{cases}$.

Let $\lambda_1^{abc}, \lambda_2^{abc}, \ldots, \lambda_n^{abc}$ be the eigen values of *ABC* matrix. Then the *ABC* energy is defined as $E_{abcs} = E_{abcs}(G)=\sum_{i=1}^{n}|\lambda_i^{abc}|$. Rodrguez [14] Proposed the geometric arithmetic matrix (*GA*) in 2016 for a graph *G* is defined as $(GA)_{xy}=\begin{cases}\frac{2\sqrt{d(x)d(y)}}{d(x)+d(y)} & if\ xy\in E(G)\\ 0 & otherwise\end{cases}$.

Let $\lambda_1^{ga}, \lambda_2^{ga}, \ldots, \lambda_n^{ga}$ be the eigen values of *GA* Matrix. The *GA*-Energy of *GA* Matrix is defined as $E_{gas} = E_{gas}(G) = \sum_{i=1}^{n} |\lambda_i^{ga}|$.

Rad et al. [15] presented the first Zagreb matrix (*FZ*) and Zhan et. all [16] proposed second Zagreb matrix (*SZ*) of a graph *G* which are respectively defined as

$(FZ)_{xy} = \begin{cases} d(x) + d(y) & if\ xy \in E(G) \\ 0 & otherwise \end{cases}$ and

$(SZ)_{xy} = \begin{cases} d(x)d(y) & if\ xy \in E(G) \\ 0 & otherwise \end{cases}$

Let $\lambda_1^{fz}, \lambda_2^{fz}, \ldots, \lambda_n^{fz}$ and $\lambda_1^{sz}, \lambda_2^{sz}, \ldots, \lambda_n^{sz}$ be eigen values of the matrices *FZ* and *SZ,* respectively. Then their energies are defined as $E_{fzs} = E_{fzs}(G) = \sum_{i=1}^{n} |\lambda_i^{fz}|$ and $E_{ezs} = E_{ezs}(G) = \sum_{i=1}^{n} |\lambda_i^{sz}|$. The Harmonic matrix *(H)* of *G* is proposed by Jahanbani et al. and defined as $(H)_{xy} = \begin{cases} \frac{2}{d(x)+d(y)} & if\ xy \in E(G) \\ 0 & otherwise \end{cases}$. Let $\lambda_1^h, \lambda_2^h, \ldots, \lambda_n^h$ be the eigen values of *H*. The energy of *H* is defined as $E_{hs} = E_{hs}(G) = \sum_{i=1}^{n} |\lambda_i^h|$. The inverse sum indeg matrix (*ISI*) of *G* is defined as $(ISI)_{xy} = \begin{cases} \frac{d(x)d(y)}{d(x)+d(y)} & if\ xy \in E(G) \\ 0 & otherwise \end{cases}$. Let $\lambda_1^{isi}, \lambda_2^{isi}, \ldots, \lambda_n^{isi}$ be the eigen values of *ISI* matrix. The energy of *ISI* is defined as $E_{isis} = E_{isis}(G) = \sum_{i=1}^{n} |\lambda_i^{isi}|$. The forgotten matrix or *F*-matrix of *G* is defined as $(F)_{xy} = \begin{cases} d^2(x)+d^2(y) & if\ xy \in E(G) \\ 0 & otherwise \end{cases}$. Let $\lambda_1^f, \lambda_2^f, \ldots, \lambda_n^f$ be the eigen values of *F*-matrix. The Energy of *F*-matrix is defined as $E_{fi} = E_{fi}(G) = \sum_{i=1}^{n} |\lambda_i^f|$.

The Symmetric division deg matrix or *SDD* matrix of *G* is defined as

$(SDD)_{xy} = \begin{cases} \frac{d^2(x)+d^2(y)}{d(x)d(y)} & if\ xy \in E(G) \\ 0 & otherwise \end{cases}$

Let $\lambda_1^{sdd}, \lambda_2^{sdd}, \ldots, \lambda_n^{sdd}$ be the eigen values of *SDD* matrix. Ther energy of *SDD* matrix is defined as $E_{sdd} = E_{sdd}(G) = \sum_{i=1}^{n} |\lambda_i^{sdd}|$.

The Sombor matrix or *SO* matrix of *G* defined as $(SO)_{xy} = \begin{cases} \sqrt{d^2(x) + d^2(y)} & if\ xy \in E(G) \\ 0 & otherwise \end{cases}$.

Let $\lambda_1^{so}, \lambda_2^{so}, \ldots, \lambda_n^{so}$ be the eigen values of *SO* matrix. Ther energy of *SO* matrix is defined as $E_{sdd} = E_{sdd}(G) = \sum_{i=1}^{n} |\lambda_i^{so}|$.

4 Quality Testing Analysis

In this section, QSPR analysis was performed to investigate the relationships between the topological indices and physicochemical properties of the selected biocontrol agents. Three regression models, namely **Linear Regression, Quadratic Regression, and Cubic Regression**, were employed to examine linear and nonlinear structure–property relationships. The calculated topological indices were used as independent variables, while the physicochemical properties were considered as dependent variables. Particular attention was given to strong correlations with (|r|>0.9), indicating potentially significant relationships between the molecular descriptors and the investigated properties.

The performance of the regression models was evaluated using the **correlation coefficient ((r)), coefficient of determination ((R^2)), F-test, p-value, and root mean square error (RMSE)**. The (R^2) value measures the proportion of variation in a physicochemical property explained by the model, while the F-test and p-value assess the statistical significance of the fitted relationship. RMSE measures the deviation between the predicted and observed values, with lower values indicating better predictive accuracy. The detailed results of the Linear, Quadratic, and Cubic regression models are presented in the following sections and corresponding tables.

Table 2. Spectral Topological Indices of Molecular Biocontrol Agents

TIs	Thiophanate-Methyl	Azoxystrobin	Trifloxystrobin	Fludioxonil	Metalaxyl	Chloropicrin	Metam Sodium	1,3-Dichloropropene	Methionine	Adenosine
Ers	1.420918	1.447974	1.401398	1.547548	1.444149	2	2.002171	1.68005	1.545667	1.516538
Ess	4.790327	5.391732	5.022929	4.309423	4.175506	2.476469	2.734579	2.536915	3.250672	4.624622
Eabcs	9.371869	10.58873	9.851547	8.345103	8.103313	4.46806	4.808517	4.604781	6.139403	9.001081
Egas	32.30445	40.15662	36.00988	24.00597	24.15233	6.186984	7.506396	7.722886	13.68578	28.21029
Efzs	1471.838	2228.886	1852.96	747.6377	810.44633	47.9309	61.094999	77.17889	245.0878	1051.631

