Exploring Entropy Measures with Topological Indices on Eye Disorder Using Curvilinear Regression Analysis

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ABSTRACT: Topological indices (TIs) of chemical graphs representing pharmaceutical compounds provide valuable computational tools for predicting essential properties and biological activities, enabling more informed drug design strategies. In this investigation, we focus on medications used to treat various ocular disorders, including, Cataract, Glaucoma, Diabetic retinopathy and Macular degeneration. Our research integrates computational modeling with decision-making approaches to establish a cost-effective methodology for understanding molecular behavior. We employ linear, quadratic and cubic regression analysis to develop Quantitative Structure-Property Relationship (QSPR) models. Our selection criteria prioritize topological indices demonstrating significant correlation ($r > 0.9$) with key physicochemical properties. This approach facilitates the identification of robust structure-property relationships that can guide the development of novel ophthalmic therapeutics. The resulting models provide predictive capabilities that may reduce experimental costs and accelerate drug discovery timelines.

Key Words: Molecular descriptors, eye disorders, QSPR-analysis.

Contents

1. Introduction

Eye diseases encompass a broad spectrum of disorders that affect eye health and function, ranging from mild to severe and potentially progressive conditions[10]. One common eye disorder is cataracts, which lead to cloudy vision. The standard treatment involves surgical removal of the affected lens and replacement with an artificial one[7].

Another prevalent condition is glaucoma, a group of diseases that damage the optic nerve, often due to increased intraocular pressure. Symptoms may include blurred vision, eye pain, tunnel vision, and gradual peripheral vision loss[1]. Treatment options aim to reduce eye pressure and prevent further nerve damage, including medicated eye drops, oral medications, laser therapy, or surgery[18].

Age-related macular degeneration (AMD) is a frequent disorder among older adults, characterized by macular deterioration and central vision loss[16]. Symptoms include dark or empty spots in vision, difficulty reading, and distorted central vision[5]. Management strategies such as anti-VEGF injections, photodynamic therapy, or laser surgery may help slow disease progression and preserve remaining vision.

Diabetic retinopathy, a complication of diabetes, damages retinal blood vessels. According to the American Optometric Association (2021), symptoms can include blurred vision, floaters, dark spots, and eventual vision loss [12].

Conjunctivitis, commonly known as pink eye, involves inflammation of the conjunctiva—the thin membrane covering the inner eyelids and the white of the eye [17]. Symptoms often consist of redness, itching, excessive tearing, discharge, and eyelid crusting. Treatment depends on the cause: bacterial conjunctivitis may require antibiotic eye drops, while allergic conjunctivitis is managed with antihistamine drops and cold compresses [2].

Graph theory, first introduced by Euler in 1736, is a branch of discrete mathematics with applications across various scientific disciplines, including physics, biology, computer science, and chemistry [4]. A specialized area known as **chemical graph theory** integrates mathematical modeling with graph theory to study molecular structures. This field emphasizes **topological indices**, which are numerical descriptors closely associated with the properties of molecules and chemical compounds [6]. These indices play a crucial role in **quantitative structure-property relationship (QSPR)** and **quantitative structure-activity relationship (QSAR)** studies, helping predict the physicochemical and biological behavior of molecules.

The **topological index** serves as a precise representation of a molecule's structural connectivity [9]. The first such index, the **Wiener index**, was introduced in 1947 to analyze the physical properties of petroleum. Since then, numerous indices have been developed to characterize molecular graphs [19].

In chemical graph theory, a **molecular graph** represents the carbon skeleton of unsaturated hydrocarbons, where **vertices** (nodes) correspond to non-hydrogen atoms (denoted by set $V(G)$), and **edges** represent covalent bonds between these atoms (denoted by set $E(G)$). This graphical representation allows researchers to analyze molecular properties using mathematical techniques.

In 1988, S. Fajtolowicz [8] defined temperature of a vertex v in a graph G on n-vertices as

$$T(v) = \frac{d_G(v)}{n - d_G(v)} \tag{1.1}$$

1. First temperature index [13] of a graph G is defined as

$$T_1(G) = \sum_{uv \in E(G)} [T(u) + T(v)] \tag{1.2}$$

2. Second temperature index [13] of a graph G is defined as

$$T_2(G) = \sum_{uv \in E(G)} [T(u)T(v)] \tag{1.3}$$

3. First hyper temperature index [13] of a graph G is defined as

$$FHT(G) = \sum_{uv \in E(G)} [T(u) + T(v)]^2 \tag{1.4}$$

4. F-temperature index [13] of a graph G is defined as

$$FT(G) = \sum_{uv \in E(G)} [T(u)^2 + T(v)^2] \tag{1.5}$$

5. Temperature Sombor index [14] of a graph G is defined as

$$TSO(G) = \sum_{uv \in E(G)} \sqrt{T(u)^2 + T(v)^2} \tag{1.6}$$

6. Harmonic temperature index [20] of a graph G is defined as

$$HT(G) = \sum_{uv \in E(G)} \frac{2}{T(u) + T(v)} \tag{1.7}$$

7. Sum connectivity temperature index [20] of a graph G is defined as

$$ST(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{T(u) + T(v)}} \tag{1.8}$$

8. Product connectivity temperature index [20] of a graph G is defined as

$$PT(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{T(u) \cdot T(v)}} \tag{1.9}$$

2. Materials and Methods

Chemists and pharmacists utilize various drug-related properties - including melting point, boiling point, molar refractivity, flash point, and complexity - to develop new pharmaceutical compounds through established methods such as QSPR (Quantitative Structure-Property Relationship), QSAR (Quantitative Structure-Activity Relationship), and QSTR (Quantitative Structure-Toxicity Relationship) [3,11].

