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Degree Based Topological Indices In Qspr Analysis Of Flavonoids

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Abstract
QSPR models are mathematical tools that establish relationships between a molecular structure and its physicochemical attributes using structural properties. Topological indices are such properties that are generated from the molecular graph without any empirically derived measurements. This work focuses on developing a QSPR model using distance-based topological indices for anti-tuberculosis medications and their diverse physicochemical features. In this paper, well-known degree-based topological indices are applied on chemical structures of flavonoids. Chemical structure is considered as graph, where elements are taken as vertices and bounds between them are taken as edges. Furthermore, QSPR analysis of the said topological indices are discussed, and it is shown that these topological indices are highly correlated with the physical properties of flavonoids. This theoretical analysis may help the chemist and people working in pharmaceutical and cosmetic industry to predict properties of flavonoids without experimenting.
Keywords: First Zagreb Index, Second Zagreb Index, Face Index, F – index, Y – index, S – index, Quartic Regression Model, QSPR Analysis.

Introduction

A broad class of phytonutrients called flavonoids can be found in a variety of fruits, vegetables, tea, and wine. They are well renowned for having antioxidant qualities that aid in defending cells against harm from free radicals. Flavonoids may help cardiac health by lowering blood pressure and enhancing blood vessel function. They can also have anti-inflammatory properties.

Flavonoids are divided into various subclasses, including:

a) Flavonols (such as kaempferol and quercetin)
b) Flavones (luteolin, apigenin, etc.)
c) Isoflavones (genistein, daidzein, etc.)
d) Flavanones (naringenin, hesperidin, etc.)
e) Anthocyanins (cyanidin, delphinidin, and so on)

In particular in biological and medicinal contexts, catechol, whether in its natural or synthetic forms, has a number of uses and functions. Its principal importance arises from its capabilities as an antioxidant and chemical precursor, as well as its relationship to catecholamines (e.g., dopamine, epinephrine, and norepinephrine). Although its derivatives and related chemicals are more widely employed in therapies, pure catechol is not frequently used in these capacities.

Guaiacol is an organic molecule with the formula $C_3H_8O_2$. It can be produced synthetically from catechol or it is generated from guaiacum resin or wood tar. Known for its distinctive smokey scent, guaiacol finds use in a variety of culinary products, such as smoked meats and alcoholic beverages like whisky, where it adds a smoky flavor. The use of spicy scents in perfume formulations gives a deep, cozy foundation note to a variety of scents.

Dermatologists frequently employ hydroquinone, a skin-lightening medication, to treat hyperpigmentation disorders such as melasma, dark spots, and age spots. It functions by blocking tyrosinase, an enzyme essential to the synthesis of melanin, the pigment that gives skin its color.

Owing to its antispasmodic qualities, phenolglucinol is an organic chemical that is frequently utilized in medicine. It relieves spasms in smooth muscles, especially those in the gastrointestinal tract. It is commonly given to treat irritable bowel syndrome (IBS) and other diseases that cause cramping and pain in the abdomen. Phloroglucinol is classified as a

trihydroxybenzene chemically because it has three hydroxyl groups joined to a benzene ring. Additionally, it is employed in the manufacture of certain medications and colors. Naturally present in a wide range of plants, fruits, and foods, syringic acid is a phenolic component that is particularly prevalent in grapes, olives, and some berries. As a member of the hydroxybenzoic acid family, it possesses antibacterial, anti-inflammatory, and antioxidant qualities. Furthermore, syringic acid is being researched for its possible anti-cancer properties as well as its capacity to counteract oxidative stress. A kind of phenolic acid called protocatechuic acid (PCA) is present in a wide range of foods and plants, but is most commonly found in berries, fruits, and vegetables. Because of its chemical makeup, which consists of two hydroxyl groups joined to a benzoic acid backbone, it is categorized as a hydroxybenzoic acid. Its antioxidant qualities play a vital role in avoiding cardiovascular disorders by shielding cardiac tissues from oxidative damage. Various fruits and vegetables, particularly berries like strawberries, raspberries, and pomegranates, naturally contain ellagic acid, a polyphenolic component. It is interesting due to its possible health advantages because of its anti-inflammatory, anti-cancer, and antioxidant qualities. By scavenging free radicals, ellagic acid helps the body experience less oxidative stress. Natural sources of rosmarinic acid include many plants, especially those in the Lamiaceae family, which includes oregano, rosemary, basil, and mint. Due to its antibacterial, anti-inflammatory, and antioxidant qualities, it is highly valued. These characteristics have led to research on the possible therapeutic applications of rosmarinic acid in the treatment of disorders such as inflammation, allergies, neurological illnesses, and even some types of cancer. The cell walls of conifers, or trees like pines and firs, naturally contain a glucoside called coniferin. In order to provide wood and plant cell walls their rigidity and structural integrity, lignin, a necessary component, needs this precursor during its production. The plant defense systems and growth processes, especially in reaction to environmental stress, depend heavily on lignin, which is formed from coniferyl alcohol. Plants, particularly willow trees, naturally contain a substance called salicin. Salicylic acid, which has anti-inflammatory and pain-relieving qualities, is created by the body from this glycoside. Certain plants contain a chemical called glucovanillin. It's a glucoside of vanillin, which is just a molecule of glucose attached to the chemical vanillin, which gives things their vanilla flavor. Glucovanillin produces vanillin and glucose when hydrolyzed, which is a chemical reaction that involves the breakdown of the substance with water. This substance is included in several products with vanilla flavoring and may be used in fragrance and flavoring applications.