Eezs	16752.94	30924.75	23823.45	5808.99	6792.47	77.99607	118.515158	186.5994	1093.027	9795.333
Ehs	1.420296	1.447778	1.40097	1.546026	1.443198	1.87598	1.963644	1.64283	1.541979	1.515915
Eisis	367.6247	557.0685	462.9565	186.5408	202.33155	10.52919	14.636221	18.62183	60.96506	262.6818
Efi	33568.08	61883.68	47705.3	11664.01	13623.45	198.337	257.99444	397.3707	2208.558	19625.08
Esdd	64.75343	80.36805	72.13007	48.24955	48.468155	17.01795	16.647044	17.09412	27.71026	56.53941
Eso	1041.221	1576.277	1310.641	529.1804	573.468	35.8793	44.093099	55.5093	173.7368	743.9344
Ecrs	2.484774	2.494171	2.490736	2.605655	2.50336	2.716515	2.661994	2.216523	2.533244	2.583229
Ecss	8.410411	9.302755	8.957102	7.302214	7.281899	3.841747	3.826796	3.478547	5.379931	7.909375
Ecabcs	16.45726	18.27103	17.56907	14.14142	14.137738	6.946417	6.822187	6.33654	10.21195	15.39859
Ecgas	56.95101	69.40244	64.43424	40.94948	42.379422	11.07	11.085689	11.01199	23.03598	48.44943
Ecfzs	2617.079	3865.869	3338.69	1292.243	1440.401	102.0531	99.295336	116.9265	424.2149	1822.237
Eceszs	30060.63	53833.03	43247.88	10196.44	12235.94	229.3877	217.95444	305.6469	1949.708	17132.48
Echs	2.483679	2.493792	2.490111	2.603999	2.501091	2.617151	2.612427	2.177818	2.526994	2.582046
Eci	653.6943	966.1657	834.2577	322.64	359.5	24.5634	24.13	28.5587	105.56	455.13
sis				88	959	1	208		34	48
Ecfi	60226.76	107734.7	86581.73	20445.05	2454 2.97	484.1057	456.97577	635.0991	3934.326	34329.41
Ecsdd	114.1534	138.914	129.0308	82.16219	85.06379	25.61507	24.111433	23.74356	46.63103	97.12357
Ecso	1851.368	2734.016	2361.401	914.3379	1019.257	73.50567	71.189933	83.62657	300.6596	1289.117

5 Linear Regression

Linear regression is one of the most fundamental and widely used statistical and machine-learning techniques for modeling the relationship between variables. It helps in understanding how a dependent variable (output) changes when one or more independent variables (inputs) vary. The main goal of linear regression is to draw a straight line (called the regression line) that best fits the data points and can be used to make predictions. In its simplest form, known as simple linear regression, the relationship between two variables is represented using a line $Y = a + bX$, **Y** is the dependent variable, **X** is the independent variable, **a** is the intercept (value of Y when X = 0) and **b** is the slope (how much Y changes for a one-unit change in X). When more than one independent variable is involved, the method is called multiple Linear Regression, which fits a hyperplane instead of a line.

Linear regression is widely used in fields such as economics, biology, finance, medicine, and engineering. It is especially useful for prediction, trend analysis, risk assessment, and identifying relationships between variables. Its simplicity, interpretability, and efficiency make it an essential technique for both beginners and advanced researchers.

Table 3. Linear regression Analysis between Molar weight and Tis

Equation	R	R^2	RMSE	F	p-value
MW = 826.3720 + -359.8751*Ers	0.73718	0.543435	70.72624	9.52213	0.014985
MW = -126.3704 + 95.8232*Ess	0.94705 2	0.89690 7	33.6080 3	69.6000 8	3.22E-05
MW = -88.1436	0.94	0.89	33.7	69.0	3.32

+ 44.9621*Eabcs	6651	6148	315	3302	E-05
MW = 62.8452 + 8.5248*Egas	0.967916	0.936861	26.3013	118.7043	4.46E-06
MW = 132.8353 + 0.1367*Efzs	0.975228	0.951071	23.1533	155.5007	1.6E-06
MW = 159.2972 + 0.0095*Eezs	0.94426	0.891628	34.4578	65.8197	3.95E-05
MW = 924.8323 + -426.9361*Ehs	0.751032	0.564049	69.1111	10.3507	0.01229
MW = 133.2493 + 0.5461*Eisis	0.975132	0.950883	23.1978	154.875	1.62E-06
MW = 159.1318 + 0.0048*Efi	0.944398	0.891888	34.4164	65.99756	3.91E-05
MW = 49.3500 + 4.4766*Esdd	0.975018	0.950661	23.2501	154.1428	1.65E-06
MW = 132.6323 + 0.1935*Eso	0.975274	0.951159	23.1323	155.7977	1.59E-06

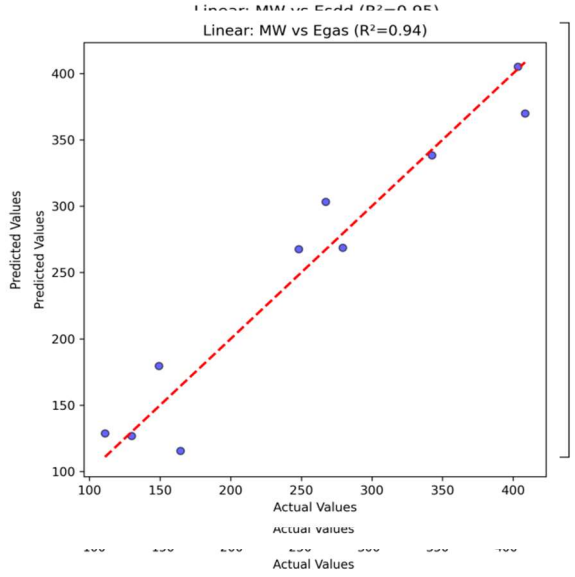


Figure 1: Scatter plot between MW and Tis

Table 4. Linear regression Analysis between BP and Tis

Equation	R	R²	RMSE	F	p-value
BP = 828.1784 + -355.9376*Ers	0.364997	0.133688	191.6414	1.26870	0.29266
BP = -42.4329 + 76.5349*Ess	0.383829	0.147325	190.4782	1.38223	0.27352
BP = -13.6071 + 36.1383*Eabcs	0.386088	0.149064	190.2839	1.40141	0.27046
BP = 122.4363 + 6.1841*Egas	0.356291	0.126943	192.7413	1.16320	0.31224
BP = 187.1251 + 0.0830*Efzs	0.300375	0.090225	196.7526	0.79338	0.39907
BP = 208.4879 + 0.0052*Eezs	0.262941	0.069138	199.0198	0.59418	0.46296
BP = 884.0103 + -395.9640*Ehs	0.353449	0.124926	192.9638	1.14208	0.31639
BP = 187.2357 + 0.3322*Eisis	0.30094	0.090565	196.7158	0.79667	0.39814
BP = 208.4599 + 0.0026*Efi	0.262649	0.068985	199.0362	0.59276	0.46347
BP = 117.3284 + 3.1432*Esdd	0.347381	0.120673	193.4322	1.09786	0.32535
BP = 187.0710 + 0.1173*Eso	0.300099	0.090059	196.7706	0.79178	0.39952

Table 5. Linear regression Analysis between Sol and Tis

Equation	R	R²	RMSE	F	p-value
Sol = 639.5748 + -123.6898*Ess	0.581102	0.33768	179.2039	4.07875	0.07810
Sol = 605.2837 + -60.0371*Eabcs	0.600868	0.361042	176.015	4.52038	0.06619
Sol = 386.1288 + -10.5854*Egas	0.571318	0.326404	180.7229	3.87655	0.08448
Sol = 277.1910 + -0.1441*Efzs	0.488724	0.238852	192.1092	2.51043	0.15175
Sol = 238.1917 + -0.0089*Eezs	0.418472	0.175119	199.9905	1.69836	0.22875
Sol = -1277.3440 + 905.5689*Ehs	0.757239	0.57341	143.8198	10.75338	0.01120

Sol = 276.8162 + -0.5761*Eisis	0.48892 1	0.23904 4	192.085	2.51308 6	0.15156 5
Sol = 238.3481 + -0.0044*Efi	0.41854 4	0.17517 9	199.9831	1.69907 3	0.22866 8
Sol = 400.8424 + -5.5132*Esdd	0.57079 8	0.32581	180.8026	3.86608 9	0.08483 6
Sol = 277.3740 + -0.2039*Eso	0.48862 5	0.23875 5	192.1214	2.50909 6	0.15185
Sol = 639.5748 + -123.6898*Ess	0.58110 2	0.33768	179.2039	4.07875 2	0.07810 8