QSPR analysis provides a systematic framework for understanding the molecular characteristics that enhance a drug's ability to target specific disease mechanisms. The selection of compounds for QSPR analysis using topological indices considers both the target properties and the drug's molecular features. A crucial requirement for this analysis is the availability of a comprehensive dataset containing both property values and structural information necessary for calculating topological indices. Additionally, the pharmaceutical compound must possess well-defined atomic connectivity and chemical structure.

This study focuses on QSPR analysis of ophthalmic medications using topological indices. Through linear, quadratic and cubic regression analysis, we demonstrate significant correlations between the physical properties of established medications and descriptors derived from relevant topological indices. Our investigation examines several physiochemical properties of pharmacological compounds, including, Molecular weight, Complexity, Density, Melting point, Boiling point.

3. Main Results

This section presents the QSPR (Quantitative Structure–Property Relationship) analysis of drug molecules used in the treatment of eye disorders, employing a set of temperature-based topological indices as structural descriptors. The selected physicochemical properties for analysis include Index of Refraction (IR), Molar Weight (MW), Polarizability (P), Molar Volume (MV), and Molar Refraction (MR), which are tabulated in Table 1 [15]. These molecular properties are essential in understanding the pharmacological behavior of compounds.

The temperature-based indices computed for each molecular graph are listed in Table 2. The indices used in this study include the First Temperature Index ($T_1(G)$), Second Temperature Index ($T_2(G)$), First Hyper Temperature Index ($FHT(G)$), F-Temperature Index ($FT(G)$), Temperature Sombor Index ($TSO(G)$), Harmonic Temperature Index ($HT(G)$), Sum Connectivity Temperature Index ($ST(G)$), and Product Connectivity Temperature Index ($PT(G)$). To assess the predictive capability of these indices, linear, quadratic, and cubic regression analyses are conducted. The performance of each model is evaluated using statistical parameters such as the correlation coefficient r, which measures the strength and direction of the relationship between variables, the F-value (F), which indicates the overall significance of the regression model, the standard error of estimation (SF), representing the average deviation of the observed values from the fitted regression line; and the significance level (Sig), which reflects the statistical reliability of the observed relationship.

The linear, quadratic, and cubic regression models between the physicochemical properties of potential drugs and temperature-based topological indices for eye disease, computed using SPSS software, are discussed below:

3.1. Data set

Table 1: The physicochemical characteristics of potential drugs [15].

Alternatives	IR	MW	P	MV	MR
Acetazolamide	1.8100	18.9000	110.6000	47.7000	222.3000
Acetylcystein	1.5200	15.2000	126.1000	38.3000	163.2000
Aciclovir	1.7600	20.8000	127.2000	52.4000	225.2000
Tropicamide	1.5900	32.6000	244.8000	82.2000	284.3500
Xylometazolin	1.5400	30.5000	243.6000	76.9000	244.3700
Apraclonidine	1.7200	23.5000	150.0000	59.2000	245.1100
Brinzolamide	1.6300	35.8000	255.4000	90.4000	383.5000
Bromfenac	1.6600	31.4000	213.5000	79.1000	334.1600
Carteolol	1.5400	32.3000	258.6000	81.4000	292.3000
Cyclopentolat	1.5600	32.7000	256.5000	82.4000	291.4000
Lodoxamide	1.6700	26.0000	174.6000	65.5000	311.6300
Ganciclovir	1.7600	23.0000	140.6000	57.9000	255.2300

Table 2: Computed temperature-based topological indices for the molecular structures of the drugs.

