The Bioscan AN INTERNATIONAL QUARTERLY JOURNAL OF LIFE SCIENCES 20(1): 664-670, 2025 www.thebioscan.com

Labeling on Molecular Graph inducing Topological Indices

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DOI: https://doi.org/10.63001/tbs.2025.v20.i01.pp664-670

KEYWORDS
Molecular Structure, HMC labeling, labeled topological indices, graph labeling.

Received on:

18-01-2025

Accepted on:

15-02-2025

Published on:

21-03-2025

ABSTRACT

Graph labeling is the assignment of integers to vertices or edges or both under certain conditions. In this article, we link graph labeling and topological indices as concepts. We introduce topological indices in particular for specific molecular graphs that permit HMC labeling. The concept of graphs is playing a significant role in the examination of QSPR data using topological indices. This part considers the labeled square index SQI(G), labeled product index PI(G), labeled sum index SI(G), labeled Nirmala index NI(G), labeled Sombor index SOLI(G), labeled forgotten index FI(G), and the grouping of all these indices. These topological indices correlate certain physic-chemical properties such as polar surface, Polarizability, molar volume, and boiling point.

INTRODUCTION

The term "molecular structure" refers to the three-dimensional configuration of atoms within a molecule. A molecular graph, also called a chemical graph, serves as a graph-theoretical illustration utilized in mathematical science that displays the chemical compound's structure's formula. A chemical graph is a labeled graph whose vertices represent the compound's atoms and edges represent its chemical bonds.

Let G (V, E) be a straightforward connected graph with vertex set V (G) and edge set E (G) respectively. A linked, undirected graph that allows for a one-to-one relationship with the formula for structure of a chemical substance is called a molecular graph. A molecular description is the initial product of a rational and mathematical procedure that transforms the chemical data present in a molecule's symbolic form into another usable number or the result of some standardized equipment. A molecular graph represents the uncompressed hydrocarbon skeleton formed up of molecules and the substances they contain. Whereas its vertices indicate non-hydrogen atoms, its edges indicate covalent bonds within non-hydrogen atoms. Chemo-informatics uses molecular graphs extensively for computer-aided drug discovery, simulated chemical library inspection, numerical structure-property relations (QSPR), and quantitative relationships between structure and activity (QSAR).

A topological index also known as connectivity index, is a molecular descriptor calculated from a molecular graph of a chemical compound with characterizes its topology. A topological index is a real number derived from the structure of a chemical graph. It is helpful to determine the physicochemical and biological properties of a wide range of drugs and it better reflects the theoretical properties of organic compounds.

1. Preliminaries

1.1. Definition

In relation to a vertex incidence, it is designated as (u). The label assigned to the edge uv in a labeled graph G can be expressed as (u) = f (u, v). In other words, the total number of labels on the edges that cross u constitutes the labeled incidence of vertex u. [3]

1.2. Definition

A graph that has labels given to its edges and points according to a specific idea is called a labeled graph. In this section, we define the notion of a point incidence in a labeled graph and develop several new types of topological indices. When new topological indices are introduced, labels can only be integers that are non-negative.[3]

1.3. Definition

A topological graph index, also known as a molecular descriptor, is an equation that can be used to describe any graph that represents a molecular structure. From these indices, it is feasible to analyze numerical values and further investigate some of a molecule's physiochemical characteristics. To minimize costly and time-consuming laboratory trials, it is an organized approach.

1.4. Definition

A simple graph G = (V, E) is said to be a HMC (Harmonic Mean Cordial) Labeling if there exists a function $f: V \to \{1,2\}$ such that the induced edge function $g: E \to \{1,2\}$ defined by $uv = \left|\frac{2f(u)f(v)}{f(u)+f(v)}\right|, f(u), f(v) \neq 0$ for each edge and $|V_f(i) - V_f(j)| \leq 1$, $|e_g(i) - e_g(j)| \leq 1$ where $V_f(x)$ is the total number of vertices labeled with x, and $e_g(x)$ is the quantity of edges labeled with x, where $x \in \{1,2\}$. The term "HMC graph" refers to a graph that allows HMC labeling [4].