Table 6. Linear regression Analysis between D and Tis

Equation	R	R^2	RMSE	F	p-value
D = 1.3194 + -0.0054*Ers	0.005465	2.99E-05	0.213364	0.000239	0.988045
D = 1.3002 + 0.0027*Ess	0.012949	0.000168	0.21335	0.001342	0.971678
D = 1.2907 + 0.0027*Eabcs	0.027471	0.000755	0.213287	0.006042	0.939953
D = 1.2949 + 0.0007*Egas	0.039992	0.001599	0.213197	0.012815	0.912657
D = 1.2927 + 0.0000*Efzs	0.073372	0.005383	0.212793	0.043301	0.84036
D = 1.2929 + 0.0000*Eezs	0.09047	0.008185	0.212493	0.06602	0.803708
D = 1.4655 + -0.0980*Ehs	0.084557	0.000715	0.212603	0.057611	0.816349
D = 1.2930 + 0.0001*Eisis	0.072454	0.000525	0.212807	0.042219	0.842336
D = 1.2928 + 0.0000*Efi	0.090793	0.008243	0.212486	0.066494	0.80302
D = 1.2838 + 0.0006*Esdd	0.064109	0.000411	0.212929	0.033015	0.860337
D = 1.2926 + 0.0000*Eso	0.073811	0.005448	0.212786	0.043823	0.839415

Table 7. Linear regression Analysis between LogP and Tis

Equation	R	R^2	RMSE	F	p-value
LogP = 6.4203 + -3.2245*Ers	0.340812	0.116153	1.907171	1.051342	0.3352
LogP = -1.4227 + 0.6821*Ess	0.347854	0.121002	1.901933	1.101274	0.324652
LogP = -1.2317 + 0.3308*Eabcs	0.359412	0.129177	1.893068	1.186713	0.307717
LogP = -0.2311 + 0.0677*Egas	0.396909	0.157536	1.861988	1.495959	0.256098
LogP = 0.2366 + 0.0012*Efzs	0.437804	0.191672	1.823875	1.896973	0.205721
LogP = 0.4335 + 0.0001*Eezs	0.44177	0.19516	1.819935	1.93987	0.201168
LogP = 8.3584 + -4.4938*Ehs	0.40788	0.166366	1.852204	1.596542	0.24197
LogP = 0.2417 + 0.0047*Eisis	0.43712	0.191074	1.82455	1.889653	0.206512
LogP = 0.4316 + 0.0000*Efi	0.442025	0.195386	1.81968	1.942656	0.200877
LogP = -0.4031 + 0.0370*Esdd	0.416037	0.173087	1.847233	1.674534	0.231757
LogP = 0.2342 + 0.0017*Eso	0.438131	0.191959	1.823551	1.900488	0.205343

Table 8. Linear regression Analysis between MV and Tis

Equation	**R**	**R^2**	**RMSE**	**F**	**p-value**
MV = 604.3860 + -263.4981*Ers	0.789624	0.623507	43.90223	13.22872	0.00659
MV = -63.2762 + 62.5480*Ess	0.904353	0.817855	30.53635	35.92095	0.000326
MV = -38.6392 + 29.3906*Eabcs	0.90526	0.819497	30.3984	36.32049	0.000314
MV = 58.8628 + 5.6268*Egas	0.934626	0.873525	25.44546	55.25359	7.38E-05
MV = 104.8001 + 0.0905*Efzs	0.944842	0.892726	23.43444	66.57562	3.79E-05
MV = 122.0033 + 0.0064*Eezs	0.919718	0.845882	28.08894	43.90812	0.000165
MV = 672.6264 + -310.1618*Ehs	0.798188	0.637104	43.10218	14.04487	0.005643
MV = 105.0608 + 0.3618*Eisis	0.94491	0.89286	23.4197	66.6693	3.77E-

	3	1	2	7	05
MV = 121.8970 + 0.0032*Efi	0.91979 5	0.84602 3	28.0760 7	43.9557	0.00016 4
MV = 50.6510 + 2.9393*Esdd	0.93654 7	0.87712	25.0812 3	57.1040 9	6.57E-05

The linear regression analysis using TIs revealed strong correlations for molecular weight (MW) and molar volume (MV) with R^2 values above 0.90, signifying high predictive accuracy. However, properties like boiling point (BP) and density (D) exhibited poor correlations, suggesting linear models cannot fully capture their complexity. Linear regression is effective for properties that exhibit straightforward, proportional relationships with TIs.

6.Quadratic Regression

Quadratic regression is a form of polynomial regression used to model relationships that follow a curved, parabolic pattern rather than a straight line. Unlike linear regression, which fits a straight line to the data, quadratic regression includes an additional squared term, allowing the model to capture curvature in the relationship between the independent and dependent variables.

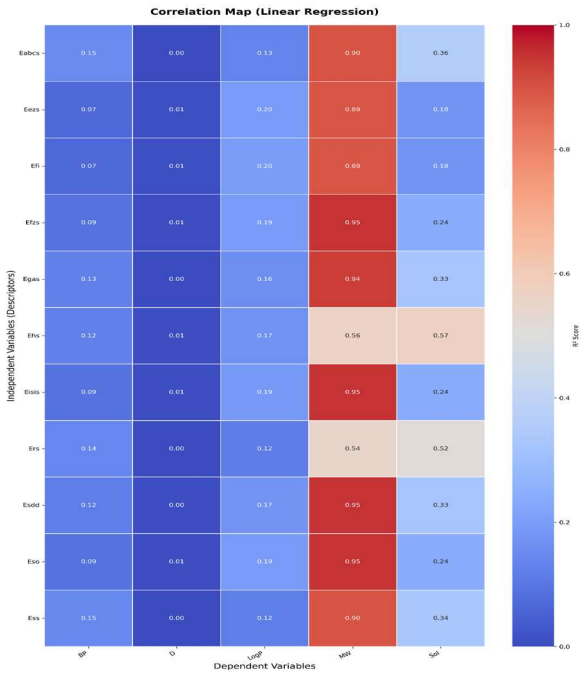


Figure 2. Correlation map of the linear regression between properties and Tis

The general form of the model is:

$$Y = a + bX + cX^2$$

where the X^2 term enables the model to represent U-shaped or inverted U-shaped trends. Quadratic regression is widely used in fields such as economics, engineering, biology, and environmental science, where data often exhibit nonlinear patterns. Its ability to model curved relationships makes it a valuable tool for prediction, pattern analysis, and understanding more complex behaviors in datasets.