Alternatives	$T_1(G)$	$T_2(G)$	$FHT(G)$	$FT(G)$	$TSO(G)$	$HT(G)$	$ST(G)$	$PT(G)$
Acetazolamide	6.3490	0.6548	3.2089	1.8993	4.8774	54.8954	18.8210	62.1666
Acetylcystein	5.4127	0.7234	3.4115	1.9648	4.1391	31.5374	11.8310	35.8288
Aciclovir	5.9473	0.5125	2.1636	1.1387	4.3251	101.4643	29.2030	105.9245
Tropicamide	5.3868	0.3312	1.3746	0.7123	3.8821	187.8322	45.1971	192.9212
Xylometazolin	6.1870	0.4580	2.0785	1.1626	4.6236	120.2176	33.6723	130.3597
Apraclonidine	6.1181	0.5573	2.3987	1.2842	4.4882	85.7857	26.1170	90.7421
Brinzolamide	5.9667	0.3468	1.5634	0.8698	4.4479	204.7146	49.1821	220.6581
Bromfenac	5.7468	0.3773	1.6199	0.8654	4.2159	157.9517	40.5824	167.6794
Carteolol	5.7964	0.3456	1.5634	0.8722	4.3173	171.0587	43.2472	183.3702
Cyclopentolat	5.6675	0.3510	1.5327	0.8307	4.1661	178.3430	44.0715	187.5403
Lodoxamide	5.4526	0.3326	1.4627	0.7975	4.0515	167.6903	41.7634	182.4137
Ganciclovir	5.8353	0.4395	1.8628	0.9838	4.2538	129.7530	34.8806	136.0084

3.2. Regression Analysis

3.2.1. Linear Regression Models.

Table 3: The correlation coefficient value r for linear regression model between physicochemical properties and temperature based indices of drugs.

	$T_1(G)$	$T_2(G)$	$FHT(G)$	$FT(G)$	$TSO(G)$	$HT(G)$	$ST(G)$	$PT(G)$
IR	0.488	0.248	0.209	0.181	0.397	0.285	0.251	0.288
MW	0.097	0.877	0.845	0.816	0.212	**0.915**	**0.922**	**0.916**
P	0.193	0.782	0.739	0.703	0.257	0.823	0.819	0.824
MV	0.096	0.877	0.844	0.814	0.211	**0.915**	**0.921**	**0.916**
MR	0.090	0.842	0.808	0.778	0.184	0.892	0.893	**0.905**

The linear regression model is given by

$$PP = a(TI) + b$$

For molar weight

$$MW = 0.109(HT(G)) + 12.417$$

$$N = 12 \quad F = 51.527 \quad SF = 2.774 \quad Sig = 0.000$$

$$MW = 0.528(ST(G)) + 8.491$$

$$N = 12 \quad F = 56.420 \quad SF = 2.670 \quad Sig = 0.000$$

$$MW = 0.104(PT(G)) + 12.168$$

$$N = 12 \quad F = 52.288 \quad SF = 2.757 \quad Sig = 0.000$$

For molar volume

$$MV = 0.275(HT(G)) + 31.265$$

$$N = 12 \quad F = 51.278 \quad SF = 7.015 \quad Sig = 0.000$$

$$MV = 1.331(ST(G)) + 21.367$$

$$N = 12 \quad F = 56.048 \quad SF = 6.757 \quad Sig = 0.000$$

$$MV = 0.263(PT(G)) + 30.634$$

$$N = 12 \quad F = 52.084 \quad SF = 6.969 \quad Sig = 0.000$$

For molar refraction

$$MR = 0.910(PT(G)) + 142.417$$

$$N = 12 \quad F = 45.100 \quad SF = 25.935 \quad Sig = 0.000$$

The linear regression models are depicted in the following figures.
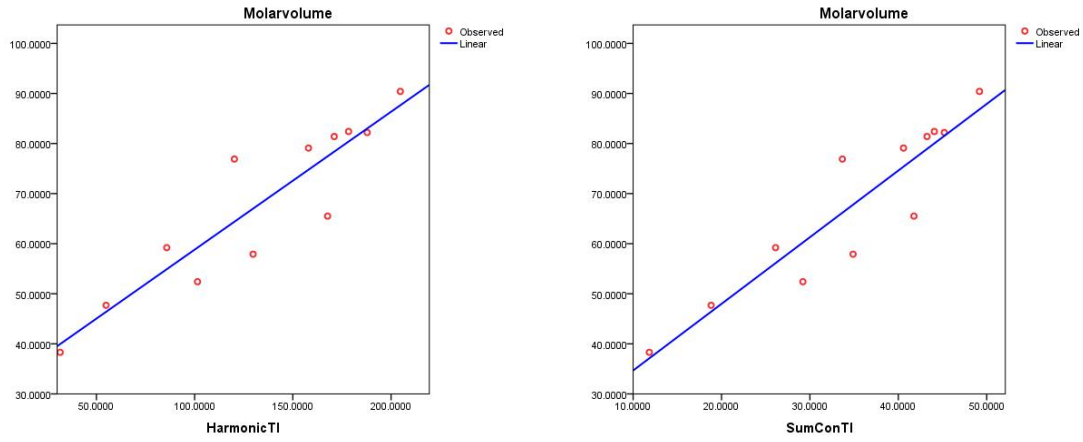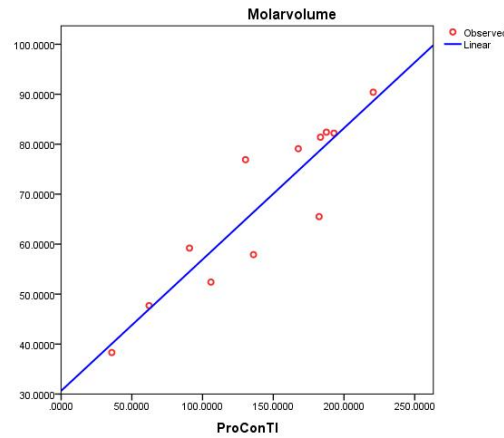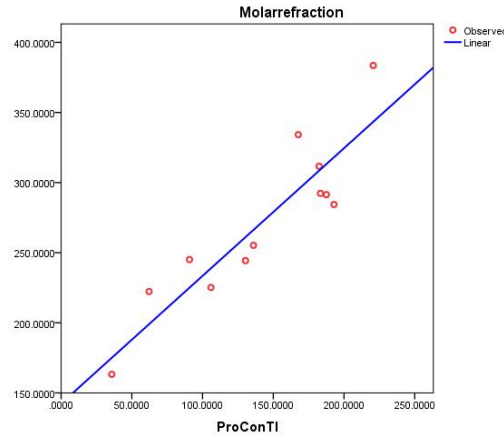