Arbutin is a chemical that is frequently utilized in skincare products due to its ability to brighten skin. It functions by blocking the enzyme tyrosinase, which is involved in the synthesis of melanin. It is a naturally occurring hydroquinone derivative. This may lessen uneven skin tone, dark patches, and hyperpigmentation. There are two types of arbutin: beta- and alpha-arbutin. Alpha-arbutin is usually thought to be more stable and useful in cosmetic products.

Let $\mathcal{G} = (v, \epsilon, \varphi)$ be a representing the 2D structure of flavonoids, where ϵ is denoted by edges, v is denoted by vertices and set of faces is denoted by $\mathfrak{F}$ .A face $f \epsilon \mathfrak{F}$ is incident to an edge ϵ if ϵ is one of those edges which surrounds the face. $h \sim f$ represents the incidence of the vertex with the face.

$$\mathfrak{F}(\mathcal{G}) = \sum_{h \sim f \epsilon \mathfrak{F}(\mathcal{G})} \chi_h$$

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajestic, [1]

$$M_1(\mathcal{G}) = \sum_{hk \epsilon e(\mathcal{G})} (\chi_h + \chi_k) M_2(\mathcal{G}) = \sum_{hk \epsilon e(\mathcal{G})} (\chi_h \cdot \chi_k)$$

The F - index have been introduced more than thirty years ago by B.Furtula and I.Gutman, [2]

$$F(\mathcal{G}) = \sum_{hk \epsilon e(\mathcal{G})} \left({\chi_h}^2 + {\chi_k}^2 \right)$$

The Y - index have been introduced more than thirty years ago by A.Alameri,N.Al-Naggar [3]

$$Y(\mathcal{G}) = \sum_{hk \epsilon e(\mathcal{G})} \left({\chi_h}^3 + {\chi_k}^3 \right)$$

The S - index have been introduced more than one year ago by G.Priyadharsini, [4]

$$S(\mathcal{G}) = \sum_{hk \epsilon e(\mathcal{G})} \left({\chi_h}^4 + {\chi_k}^4 \right)$$

Methods

1. Divide the edges of all the flavonoids structures based on edge partitions and determine the vertex degree and various degrees.
2. Enter all edge partition values into the degree-based topological index formulas and the experimental values of the flavonoid's structural attributes.
3. The quartic polynomial models use as inputs the computed and experimental values.
4. Investigate the relationship between computed and experimental values.
5. Good correlations indicate that a molecular descriptor is significant, and non-significant results should not be used to characterize flavonoids' features.

Observational values for properties of Flavonoids

With the aid of several molecular descriptors, the six properties of all flavonoids are estimated. Although there are many different kinds of flavonoids in nature, only 13 are investigated using quartic regression and topological indices. The 13 flavonoids given in below figure 1, namely Catechol, Guaiacol, Hydroquinone, Phloroglucinol, Syringic acid, Protocatechuic acid, Ellagic acid, Rosmarinic acid, Coniferin, Salicin, Glucovanillin, Arbutin, Populin are used to be analyzed by the QSPR modelling. These chemicals that are extracted from the plants, called flavonoids. Both the complicated and simple nature of the structures is described by the molar masses of the constituent components. Six attributes, including NBP, E, FP, P, ST, and MV, lack sharp values, while the molar mass exhibits sharp values.