Table 9. Quadratic between MW and Tis

Equation	R	R^2	RMSE	F	p-value
MW = 6355.1946 + 0.0000*Ers^1 + -6932.9273*Ers^2	0.924374	0.854467	39.9309 99	46.9702 9	0.00001 31
MW = 247.1150 + 0.0000*Ess^1 + -115.3438*Ess^2	0.966421	0.933397	26.8967 7	113.156 8	5.34E-06
MW = 228.7627 + 0.0000*Eabcs^1 + -51.1668*Eabcs^2	0.968333	0.937663	26.1336 7	120.356	4.24E-06
MW = 101.8917 + 0.0000*Egas^1 + 3.4543*Egas^2	0.975078	0.950777	23.2226 3	154.526 9	1.64E-06
MW = 119.8910 + 0.0000*Efzs^1 + 0.1913*Efzs^2	0.982086	0.964493	19.7237 1	217.305	4.41E-07
MW = 135.6737 + 0.0000*Eezs^1 + 0.0189*Eezs^2	0.983232	0.966745	19.0888	232.562 1	3.39E-07
MW = 6566.2850 + 0.0000*Ehs^1 + -7250.4705*Ehs^2	0.903549	0.816402	44.8501 1	35.573 37	0.00003 37
MW = 120.6307 + 0.0000*Eisis^1 + 0.7611*Eisis^2	0.981854	0.964037	19.8498 8	214.499 9	4.64E-07
MW = 135.3980 + 0.0000*Efi^1 + 0.0094*Efi^2	0.983298	0.966875	19.0506 1	233.507 4	3.34E-07
MW = 81.6811 + 0.0000*Esdd^1 + 2.5604*Esdd^2	0.978224	0.956922	21.7247 3	177.711 8	9.58E-07

MW = 119.5291 + 0.0000*Eso^1 + 0.2712*Eso^2	0.982196	0.964709	19.6634	218.688	4.3E-07

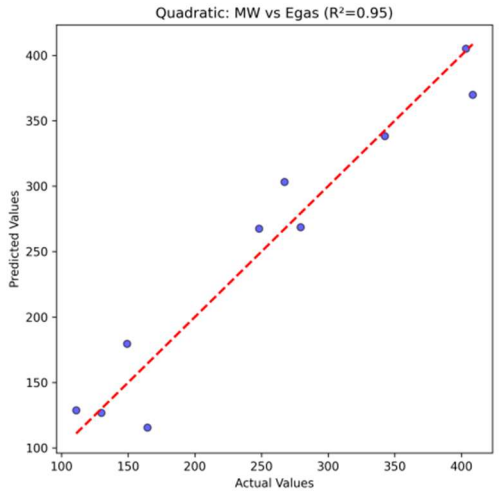
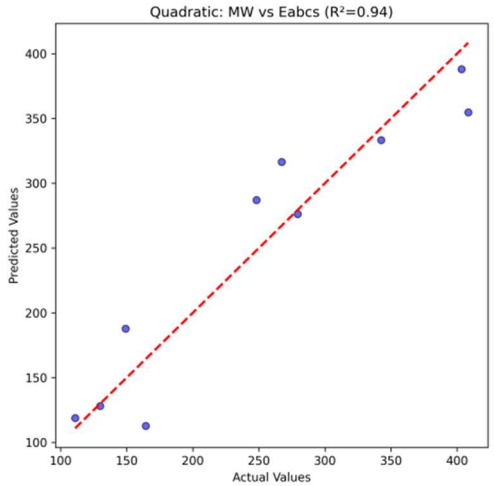


Figure 3. Scatter plot between MW and Topological coindices

Table 10. Quadratic between BP and Tis

Equation	R	R²	RMSE	F	p-value
BP = -2898.4597 + 0.0000*Ers^1 + 4074.5512*Ers^2	0.416252	0.173266	187.5584	1.676632	0.231491
BP = -347.0638 + 0.0000*Ess^1 + 248.7718*Ess^2	0.392012	0.153674	189.7678	1.452618	0.262546
BP = -312.7551 + 0.0000*Eabcs^1 + 126.8805*Eabcs^2	0.398233	0.158589	189.2159	1.507842	0.254369
BP = 33.1214 + 0.0000*Egas^1 + 17.7824*Egas^2	0.381695	0.145691	190.6066	1.364298	0.276423



BP = 163.4150 + 0.0000*Efzs^1 + 0.1829*Efzs^2	0.319093	0.101823	195.4948	0.906905	0.368819
BP = 204.2355 + 0.0000*Eezs^1 + 0.0069*Eezs^2	0.26413	0.069764	198.9528	0.599972	0.460866
BP = -3727.6127 + 0.0000*Ehs^1 + 5181.9552*Ehs^2	0.4103	0.168346	188.1157	1.619382	0.238915
BP = 163.7685 + 0.0000*Eisis^1 + 0.7318*Eisis^2	0.319811	0.102279	195.4448	0.911458	0.367682
BP = 204.1595 + 0.0000*Efi^1 + 0.0035*Efi^2	0.263853	0.069619	198.9684	0.598624	0.461353
BP = 13.9210 + 0.0000*Esdd^1 + 9.2719*Esdd^2	0.37036	0.137167	191.6095	1.271778	0.292118
BP = 163.2424 + 0.0000*Eso^1 + 0.2587*Eso^2	0.318743	0.101595	195.5193	0.904693	0.369374

Table 11. Quadratic between Sol and Tis

Equation	R	R²	RMSE	F	p-value
Sol = 2170.3257 + 0.0000*Ers^1 + -3064.0276*Ers^2	0.734448	0.539413	149.4408	9.369151	0.001561
Sol = 1446.3024 + 0.0000*Ess^1 + -579.8099*Ess^2	0.613802	0.376753	173.8376	4.835993	0.059078
Sol = 1432.4729 + 0.0000*Eabcs^1 + -310.9529*Eabcs^2	0.651885	0.424954	166.9801	5.911932	0.041109
Sol = 602.1561 + 0.0000*Egas^1 + -38.6386*Egas^2	0.650121	0.422657	167.3132	5.855689	0.041848
Sol = 352.6645 + 0.0000*Efzs^1 + -0.4623*Efzs^2	0.584771	0.341958	178.6242	4.157273	0.075799
Sol = 284.8889 + 0.0000*Eezs^1 + -	0.491	0.241	191.7	2.546	0.149

0.0273*Eezs^2	367	441	821	315	218
Sol = 6646.8046 + 0.0000*Ehs^1 + -8678.9659*Ehs^2	0.828198	0.685913	123.4067	17.47062	0.003081
Sol = 350.9720 + 0.0000*Eisis^1 + -1.8390*Eisis^2	0.584546	0.341694	178.66	4.152407	0.075939
Sol = 285.3626 + 0.0000*Efi^1 + -0.0137*Efi^2	0.491596	0.241666	191.7537	2.549446	0.149
Sol = 700.3644 + 0.0000*Esdd^1 + -23.2654*Esdd^2	0.668763	0.447245	163.7118	6.472948	0.034485
Sol = 353.4899 + 0.0000*Eso^1 + -0.6555*Eso^2	0.584869	0.342071	178.6088	4.159371	0.075738

Table 12. Quadratic between D and Tis

Equation	R	R²	RMSE	F	p-value
D = 4.0016 + 0.0000*Ers^1 + -3.1941*Ers^2	0.132837	0.017646	0.211477	0.143701	0.714493
D = 1.9583 + 0.0000*Ess^1 + -0.3694*Ess^2	0.166903	0.027856	0.210375	0.229237	0.644902
D = 1.6756 + 0.0000*Eabcs^1 + -0.1141*Eabcs^2	0.124465	0.015492	0.211708	0.125883	0.731911
D = 1.3830 + 0.0000*Egas^1 + -0.0107*Egas^2	0.136454	0.01862	0.211372	0.151783	0.707004
D = 1.3139 + 0.0000*Efzs^1 + -0.0001*Efzs^2	0.11865	0.014078	0.21186	0.114231	0.744076
D = 1.3046 + 0.0000*Eezs^1 + -0.0000*Eezs^2	0.112052	0.012556	0.212024	0.101722	0.757941
D = -1.8137 + 0.0000*Ehs^1 + 3.8683*Ehs^2	0.166339	0.027669	0.210395	0.227649	0.646034
D = 1.3144 + 0.0000*Eisis^1 + -0.0003*Eisis^2	0.119971	0.014393	0.211827	0.116825	0.741309
D = 1.3044 + 0.0000*Efi^1 + -0.0000*Efi^2	0.111965	0.012536	0.212026	0.101562	0.758124
D = 1.3302 + 0.0000*Esdd^1 + -0.0022*Esdd^2	0.084976	0.007221	0.212596	0.058187	0.815452
D = 1.3137 + 0.0000*Eso^1 + -0.0001*Eso^2	0.118039	0.013933	0.211876	0.113041	0.745358