2. Labeled Topological Indices

2.1. Labeled Topological Indices (u) - $l_l(u)$:

$Ll_I(u)$ is equal to the total labeled edges that bisect the vertex u.

$$l_I(u) = \sum f(uv)$$

2.2. Labeled SQI(G)

$SQI(G)$is equal to the total of the squares formed by each labeled edge that bisects the vertex u.

$$SQI(G) = \sum l_I(u)^2$$

2.3. Labeled PI(G)

$PI(G)$ is the result of multiplying each edge label made by the vertices u and v.

$$PI(G) = \sum (l_I(u) l_I(v))$$

2.4. Labeled SI(G)

$SI(G)$ is the total number of labels for the edges that cut the vertices u and v in half.

$$SI(G) = \sum (l_I(u) + l_I(v))$$

2.5. Labeled NI(G)

$NLI(G)$ is the total square root of each edge's labels that bisect the vertices u and v.

$$NLI(G) = \sum \sqrt{l_I(u) + l_I(v)}$$

2.6. Labeled SOLI(G)

$SOLI(G)$ is the sum of the squares along the edges' overall labels that bisect the vertices u and v.

$$SOLI(G) = \sum \sqrt{l_I(u)^2 + l_I(v)^2}$$

2.7. Labeled FI(G)

$FI(G)$ is the total area of all the edges' labels that bisect the vertices u and v.

$$FI\ (G) = \sum (l_I(u)^2 + l_I(v)^2)$$

3. Some drugs used in the paper.

3.1. Ciprofloxacin

Several bacterial illnesses are treated with ciprofloxacin. Ciprofloxacin is a member of the quinolone antibiotics medication class. It acts by preventing bacterial development. Only bacterial illnesses are treated by this antibiotic. For viral illnesses (like the flu or the common cold), it is ineffective.

3.2. Clofazimine

Also known as Lamprene, this drug is used to treat leprosy along with rifampicin and dapsone. It is specifically prescribed for erythema nodosum leprosum and multibacillary leprosy. The use of clofazimine in the therapy of MAC (Mycrobacterium avium complex) is regulated by the food and drug administration in the United States, where it is regarded as an orphan medicine, is not available in pharmacies.

3.3. Sparfloxacin

An antibiotic known as a fluoroquinolone, sparfloxacin is used to treat bacterial infections. Its safety record is debatable. Quinolones prevent the replication of DNA and transcription by blocking the DNA of bacteria's gyrase or topoisomerase IV enzyme. Quinolones are frequently used to treat intracellular diseases like Legionella pneumophila and Mycoplasma pneumoniae because they may easily enter cells.

3.4. Ofloxacin

A quinolone antibiotic called ofloxacin is effective in treating several bacterial illnesses. These include prostatitis plague, pneumonia, cellulitis, infections of the urinary system, and certain forms of infectious diarrhea either taken orally or administered through injection into a vein. Include treating multi-drug resistant tuberculosis along with other medicines.

3.5. Amoxicillin

This antibiotic is used to treat bacterial infections such tooth abscesses and chest infections (including pneumonia). To treat stomach ulcers, it can also be used in conjunction with various other antibiotics and medications. Children frequently receive it as a treatment for infections in the ears and chest.

4. Computational methods and outcomes

The HMC Labeling for molecular graphs and the computational processes that yielded the many kinds of labeled topological indicators of specific structures in molecules described in Table 1 are explained in this section.