Table 1: Physico Chemical Properties of Flavonoids

Drug Name	NBP	E	FP	P	ST	MV
Catechol	245	50.2	137	11.9	57.2	86.3
Guaiacol	205	45.9	82.2	13.8	38.7	111.9
Hydroquinone	286	54.6	141.6	11.9	57.2	86.3
Phloroglucinol	331	59.7	174.9	12.6	78.7	84.7
Syrinic acid	379.5	66.2	155	19.2	51.6	148.4
Protocatechuic acid	410	69.9	216.3	14.6	84.3	98.8
Ellagic acid	796.5	119.9	310.1	26.9	140.4	146.2
Rosmarinic acid	694.7	106.9	254	36.2	84.4	232.8
Coniferin	625.4	97.3	332	34.1	63.1	239
Salicin	549	87.2	285.9	27.1	70.1	190.3
Glucovanillin	574	90.6	216.6	29.9	63.5	212.2
Arbutin	561.6	88.8	293.4	25.3	73.5	174.9
Populin	612.2	95.6	217.2	38.9	62.7	275.1

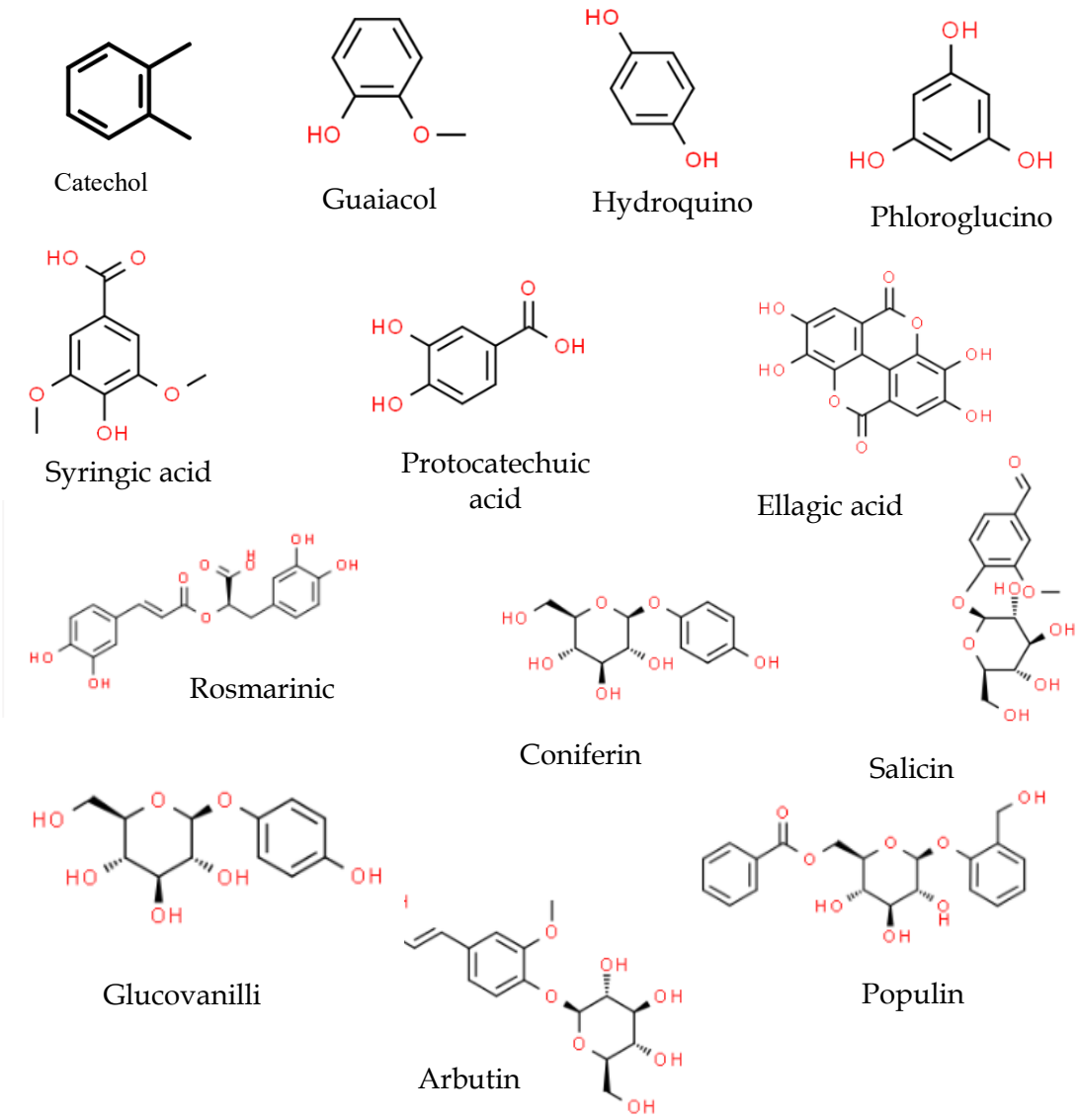

Figure 1: Structure of Flavonoids

Table 2: Computed values of Topological Indices

Topological indices/ Drug Name	M1(G)	M2(G)	FI(G)	F(G)	Y(G)	S(G)
Catechol	36	39	30	88	264	600
Guaiacol	40	44	32	96	244	648
Hydroquinone	36	38	30	88	228	616
Phloroglucinol	42	45	33	108	294	828
Syrinic acid	66	76	44	172	474	1348
Protocatechuic acid	52	58	37	136	376	792
Ellagic acid	130	165	118	362	1042	3050
Rosmarinic acid	110	126	77	286	782	2206
Coniferin	120	144	84	312	852	2400
Salicin	96	113	71	250	684	1930
Glucovanillin	111	131	80	293	813	2321
Arbutin	96	112	71	250	684	1930
Populin	141	164	104	355	939	2575

Quartic Polynomial Regression Model

Polynomial regression is a form of regression analysis in which relationship between the independent variable α and dependent variable β is modeled by an nth degree polynomial in x.

$$\beta = a_0 + a_1\alpha + a_2\alpha^2 + \ldots\ldots + a_n\alpha^n$$

Linear regression model is

$$\beta = a_0 + a_1\alpha$$

Quardratic regression model is