Table13. Quadratic between LogP and Tis

Equation	R	R²	RMSE	F	p-value
LogP = 52.5292 + 0.0000*Ers^1 + -58.0420*Ers^2	0.416828	0.173745	1.843988	1.682246	0.23078
LogP = 9.5075 + 0.0000*Ess^1 + -5.4978*Ess^2	0.453333	0.20551	1.808195	2.069359	0.188233
LogP = 6.6944 + 0.0000*Eabcs^1 + -2.0734*Eabcs^2	0.445325	0.198314	1.816366	1.978972	0.197138
LogP = 0.9493 + 0.0000*Egas^1 + -0.0855*Egas^2	0.43749	0.191398	1.824184	1.893615	0.206083
LogP = 0.3033 + 0.0000*Efzs^1 + 0.0009*Efzs^2	0.438885	0.19262	1.822805	1.908596	0.204474
LogP = 0.3476 + 0.0000*Eezs^1 + 0.0001*Eezs^2	0.444755	0.197807	1.816941	1.972657	0.197781
LogP = 24.4160 + 0.0000*Ehs^1 + -23.9160*Ehs^2	0.414499	0.171809	1.846147	1.659612	0.233664
LogP = 0.3120 + 0.0000*Eisis^1 + 0.0035*Eisis^2	0.438359	0.192159	1.823326	1.902934	0.20508
LogP = 0.3447 + 0.0000*Efi^1 + 0.0001*Efi^2	0.445042	0.198062	1.816651	1.975835	0.197457
LogP = 0.5668 + 0.0000*Esdd^1 + -0.0205*Esdd^2	0.433694	0.18809	1.827911	1.853312	0.210501
LogP = 0.2991 + 0.0000*Eso^1 + 0.0013*Eso^2	0.439142	0.192845	1.822551	1.911359	0.204179

Table 14. Quadratic between MV and Tis

Equation	R	R²	RMSE	F	p-value
MV = 3956.3440 + 0.0000*Ers^1 + -4248.5410*Ers^2	0.93176	0.868176	25.97797	52.68697	8.73E-05
MV = 175.2176 + 0.0000*Ess^1 + -72.2953*Ess^2	0.92206	0.85019	27.6928	45.4037	0.00014

	2	8		9	7
MV = 162.1366 + 0.0000*Eabcs^1 + -31.5118*Eabcs^2	0.924748	0.855159	27.2304	47.2329	0.00012 8
MV = 84.7261 + 0.0000*Egas^1 + 2.2682*Egas^2	0.94159	0.886592	24.09515	62.5418	4.74E-05
MV = 98.7357 + 0.0000*Efzs^1 + 0.1161*Efzs^2	0.948173	0.899031	22.73533	71.2325	2.96E-05
MV = 109.4068 + 0.0000*Eezs^1 + 0.0113*Eezs^2	0.94424	0.891591	23.55828	65.7936 1	3.95E-05
MV = 4376.3263 + 0.0000*Ehs^1 + -4789.9163*Ehs^2	0.932674	0.86988	25.80948	53.4819	8.28E-05
MV = 99.1312 + 0.0000*Eisis^1 + 0.4627*Eisis^2	0.948197	0.899077	22.73013	71.2687 3	2.96E-05
MV = 109.2493 + 0.0000*Efi^1 + 0.0057*Efi^2	0.94424 4	0.891596	23.55755	65.7982	3.95E-05
MV = 77.0412 + 0.0000*Esdd^1 + 1.3752*Esdd^2	0.94130 1	0.886048	24.15283	62.2052 7	4.84E-05
MV = 98.5420 + 0.0000*Eso^1 + 0.1645*Eso^2	0.948016	0.899008	22.73798	71.2144	2.97E-05

Adding squared terms significantly improved model accuracy for MW and MV ($R^2 > 0.95$). The model effectively captured smooth curvature but still fell short for D and BP. Conclusion: Suitable for mildly non-linear patterns in molecular–property relationships.

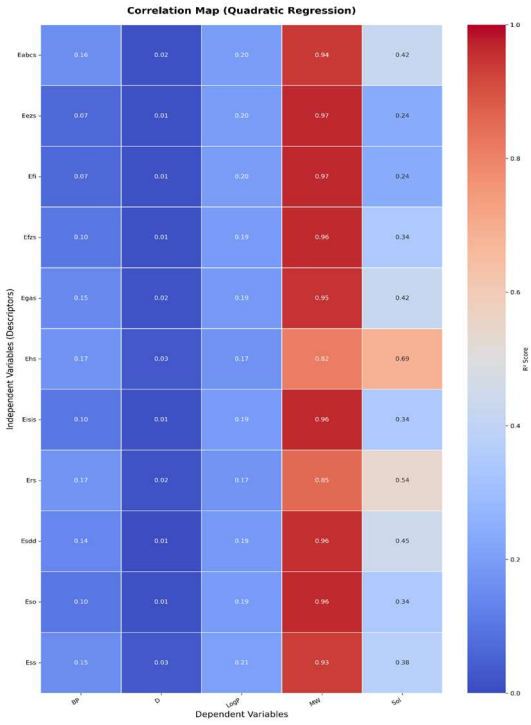


Figure 4. Correlation map of the quadratic regression between properties and Tis

7 Cubic Regression

Cubic regression is a type of polynomial regression used to model complex nonlinear relationships between a dependent variable and an independent variable. Unlike linear or quadratic regression, cubic regression includes a third-degree polynomial term, allowing the model to capture S-shaped or wave-like patterns in the data. The general form of the model is:

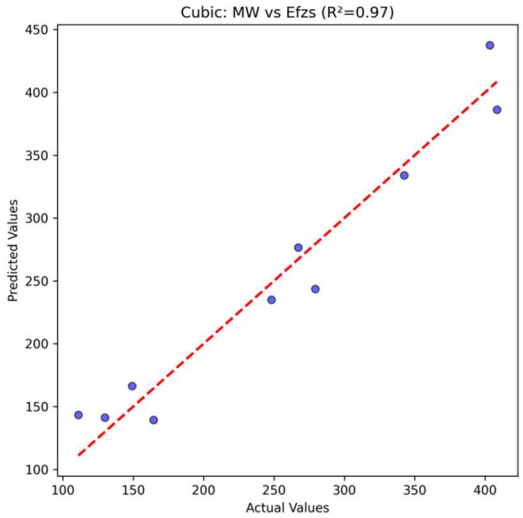
$$Y = a + bX + cX^2 + dX^3$$

where the X^3 term makes cubic regression capable of fitting more flexible curves, especially when the data show multiple bends or inflection points. This method is commonly applied in fields such as engineering, environmental science, economics, and biological modeling, where trends may change direction more than once. By providing a better fit for complex patterns, cubic regression enhances predictive accuracy and helps researchers understand intricate relationships within the data.

Table 15. Cubic between MW and Tis

Equation	**R**	**R²**	**RMSE**	**F**	**p-value**
MW = 4741.0484 +	0.	0.	39	47	0.