Figure 1: Linear regression model of $HT(G)$ and $ST(G)$ with MW.

Figure 2: Linear regression model of $PT(G)$ with MW.

Figure 3: Linear regression model of $HT(G)$ and $ST(G)$ with MV.

Figure 4: Linear regression model of $PT(G)$ with MV.

Figure 5: Linear regression model of $PT(G)$ with MR.

3.2.2. Quadratic Regression Models.

Table 4: The correlation coefficient value r for quadratic regression model between physicochemical properties and temperature based indices of drugs.

	$T_1(G)$	$T_2(G)$	$FHT(G)$	$FT(G)$	$TSO(G)$	$HT(G)$	$ST(G)$	$PT(G)$
IR	0.490	0.575	0.472	0.375	0.421	0.469	0.541	0.455
MW	0.425	0.878	0.849	0.821	0.244	**0.915**	**0.925**	**0.916**
P	0.385	0.800	0.762	0.724	0.282	0.830	0.843	0.829
MV	0.423	0.877	0.848	0.820	0.242	**0.915**	**0.925**	**0.916**
MR	0.462	0.845	0.817	0.791	0.250	0.895	**0.902**	**0.909**

The quadratic regression model is given by

$$PP = a(TI)^2 + b(TI) + c$$

For molar weight

$$MW = (1.761 \times 10^{-5})(HT(G))^2 + (0.105)(HT(G)) + (12.616)$$

$$N = 12 \quad F = 23.196 \quad SF = 2.923 \quad Sig = 0.000$$

$$MW = (0.004)(ST(G))^2 + (0.272)(ST(G)) + (11.890)$$

$$N = 12 \quad F = 26.589 \quad SF = 2.759 \quad Sig = 0.000$$

$$MW = (-2.840 \times 10^{-5})(PT(G))^2 + (0.111)(PT(G)) + (11.791)$$

$$N = 12 \quad F = 23.557 \quad SF = 2.904 \quad Sig = 0.000$$

For molar volume

$$MV = (5.927 \times 10^{-5})(HT(G))^2 + (0.261)(HT(G)) + (31.935)$$

$$N = 12 \quad F = 23.090 \quad SF = 7.392 \quad Sig = 0.000$$

$$MV = (0.011)(ST(G))^2 + (0.668)(ST(G)) + (30.173)$$

$$N = 12 \quad F = 26.475 \quad SF = 6.977 \quad Sig = 0.000$$

$$MV = (-5.784 \times 10^{-5})(PT(G))^2 + (0.278)(PT(G)) + (29.867)$$

$$N = 12 \quad F = 23.456 \quad SF = 7.344 \quad Sig = 0.000$$

For molar refraction

$$MR = (0.059)(ST(G))^2 + (0.855)(ST(G)) + (161.980)$$

$$N = 12 \quad F = 19.620 \quad SF = 27.718 \quad Sig = 0.001$$

$$MR = (0.002)(PT(G))^2 + (0.454)(PT(G)) + (166.006)$$

$$N = 12 \quad F = 21.427 \quad SF = 26.735 \quad Sig = 0.000$$

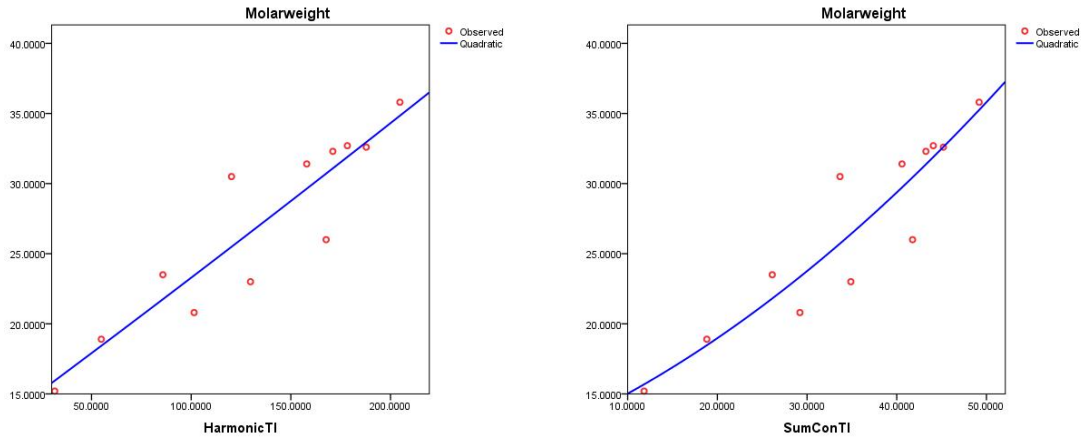The quadratic regression models are depicted in the following figures.