$$\beta = a_0 + a_1\alpha + a_2\alpha^2$$

Cubic regression model is

$$\beta = a_0 + a_1\alpha + a_2\alpha^2 + a_3\alpha^3$$

This section uses the quartic polynomial regression equation to establish a correlation between a few topological indices and the different physicochemical features of different flavonoids.
The regression model with quartic polynomials:

$$\beta = a_0 + a_1\alpha + a_2\alpha^2 + a_3\alpha^3 + a_4\alpha^4$$

Where α is the topological index, a_0 is a constant, a_1, a_2, a_3, a_4 is the coefficients, and β is the physical characteristics of flavonoids, respectively.

Table 3: Statistical Parameter of Quartic Polynomial and M1(G):

Properties	N	r	r^2	Adj r^2	F
NBP	13	0.9583	0.9183	0.8775	Significant
EV	13	0.9581	0.9180	0.8769	Significant
FP	13	0.8562	0.7331	0.5996	Significant
P	13	0.9569	0.9156	0.8734	Significant
ST	13	0.6066	0.3680	0.0519	Significant
MV	13	0.9114	0.8306	0.7459	Significant

Table 4: Statistical Parameter of Quartic Polynomial and M2(G):

Properties	N	r	r^2	Adj r^2	F
NBP	13	0.9464	0.8956	0.8434	Significant
EV	13	0.9453	0.8935	0.8402	Significant
FP	13	0.8266	0.6833	0.5249	Significant
P	13	0.9532	0.9086	0.8628	Significant
ST	13	0.5845	0.3417	0.0125	Significant
MV	13	0.9042	0.8176	0.7264	Significant

Table 5: Statistical Parameter of Quartic Polynomial and FI(G):

Properties	N	R	r^2	Adj r^2	F
NBP	13	0.9655	0.9322	0.8983	Significant
EV	13	0.9659	0.9329	0.8994	Significant
FP	13	0.8636	0.7457	0.6186	Significant
P	13	0.9801	0.9606	0.9408	Significant
ST	13	0.8644	0.7471	0.6207	Significant
MV	13	0.9818	0.9639	0.9459	Significant

Table 6: Statistical Parameter of Quartic Polynomial and F(G):