0.0000*Ers^1 + 3990.3431*Ers^2 + 142.1485*Ers^3	-	92 44 26	85 45 63	.9 17 82	.0 06 58	00 01 3
MW = 1172.5798 + 0.0000*Ess^1 + 871.1225*Ess^2 + 224.3046*Ess^3	- +	0. 97 04 45	0. 94 17 63	25 .2 59 79	12 9. 36 9	3. 22 E-06
MW = 898.1814 + 0.0000*Eabcs^1 + 342.4942*Eabcs^2 + 46.4836*Eabcs^3	- +	0. 97 18 94	0. 94 45 79	24 .6 41 48	13 6. 34 93	2. 64 E-06
MW = 214.5412 + 0.0000*Egas^1 + 18.6936*Egas^2 + 1.2086*Egas^3	- +	0. 98 24 53	0. 96 52 13	19 .5 22 49	22 1. 97 35	4. 06 E-07



MW = 126.1511 + 0.0000*Efzs^1 + 0.1288*Efzs^2 + 0.0001*Efzs^3	+ +	0. 98 35 3	0. 96 73 32	18 .9 18 67	23 6. 88 78	3. 16 E-07
MW = 133.6151 + 0.0000*Eezs^1 + 0.0209*Eezs^2 + 0.0000*Eezs^3	+ -	0. 98 37 59	0. 96 77 81	18 .7 88 23	24 0. 29 99	2. 99 E-07
MW = 23016.1647 + 0.0000*Ehs^1 + 37458.0490*Ehs^2 + 20386.6526*Ehs^3	- +	0. 91 20 06	0. 83 17 56	42 .9 33 79	39 .5 49 91	0. 00 02 36
MW = 126.8539 + 0.0000*Eisis^1 + 0.5055*Eisis^2 + 0.0009*Eisis^3	+ +	0. 98 33 97	0. 96 70 69	18 .9 94 58	23 4. 93 43	3. 26 E-07
MW = 133.2976 + 0.0000*Efi^1 + 0.0105*Efi^2 + 0.0000*Efi^3	+ -	0. 98 38 32	0. 96 79 25	18 .7 46 24	24 1. 41 35	2. 93 E-07
MW = 188.6653 +		0.	0.	20	20	5.

0.0000*Esdd^1 + 6.8157*Esdd^2 + 0.2406*Esdd^3	- +	98 13 54	96 30 56	.1 18 87	8. 54 15	17 E-07
MW = 125.8046 + 0.0000*Eso^1 + 0.1837*Eso^2 + 0.0001*Eso^3	+ +	0. 98 35 95	0. 96 74 59	18 .8 81 81	23 7. 84 48	3. 11 E-07

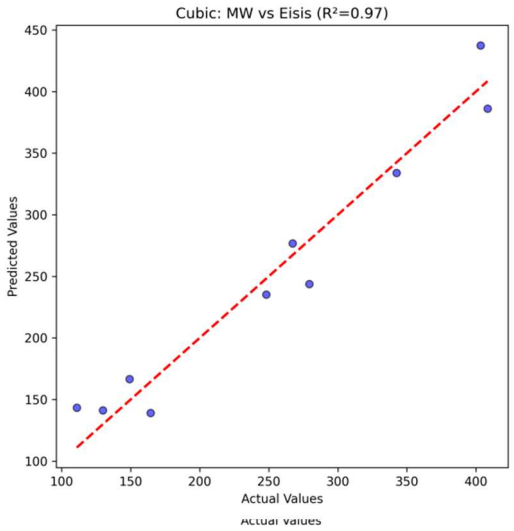


Figure 5. Scatter plot between Properties and Topological coindices

Table 16. Cubic between BP and Tis

Equation	R	R^2	RMSE	F	p-value
BP = -188548.3903 + 0.0000*Ers^1 + 342513.8881*Ers^2 + 205101.2845*Ers^3	-	0. 70 72 85	0. 50 02 52	14 5. 82 4	8. 00 80 83	0. 02 21 55
BP = -7782.7216 + 0.0000*Ess^1 + 6321.0857*Ess^2 + 1602.6854*Ess^3	-	0. 53 21 67	0. 28 32 02	17 4. 64 33	3. 16 07 43	0. 11 33 22
BP = -6448.1684 + 0.0000*Eabcs^1 + 2796.9791*Eabcs^2 + 371.6854*Eabcs^3	-	0. 55 51 26	0. 30 81 65	17 1. 57 53	3. 56 34 58	0. 09 57 62
BP = -681.8893 + 0.0000*Egas^1 + 158.3593*Egas^2 + 7.2004*Egas^3	-	0. 54 35 44	0. 29 54 41	17 3. 14 6	3. 35 46 13	0. 10 43 87
BP = 51.8806 + 0.0000*Efzs^1 + 1.2970*Efzs^2 + 0.0015*Efzs^3	-	0. 57 78 4	0. 33 39	16 8. 35 4	4. 01 02 01	0. 08 01 99

BP = 133.0620 + 0.0000*Eezs^1 + 0.0788*Eezs^2 + -0.0000*Eezs^3	0.62 34 88	0.38 87 37	16 1. 27 52	5. 08 76 62	0. 05 40 94
BP = -112405.8442 + 0.0000*Ehs^1 + 204752.1816*Ehs^2 + -122927.7925*Ehs^3	0. 58 38 7	0. 34 09 04	16 7. 46 65	4. 13 78 3	0. 07 63 62
BP = 56.5085 + 0.0000*Eisis^1 + 5.1359*Eisis^2 + -0.0231*Eisis^3	0. 57 81 25	0. 33 42 28	16 8. 31 25	4. 01 61 26	0. 08 00 15
BP = 132.0441 + 0.0000*Efi^1 + 0.0395*Efi^2 + -0.0000*Efi^3	0. 62 31 79	0. 38 83 52	16 1. 32 6	5. 07 94 24	0. 05 42 48
BP = -1117.3691 + 0.0000*Esdd^1 + 108.4187*Esdd^2 + -2.3877*Esdd^3	0. 56 01 3	0. 31 37 45	17 0. 88 2	3. 65 74 78	0. 09 21 82
BP = 49.6166 + 0.0000*Eso^1 + 1.8430*Eso^2 + -0.0029*Eso^3	0. 57 76 85	0. 33 37 2	16 8. 37 67	4. 00 69 63	0. 08 02 99

Table 17. Cubic between Sol and Tis

Equation	R	R²	RMSE	F	p-value
Sol = 88755.1577 + 0.0000*Ers^1 + 160907.9492*Ers^2 + 96162.0686*Ers^3	0. 77 57 77	0. 60 18 3	13 8. 94 65	12 .0 91 94	0. 00 83 52
Sol = 1615.5372 + 0.0000*Ess^1 + 718.0151*Ess^2 + 95.6552*Ess^3	0. 61 38 5	0. 37 68 11	17 3. 82 94	4. 83 72 06	0. 05 90 52
Sol = 3436.4998 + 0.0000*Eabcs^1 + 1183.0946*Eabcs^2 + 136.6220*Eabcs^3	0. 66 25 39	0. 43 89 59	16 4. 93 43	6. 25 91 96	0. 03 68 36
Sol = 1129.5283 + 0.0000*Egas^1 + 142.3242*Egas^2 + 5.7568*Egas^3	0. 70 29 57	0. 49 41 49	15 6. 61 2	7. 81 49 25	0. 02 33 59
Sol = 457.1600 + 0.0000*Efzs^1 + 1.5060*Efzs^2 + 0.0015*Efzs^3	0. 72 16 14	0. 52 07 27	15 2. 44 21	8. 69 19 58	0. 01 84 76
Sol = 337.0899 + 0.0000*Eezs^1 + 0.0800*Eezs^2 + 0.0000*Eezs^3	0. 62 61 13	0. 39 20 18	17 1. 69 55	5. 15 82 75	0. 05 27 93
Sol = -38190.9825 +	0.	0.	11	19	0.