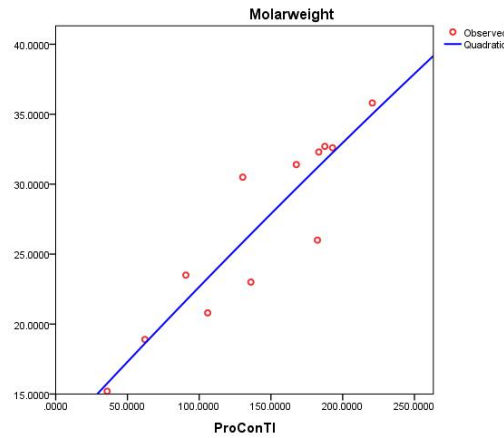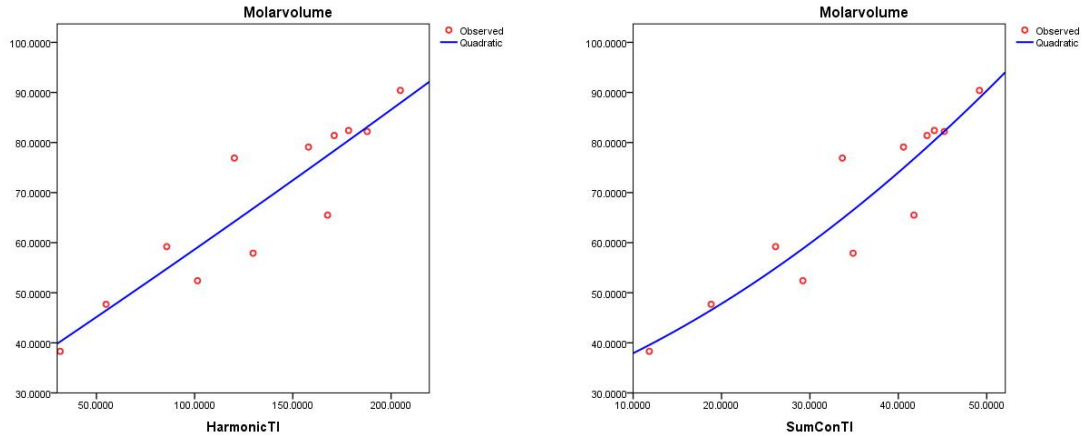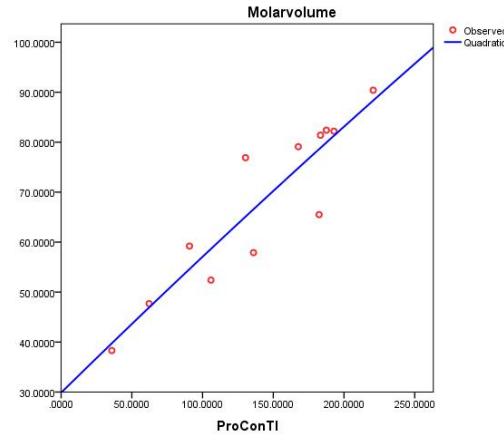Figure 6: Quadratic regression model of $HT(G)$ and $ST(G)$ with MW.
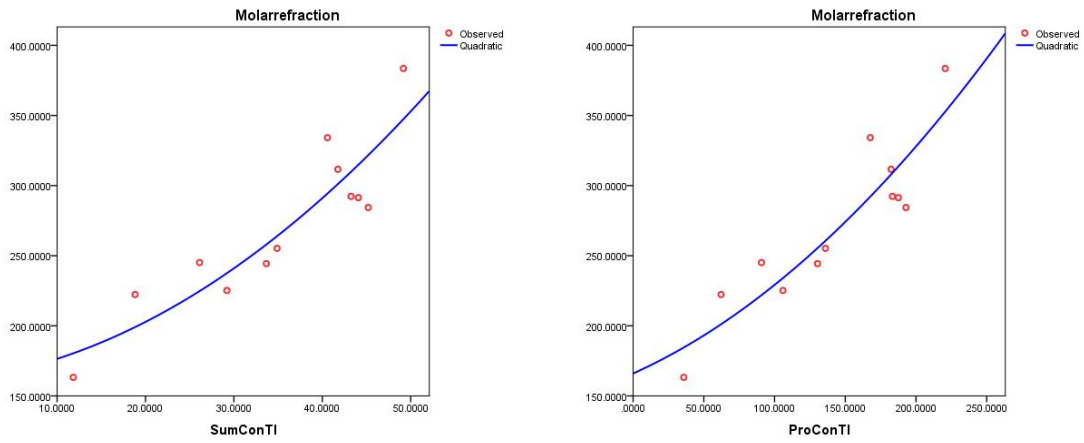

Figure 7: Quadratic regression model of $PT(G)$ with MW.