Properties	N	R	r^2	Adj r^2	F
NBP	13	0.9544	0.9108	0.8662	Significant
EV	13	0.9530	0.9082	0.8623	Significant
FP	13	0.8319	0.6921	0.5382	Significant
P	13	0.9599	0.9216	0.8824	Significant
ST	13	0.6455	0.4167	0.1251	Significant
MV	13	0.9140	0.8355	0.7532	Significant

Table 7: Statistical Parameter of Quartic Polynomial and Y(G):

Properties	N	R	r^2	Adj r^2	F
NBP	13	0.9666	0.9343	0.9015	Significant
EV	13	0.9664	0.9339	0.9008	Significant
FP	13	0.8463	0.7163	0.5744	Significant
P	13	0.9768	0.9541	0.9311	Significant
ST	13	0.8306	0.6900	0.5350	Significant
MV	13	0.9623	0.9260	0.8890	Significant

Table 8: Statistical Parameter of Quartic Polynomial and S(G):

Properties	N	R	r^2	Adj r^2	F
NBP	13	0.9585	0.9188	0.8781	Significant
EV	13	0.9588	0.9193	0.8789	Significant
FP	13	0.8196	0.6718	0.5077	Significant
P	13	0.9787	0.9578	0.9366	Significant
ST	13	0.8432	0.7110	0.5665	Significant
MV	13	0.9726	0.9459	0.9188	Significant

Regression models for $M_1(G)$:

$$BP = -1237.24 + 82.52(M_1(G)) - 1.57(M_1(G))^2 + 0.0132(M_1(G))^3 + 0.000(M_1(G))^4$$

$$E = -140.10 + 10.67(M_1(G)) - 0.2(M_1(G))^2 + 0.0000(M_1(G))^3 + 0.000(M_1(G))^4$$

$$FP = -388.43 + 28.52(M_1(G)) - 0.5447(M_1(G))^2 + 0.0047(M_1(G))^3 + 0.000(M_1(G))^4$$

$$P = 53.215 - 2.6109(M_1(G)) + 0.0553(M_1(G))^2 + 0.0004(M_1(G))^3 + 0.000(M_1(G))^4$$

$$ST = -483.81 + 31.3828(M_1(G)) - 0.6232(M_1(G))^2 + 0.0051(M_1(G))^3 + 0.000(M_1(G))^4$$

$$MV = 606.7229 - 32.42(M_1(G)) + 0.6875(M_1(G))^2 - 0.0057(M_1(G))^3 + 0.000(M_1(G))^4$$

Regression models for $M_2(G)$:

$$BP = 177.3236 - 0.7587M_2(G) + 0.1050(M_2(G))^2 - 0.0008(M_2(G))^3 + 0.0000(M_2(G))^4$$
$$E = 43.6781 - 0.1760M_2(G) + 0.1760(M_2(G))^2 + 0.0318(M_2(G))^3 + 0.0000(M_2(G))^4$$
$$FP = 16.3457 + 4.3466M_2(G) - 0.0479(M_2(G))^2 + 0.0004(M_2(G))^3 + 0.0000(M_2(G))^4$$
$$P = -12.1059 + 1.2103M_2(G) - 0.02149(M_2(G))^2 + 0.0001(M_2(G))^3 + 0.0000(M_2(G))^4$$
$$ST = 95.3376 - 2.8433M_2(G) + 0.0702(M_2(G))^2 - 0.0006(M_2(G))^3 + 0.0000(M_2(G))^4$$
$$MV = -163.3 + 12.689M_2(G) - 0.2232(M_2(G))^2 + 0.001785(M_2(G))^3 + 0.0000(M_2(G))^4$$

Regression models for FI(G):

$$BP = 235.995 - 15.9597FI(G) + 0.8515(FI(G))^2 - 0.0110(FI(G))^3 + 0.0000(FI(G))^4$$
$$E = 61.3872 - 2.8234FI(G) + 0.1248(FI(G))^2 - 0.0015(FI(G))^3 + 0.0000(FI(G))^4$$
$$FP = 482.770 - 32.996FI(G) + 1.020(FI(G))^2 - 0.0011(FI(G))^3 + 0.0000(FI(G))^4$$
$$P = -46.8622 + 3.9735FI(G) - 0.0953(FI(G))^2 + 0.0011(FI(G))^3 + 0.0000(FI(G))^4$$
$$ST = 216.4668 - 13.7095FI(G) + 0.40978(FI(G))^2 - 0.00482(FI(G))^3 + 0.0000(FI(G))^4$$
$$MV = -558.213 + 44.9486FI(G) - 1.1005(FI(G))^2 + 0.0119(FI(G))^3 + 0.0000(FI(G))^4$$