0.0000*Ehs^1 + 73658.4737*Ehs^2 + -47178.5792*Ehs^3	84 36 16	71 16 89	8. 23 45	.7 47 79	00 21 57
Sol = 450.7459 + 0.0000*Eisis^1 + 5.9356*Eisis^2 + 0.0232*Eisis^3	0. 71 95 99	0. 51 78 23	15 2. 90 32	8. 59 14 25	0. 01 89 66
Sol = 338.3744 + 0.0000*Efi^1 + 0.0401*Efi^2 + 0.0000*Efi^3	0. 62 67 48	0. 39 28 14	17 1. 58 31	5. 17 55 26	0. 05 24 81
Sol = 1922.1846 + 0.0000*Esdd^1 + 130.3462*Esdd^2 + 2.7018*Esdd^3	0. 79 24 63	0. 62 79 97	13 4. 30 33	13 .5 05 22	0. 00 62 65
Sol = 460.3027 + 0.0000*Eso^1 + 2.1448*Eso^2 + 0.0030*Eso^3	0. 72 25 5	0. 52 20 78	15 2. 22 71	8. 73 91 38	0. 01 82 52

Table 18. Cubic between D and Tis

Equation	R	R²	RMSE	F	p-value
D = 24.8814 + 0.0000*Ers^1 + 41.2581*Ers^2 + 23.8510*Ers^3	0.1 46 66 8	0.0 21 51 2	0.2 11 06	0.1 75 87 5	0.6 85 97 7
D = 6.9210 + 0.0000*Ess^1 + 4.4222*Ess^2 + 1.1033*Ess^3	0.2 85 97 9	0.0 81 78 4	0.2 04 45 7	0.7 12 54 6	0.4 23 12 2
D = 4.0619 + 0.0000*Eabcs^1 + 1.1526*Eabcs^2 + 0.1502*Eabcs^3	0.1 91 41 6	0.0 36 64	0.2 09 42 2	0.3 04 27 1	0.5 96 28 4
D = 1.5805 + 0.0000*Egas^1 + 0.0495*Egas^2 + 0.0022*Egas^3	0.1 71 17 7	0.0 29 30 2	0.2 10 21 8	0.2 41 48 8	0.6 36 33 1
D = 1.3273 + 0.0000*Efzs^1 + 0.0002*Efzs^2 + 0.0000*Efzs^3	0.1 31 16 7	0.0 17 20 5	0.2 11 52 4	0.1 40 04 7	0.7 17 95 8
D = 1.3231 + 0.0000*Eezs^1 + 0.0000*Eezs^2 + 0.0000*Eezs^3	0.1 80 95 8	0.0 32 74 6	0.2 09 84 5	0.2 70 83 4	0.6 16 86 5
D = 178.6561 + 0.0000*Ehs^1 + 327.5356*Ehs^2 + 200.1944*Ehs^3	0.6 87 32 2	0.4 72 41 1	0.1 54 98	7.1 63 32 4	0.0 28 08 1
D = 1.3285 + 0.0000*Eisis^1 + 0.0009*Eisis^2 +	0.1 34 53	0.0 18 1	0.2 11 42	0.1 47 47	0.7 10 96

0.0000*Eisis^3	7		8	2	9
D = 1.3231 + 0.0000*Efi^1 + -0.0000*Efi^2 + 0.0000*Efi^3	0.180063	0.032423	0.20988	0.268075	0.618636
D = 1.0485 + 0.0000*Esdd^1 + 0.0225*Esdd^2 + -0.0005*Esdd^3	0.132115	0.017454	0.211497	0.142116	0.71599
D = 1.3268 + 0.0000*Eso^1 + -0.0003*Eso^2 + 0.0000*Eso^3	0.129625	0.016803	0.211567	0.136717	0.721163

Table 19. Cubic between LogP and Tis

Equation	R	R²	RMSE	F	p-value
LogP = 1490.4633 + 0.0000*Ers^1 + -2679.3921*Ers^2 + 1594.5632*Ers^3	0.613654	0.376571	1.60175	4.832255	0.059156
LogP = 98.6794 + 0.0000*Ess^1 + -78.3198*Ess^2 + 19.7586*Ess^3	0.63097	0.398124	1.573819	5.291766	0.050441
LogP = 66.0960 + 0.0000*Eabcs^1 + -27.9247*Eabcs^2 + 3.7035*Eabcs^3	0.585904	0.343283	1.643956	4.181814	0.075095
LogP = 5.4541 + 0.0000*Egas^1 + -0.9712*Egas^2 + 0.0472*Egas^3	0.502849	0.252857	1.753489	2.707454	0.138499
LogP = 0.4261 + 0.0000*Efzs^1 + -0.0003*Efzs^2 + 0.0000*Efzs^3	0.442183	0.195526	1.819522	1.944388	0.200697
LogP = 0.4035 + 0.0000*Eezs^1 + 0.0001*Eezs^2 + 0.0000*Eezs^3	0.447042	0.199847	1.814629	1.998087	0.195207
LogP = 1728.4647 + 0.0000*Ehs^1 + -3153.1295*Ehs^2 + 1907.2247*Ehs^3	0.781319	0.61046	1.266128	12.53702	0.007611
LogP = 0.4394 + 0.0000*Eisis^1 + -0.0017*Eisis^2 + 0.0000*Eisis^3	0.442203	0.195543	1.819502	1.944598	0.200675
LogP = 0.4001 + 0.0000*Efi^1 + 0.0000*Efi^2 + 0.0000*Efi^3	0.447219	0.200005	1.81445	2.000061	0.195009
LogP = 4.1360 + 0.0000*Esdd^1 + -0.3333*Esdd^2 + 0.0080*Esdd^3	0.454162	0.206263	1.807338	2.078911	0.187324
LogP = 0.4194 + 0.0000*Eso^1 + -0.0004*Eso^2 + 0.0000*Eso^3	0.442194	0.195536	1.819511	1.944504	0.200685

Table 20. Cubic between MV and Tis

Equation	R	R²	RMSE	F	p-value
MV = 15684.7146 + 0.0000*Ers^1 + -25629.3299*Ers^2 + 14036.2128*Ers^3	0.937562	0.879023	24.88625	58.12822	6.16E-05
MV = 165.0037 + 0.0000*Ess^1 + -63.9542*Ess^2 + 15.4761*Ess^3	0.922063	0.8502	27.69262	45.40451	0.000147
MV = 113.7491 + 0.0000*Eabcs^1 + -10.4538*Eabcs^2 + 1.3062*Eabcs^3	0.92479	0.855236	27.22313	47.26241	0.000128
MV = 86.6381 + 0.0000*Egas^1 + 1.8923*Egas^2 + 0.0954*Egas^3	0.941595	0.886601	24.09421	62.54734	4.74E-05
MV = 96.4500 + 0.0000*Efzs^1 + 0.1389*Efzs^2 + -0.0000*Efzs^3	0.9486	0.899841	22.64394	71.87334	2.87E-05
MV = 105.8590 + 0.0000*Eezs^1 + 0.0149*Eezs^2 + -0.0000*Eezs^3	0.947722	0.898177	22.8313	70.56779	3.07E-05
MV = 12760.7079 + 0.0000*Ehs^1 + -20186.4950*Ehs^2 + 10689.1584*Ehs^3	0.937239	0.878417	24.9485	57.79865	6.29E-05
MV = 96.9823 + 0.0000*Eisis^1 + 0.5510*Eisis^2 + -0.0006*Eisis^3	0.948605	0.899851	22.64283	71.8812	2.87E-05
MV = 105.6517 + 0.0000*Efi^1 + 0.0075*Efi^2 + -0.0000*Efi^3	0.947729	0.898189	22.82992	70.5773	3.07E-05
MV = 74.6748 + 0.0000*Esdd^1 + 1.5826*Esdd^2 + 0.0124*Esdd^3	0.941305	0.886055	24.15215	62.20923	4.84E-05
MV = 96.1889 +	0.	0.	22	71	2.