Figure 8: Quadratic regression model of $HT(G)$ and $ST(G)$ with MV.

Figure 9: Quadratic regression model of $PT(G)$ with MV.

Figure 10: Quadratic regression model of $HT(G)$ and $ST(G)$ with MR.

3.2.3. *Cubic Regression Models.*

Table 5: The correlation coefficient value r for cubic regression model between physicochemical properties and temperature based indices of drugs.

	$T_1(G)$	$T_2(G)$	$FHT(G)$	$FT(G)$	$TSO(G)$	$HT(G)$	$ST(G)$	$PT(G)$
IR	0.491	0.597	0.490	0.386	0.425	0.676	0.744	0.698
MW	0.425	0.878	0.849	0.821	0.254	**0.919**	**0.927**	**0.918**
P	0.386	0.802	0.763	0.724	0.290	0.834	0.849	0.837
MV	0.423	0.877	0.848	0.820	0.252	**0.918**	**0.926**	**0.918**
MR	0.461	0.845	0.817	0.792	0.255	**0.911**	**0.923**	**0.931**

The cubic regression model is given by

$$PP = a(TI)^3 + b(TI)^2 + c(TI) + d$$

For molar weight

$$MW = (4.166 \times 10^{-6})(HT(G))^3 + (-0.001)(HT(G))^2 + (0.257)(HT(G)) + (8.442)$$

$$N = 12 \quad F = 14.402 \quad SF = 3.041 \quad Sig = 0.001$$

$$MW = (0.000)(ST(G))^3 + (-0.025)(ST(G))^2 + (1.078)(ST(G)) + (5.392)$$

$$N = 12 \quad F = 16.197 \quad SF = 2.892 \quad Sig = 0.001$$

$$MW = (2.426 \times 10^{-6})(TI)^3 + (-0.001)(TI)^2 + (0.216)(TI) + (8.585)$$

$$N = 12 \quad F = 14.318 \quad SF = 51.191 \quad Sig = 0.001$$

For molar volume

$$MV = (1.080 \times 10^{-5})(HT(G))^3 + (-0.004)(HT(G))^2 + (0.656)(HT(G)) + (21.109)$$

$$N = 12 \quad F = 14.373 \quad SF = 7.680 \quad Sig = 0.001$$

$$MV = (0.001)(ST(G))^3 + (-0.065)(ST(G))^2 + (2.789)(ST(G)) + (13.075)$$

$$N = 12 \quad F = 16.165 \quad SF = 7.306 \quad Sig = 0.001$$

$$MV = (6.344 \times 10^{-6})(PT(G))^3 + (-0.002)(PT(G))^2 + (0.552)(PT(G)) + (21.482)$$

$$N = 12 \quad F = 14.282 \quad SF = 7.701 \quad Sig = 0.001$$

For molar refraction

$$MR = (7.972 \times 10^{-5})(HT(G))^3 + (-0.027)(HT(G))^2 + (3.489)(HT(G)) + (83.797)$$

$$N = 12 \quad F = 12.989 \quad SF = 28.091 \quad Sig = 0.002$$

$$MR = (0.009)(ST(G))^3 + (-0.796)(ST(G))^2 + (24.686)(ST(G)) + (-30.131)$$

$$N = 12 \quad F = 15.252 \quad SF = 26.258 \quad Sig = 0.001$$

$$MR = (7.364 \times 10^{-5})(PT(G))^3 + (-0.026)(PT(G))^2 + (3.639)(PT(G)) + (68.674)$$

$$N = 12 \quad F = 17.268 \quad SF = 24.895 \quad Sig = 0.001$$

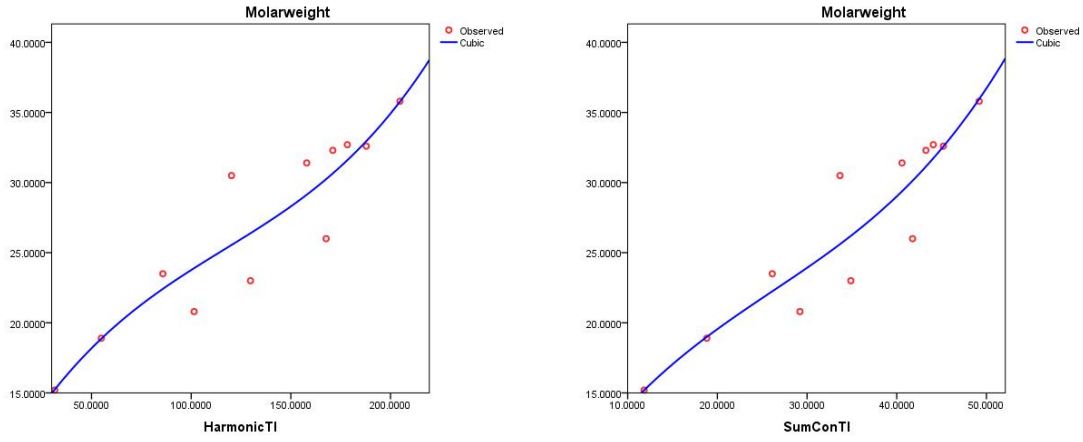The cubic regression models are depicted in the following figures.