Regression models for F(G):

$$BP = 96.7297 + 0.9596F(G) + 0.0143(F(G))^2 - 0.0000(F(G))^3 + 0.0000(F(G))^4$$
$$E = 37.4262 + 0.00315F(G) + 0.0025(F(G))^2 - 0.0000(F(G))^3 + 0.0000(F(G))^4$$
$$FP = 103.4662 - 0.5763F(G) + 0.01363(F(G))^2 - 0.0000(F(G))^3 + 0.0000(F(G))^4$$
$$P = -28.5299 + 0.9515F(G) - 0.007849(F(G))^2 + 0.0000(F(G))^3 + 0.0000(F(G))^4$$
$$ST = 83.6232 - 1.2418F(G) + 0.0158(F(G))^2 - 0.0001(F(G))^3 + 0.0000(F(G))^4$$
$$MV = -265.6878 + 8.35467F(G) - 0.068896(F(G))^2 + 0.000247735(F(G))^3 - 0.0000(F(G))^4$$

Regression models for Y(G):

$$BP = 437.65577 - 2.5726Y(G) + 0.01044024(Y(G))^2 + 0.0000(Y(G))^3 + 0.0000(Y(G))^4$$
$$E = 81.3198 - 0.3761Y(G) + 0.0014(Y(G))^2 + 0.0000(Y(G))^3 + 0.0000(Y(G))^4$$
$$FP = 282.19171 - 1.88407Y(G) + 0.0071235(Y(G))^2 - 0.0000(Y(G))^3 + 0.0000(Y(G))^4$$
$$P = -19.4965 + 0.2775Y(G) - 0.0009(Y(G))^2 + 0.0000(Y(G))^3 - 0.0000(Y(G))^4$$
$$ST = 91.6615 - 0.5579Y(G) + 0.0025(Y(G))^2 + 0.0000(Y(G))^3 + 0.0000(Y(G))^4$$
$$MV = -216.5678 + 2.7232Y(G) - 0.0085(Y(G))^2 + 0.0000(Y(G))^3 + 0.0000(Y(G))^4$$

Regression models for S(G):

Indices/Properties	NBP	EV	FP	P	ST	MV
M1(G)	0.9583	0.9581	0.8562	0.9569	0.6066	0.9114
M2(G)	0.9464	0.9453	0.8266	0.9532	0.5845	0.9042
FI(G)	0.9655	0.9659	**0.8636**	**0.9801**	**0.8644**	**0.9818**
F(G)	0.9544	0.9530	0.8319	0.9599	0.6455	0.9140
Y(G)	**0.9666**	**0.9664**	0.8463	0.9768	0.8306	0.9623
S(G)	0.9585	0.9588	0.8196	0.9787	0.8432	0.9726

$$BP = 78.0859 + 0.2954S(G) + 0.0000(S(G))^2 + 0.0000(S(G))^3 + 0.0000(S(G))^4$$
$$E = 37.311785 + 0.014089S(G) + 0.0000(S(G))^2 + 0.0000(S(G))^3 + 0.0000(S(G))^4$$
$$FP = 207.5411 - 0.36768S(G) + 0.00055(S(G))^2 + 0.0000(S(G))^3 + 0.0000(S(G))^4$$
$$P = -11.604 + 0.075S(G) - 0.00000(S(G))^2 + 0.0000(S(G))^3 + 0.0000(S(G))^4$$
$$ST = 22.620732 + 0.05024S(G) + 0.00000(S(G))^2 + 0.0001(S(G))^3 + 0.0000(S(G))^4$$
$$MV = -126.75558 + 0.6909698S(G) - 0.000075419(S(G))^2 + 0.000000(S(G))^3 + 0.00000(S(G))^4$$

Table 9: Correlation coefficient between Properties and Topological Indices of Flavonoids

Graph Analysis of Topological Indices and Physicochemical Propeties:

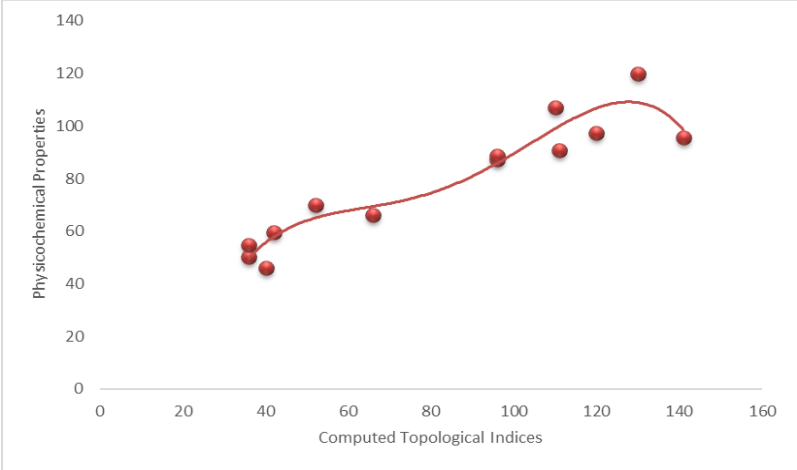

Figure 2: Polynomial curves for E against M1(G)

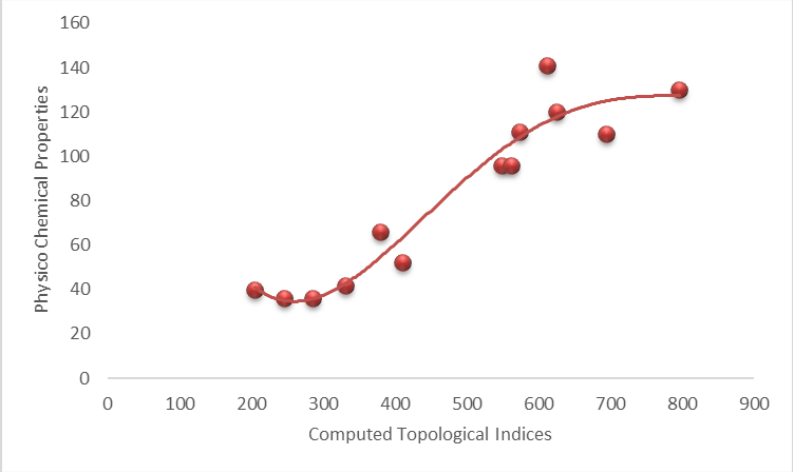

Figure 3: Polynomial curves for NBP against M1(G)

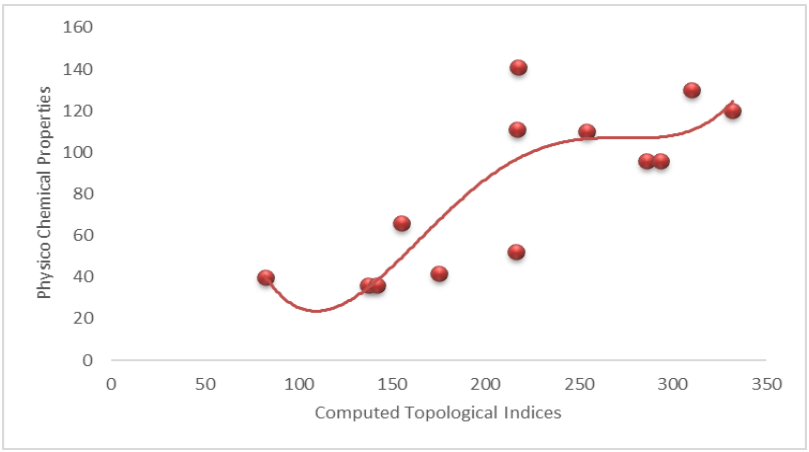

Figure 4: Polynomial curves for FP against M1(G)

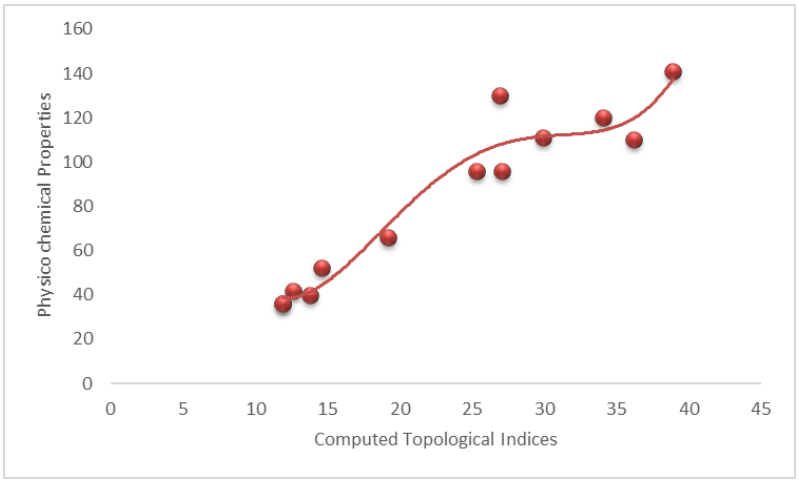

Figure 5: Polynomial curves for P against M1(G)