0.0000*Eso^1		+	94	89	.6	.8	87
0.1973*Eso^2	+	-	85	98	44	68	E-
0.0001*Eso^3			96	35	64	4	05

Cubic regression added third-order terms that modeled complex curvature effectively. It achieved R^2 values above 0.96 for MW, MV, and Sol, although risk of overfitting increases with limited data. Conclusion: Best for intricate non-linear interactions between TIs and physical properties.

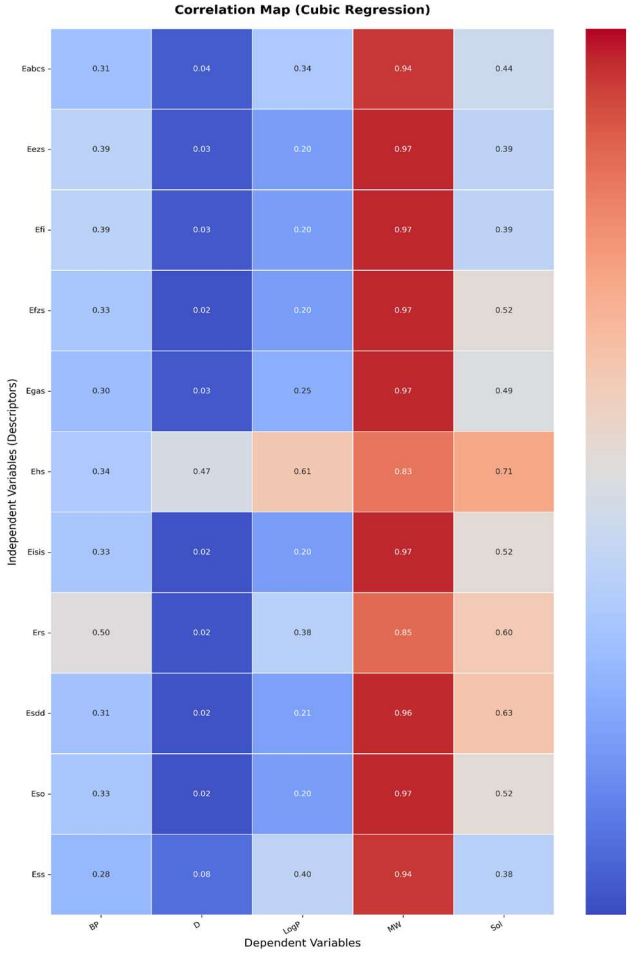


Figure 6. Correlation map of the cubic regression between properties and Tis

8 Conclusion

The present study demonstrates the effectiveness of degree-based spectral topological descriptors in the QSPR analysis of molecular biocontrol agents associated with Fusarium wilt disease. Linear, quadratic, and cubic regression models revealed meaningful relationships between the investigated descriptors and physicochemical properties. In particular, molecular weight and molar volume exhibited strong predictive relationships with several spectral descriptors, whereas some other properties showed comparatively weaker associations. The regression analysis showed that MW and MV had strong relationships with the topological indices. Linear regression produced (R^2>0.90), while quadratic regression improved the prediction with (R^2>0.95). Cubic regression showed the best performance, achieving (R^2>0.96) for MW, MV, and Sol by effectively capturing nonlinear relationships. However, BP and D showed comparatively weaker associations. Overall, polynomial regression provides an effective approach for studying the relationship between topological indices and physicochemical properties.

References

[1] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons," *Chemical Physics Letters*, vol. 17, no. 4, pp. 535–538, 1972.

[2] M. Randić, "On characterization of molecular branching," *Journal of the American Chemical Society*, vol. 97, pp. 6609–6615, 1975.

[3] E. Estrada, L. Torres, L. Rodríguez and I. Gutman, "An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes," *Indian Journal of Chemistry*, vol. 37A, pp. 849–855, 1998.

[4] B. Zhou and N. Trinajstić, "On a novel connectivity index," *Journal of Mathematical Chemistry*, vol. 46, pp. 1252–1270, 2009.

[5] D. Vukičević and B. Furtula, "Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges," *Journal of Mathematical Chemistry*, vol. 46, pp. 1369–1376, 2009.

[6] D. Vukičević and M. Gašperov, "Bond additive modeling 1. Adriatic indices," *Croatica Chemica Acta*, vol. 83, pp. 243–260, 2010.

[7] B. Furtula and I. Gutman, "A forgotten topological index," *Journal of Mathematical Chemistry*, vol. 53, pp. 1184–1190, 2015.

[8] I. Gutman, "Geometric approach to degree-based topological indices: Sombor indices," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 86, pp. 11–16, 2021.

[9] S. Fajtlowicz, "On conjectures of Graffiti-II," *Congressus Numerantium*, vol. 60, pp. 187–197, 1987.

[10] O. Favaron, M. Mahéo and J.-F. Saclé, "Some eigenvalue properties in graphs (conjectures of Graffiti-II)," *Discrete Mathematics*, vol. 111, pp. 197–220, 1993.

[11] Y. Pan and J. Li, "Graphs that minimizing symmetric division deg index," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 82, pp. 43–55, 2019.

[12] M. W. Rasheed, A. Mahboob and I. Hanif, "Uses of degree-based topological indices in QSPR

analysis of alkaloids with poisonous and healthful nature," *Frontiers in Physics*, vol. 12, 1381887, 2024.
[13] U. P. Preetha, M. Suresh, F. T. Tolasa and E. Bonyah, "QSPR/QSAR study of antiviral drugs modeled as multigraphs by using TI's and MLR method to treat COVID-19 disease," *Scientific Reports*, vol. 14, 13150, 2024.
[14] V. Kumar and S. Das, "Comparative study of GQ and QG indices as potentially favorable molecular descriptors," *International Journal of Quantum Chemistry*, 2024.
[15] A. R. Khan, S. A. Bhatti, F. Tawfiq *et al.*, "On degree-based operators and topological descriptors of molecular graphs and their applications to QSPR analysis of carbon derivatives," *Scientific Reports*, vol. 14, 21543, 2024.
[16] Dobrynin, A.A.; Entringer, R.; Gutman, I.Wiener index of trees: Theory and applications. Acta Appl. Math. **2001**, 66, 211–249.
[17] K. Pattabiraman, P. Danesh, Energy-Based Indices and their QSPR Studies of Certain Drugs Used for Kidney Cancer, *Int. J. Appl. Comput. Math.,* **11**(2025) 188.
[18] K. Pattabiraman, P. Danesh, Spectrum-Based Topological Indices and Their QSPR Studies of Nonsteroidal Anti-Inflammatory Drugs, *International Journal of Quantum Chemistry*, 124 (2024) e27472.
[19] K. Pattabiraman, Empowerments of blood cancer therapeutics via molecular descriptors, *Chemometrics and Intelligent Laboratory Systems*, 252(2025) 105180.
[20] K. Pattabiraman, P. Danesh, T.J. Zia, Quality Analysis of COVID-19 Drugs through Graph Polynomial. *Polycyclic Aromatic Compounds*, *44*(6) (2024) 4103–4126.
[21] K. Pattabiraman, S. Sudharsan, M. Cancan, *QSPR* Modeling with Topological Indices of Some Potential Drugs against Cancer. *Polycyclic Aromatic Compounds*, *44*(2)(2024) 1181–1208.