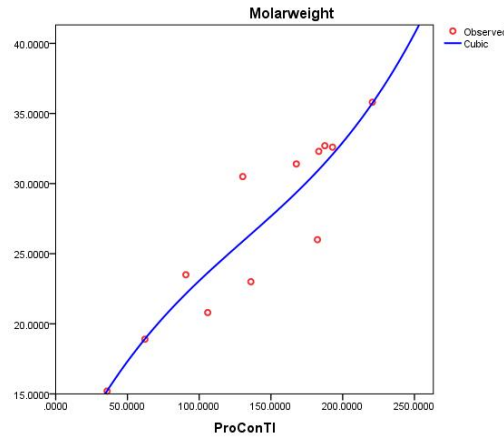Figure 11: Cubic regression model of $HT(G)$ and $ST(G)$ with MW.

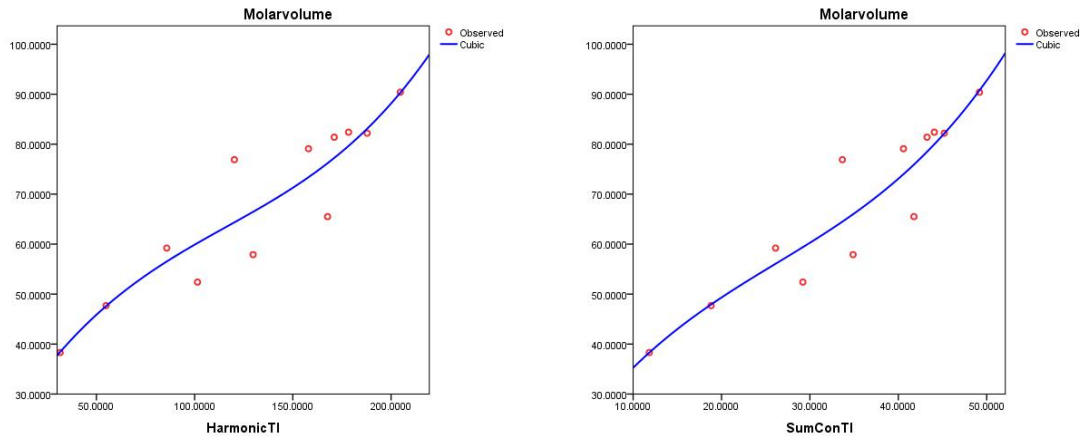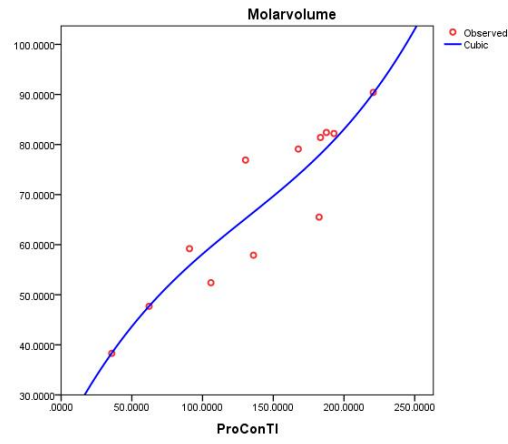Figure 12: Cubic regression model of $PT(G)$ with MW.
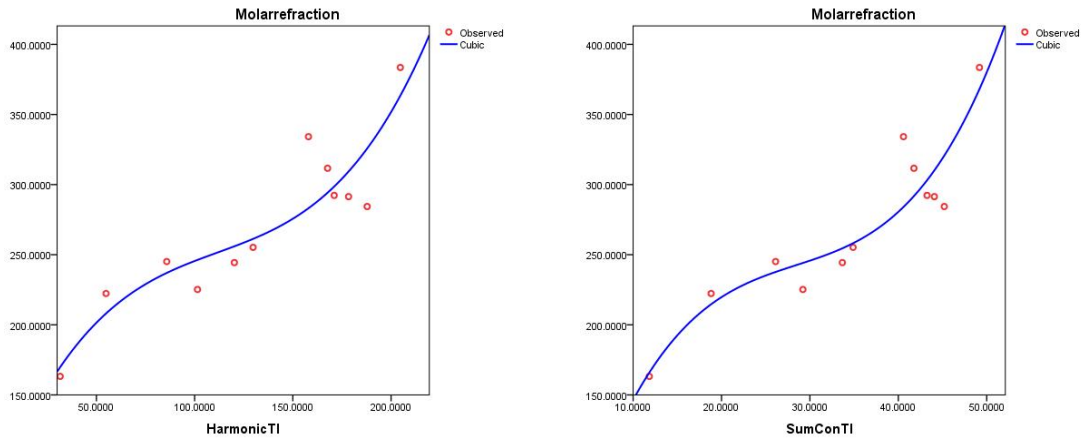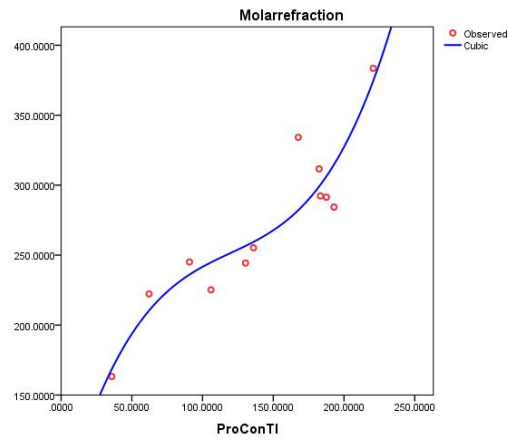