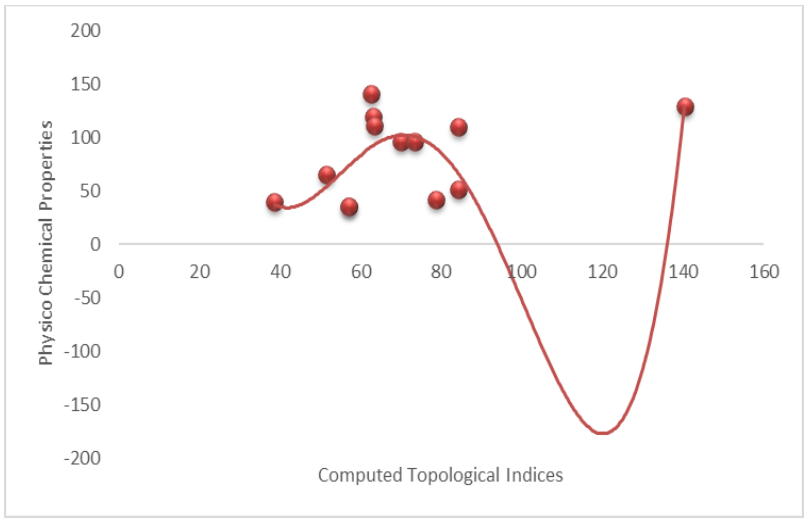

Figure 6: Polynomial curves for ST against M1(G)

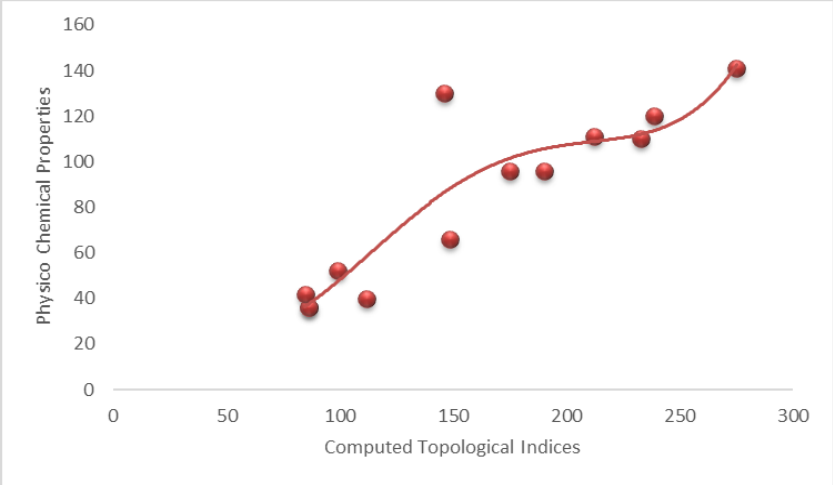

Figure 7: Polynomial curves for MV against M1(G)

Conclusion

In this study, we examined six physico chemical properties of the chemical structure called flavonoids with the help of topological indices and regression models. In QSPR studies, the indices are useful for predicting the characteristics of flavonoids. The novel indices defined in this manuscript have a strong correlation with all six properties of flavonoids.It is important to note that newly defined indices has the highest values of correlations with tha properties of flavonoids. All the correlation values are above 0.8 and p values are less than 0.001 so it is mentioned as significant. The quartic polynomial regression model is more efficient for studying flavonoid structures while compare with logarithmic and exponential regression models. A large number of molecular descriptors have been defined, but still, some properties of the complicated structures cannot be described with the help of the QSPR model method for future research.

Conflict of Interests

The authors declare that they have no conflicts of interest regarding the publication of this article.

Author Contributions

All Authors developed the theoretical formalism and performed the analytic calculations and supervised the article. All authors discussed the results and contributed to the final manuscript.

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