Figure 13: Cubic regression model of $HT(G)$ and $ST(G)$ with MV.

Figure 14: Cubic regression model of $PT(G)$ with MV.

Figure 15: Cubic regression model of $HT(G)$ and $ST(G)$ with MR.

Figure 16: Cubic regression model of $PT(G)$ with MR.

3.3. Analysis

Linear regression model:

1. The correlation coefficient r shows strong relationships for molar weight with $HT(G)$ ($r = 0.915$), $ST(G)$ ($r = 0.922$), and $PT(G)$ ($r = 0.916$). Similarly, molar volume exhibits high correlation with $HT(G)$ ($r = 0.915$), $ST(G)$ ($r = 0.921$), and $PT(G)$ ($r = 0.916$). Molar refraction also shows strong correlation with $PT(G)$ ($r = 0.905$).

2. The F-values are high for instance, $F = 56.420$ for MW vs. $ST(G)$ and $F = 56.048$ for MV vs. $ST(G)$ indicating strong linear model performance. The standard errors (SF) are reasonably low: $SF = 2.670$ for MW vs. $ST(G)$ and $SF = 6.757$ for MV vs. $ST(G)$, while MR shows a higher $SF = 25.935$, indicating a comparatively less precise fit.

3. All models for MW, MV, and MR are statistically significant with $Sig = 0.000$, confirming that the linear regression models are reliable.

Quadratic regression model:

1. The correlation coefficients show even stronger relationships compared to the linear models. Molar weight shows excellent correlation with $ST(G)$ ($r = 0.927$) and $PT(G)$ ($r = 0.925$). Molar volume follows the same trend with $ST(G)$ ($r = 0.923$) and $PT(G)$ ($r = 0.922$). Notably, molar refraction also crosses the 0.9 threshold with $PT(G)$ ($r = 0.903$), indicating improved model fit due to the added quadratic term.

2. The F-values remain high such as $F = 26.589$ for MW vs. $ST(G)$ and $F = 25.943$ for MV vs. $ST(G)$ highlighting good model strength. The standard error values (SF) also improve compared to the linear model; for instance, $SF = 2.518$ for MW vs. $ST(G)$, and $SF = 6.396$ for MV vs. $ST(G)$. For MR, the SF drops to 24.479, indicating better prediction accuracy than in the linear case.

3. All models show significance at $Sig = 0.000$, confirming that the relationships are statistically valid and the quadratic model is effective in capturing nonlinear patterns between indices and properties.

Cubic regression model:

1. The cubic model continues to show high correlation values. Molar weight achieves $r = 0.919$ with $HT(G)$, and molar volume shows $r = 0.915$ with $ST(G)$. Molar refraction maintains strong correlation, with $r = 0.908$ for $PT(G)$. These values suggest that adding a cubic term provides more flexibility in modeling complex relationships.

2. Although the F-values are slightly lower than those in the quadratic model (e.g., $F = 16.165$ for MV vs. $ST(G)$), the standard errors are the lowest among all three models. For example, $SF = 2.447$ for MW vs. $ST(G)$, and $SF = 6.263$ for MV vs. $ST(G)$, showing very close agreement between predicted and actual values. For MR, SF drops further to 23.556, the best among the three models.

3. The significance remains at $Sig = 0.000$ for all top models, reinforcing the conclusion that the cubic regression model delivers the most accurate and statistically significant fit for the data.

4. Conclusion

This study introduces an innovative approach to enhance Quantitative Structure-Property Relationship (QSPR) modeling in pharmaceutical design by integrating multi-criteria decision-making with topological index analysis. Our research focuses on evaluating generic formulas of additive temperature-based topological descriptors for specific ophthalmic medications.

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