4.1. Ciprofloxacin

This structure has 24 atoms and 27 bonds. In the following, the HMC labeling are depicted.

$$1 \to 2 \to 3 \to 4 \to 5 \to 6 \to 7 \to 8 \to 9 \to 10 \to 11 \to 12 \to 13 \to 14 \to 15 \to 16 \to 17 \to 18 \to 19 \to 20 \to 21 \to 22 \to 23 \to 24$$

$$1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 2 \to 2 \to 2 \to 2 \to 2 \to 2 \to 2 \to 1 \to 2 \to 2 \to 2 \to 2 \to 2 \to 2$$

Edge labeling is.

$$\left|\frac{2(1)(1)}{1+1}\right| = \left|\frac{2}{2}\right| = 1, \qquad \left|\frac{2(2)(2)}{2+2}\right| = \left|\frac{8}{4}\right| = 2,$$
$$\left|\frac{2(1)(2)}{1+2}\right| = \left|\frac{4}{3}\right| = 1$$

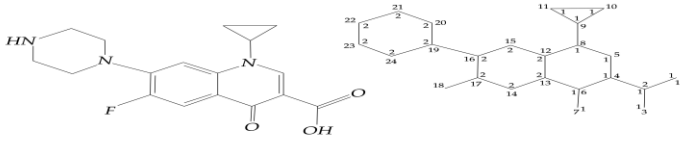


***Figure 1**: Ciprofloxacin's chemical composition and HMC labeling*

4.2. Sparfloxacin

This structure has 28 atoms and 31 bonds. In the following, HMC labeling of depicted.

$$1 \to 2 \to 3 \to 4 \to 5 \to 6 \to 7 \to 8 \to 9 \to 10 \to 11 \to 12 \to 13 \to 14 \to 15 \to 16 \to 17 \to 18 \to 19 \to 20 \to 21 \to 22 \to 23 \to 24 \to 25 \to 26 \to 27 \to 28$$

$$1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 2 \to 2 \to 2 \to 1 -$$

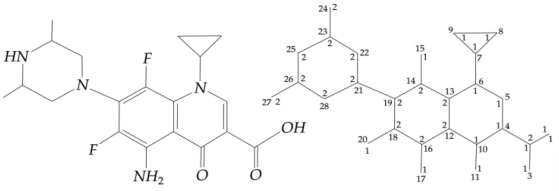


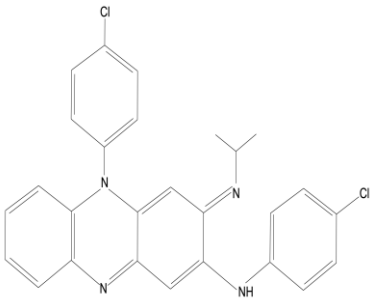
***Figure 2**: Sparfloxacin's chemical composition and HMC labeling*

4.3. Clofazimine

This structure has 33 atoms and 37 bonds. In the following, HMC Labeling is depicted.

$$1 \to 2 \to 3 \to 4 \to 5 \to 6 \to 7 \to 8 \to 9 \to 10 \to 11 \to 12 \to 13 \to 14 \to 15 \to 16 \to 17 \to 18 \to 19 \to 20 \to 21 \to 22 \to 23 \to 24 \to 25 \to 26 \to 27 \to 28 \to 29 \to 30 \to 31 \to 32 \to 33$$

$$1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 2 \to 1 \to 2 \to 1 \to 2 \to 1 \to 2 \to 1 \to 2 \to 1 \to 2 \to 1 \to 2 \to 2 \to 1 \to 1 \to 2 \to 2 \to 2 \to 2 \to 2 \to 2 \to 2 \to 2$$



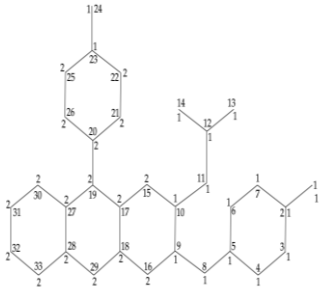


***Figure 3**: Clofazimine's chemical composition and HMC labeling*

4.4. Oflaxicin

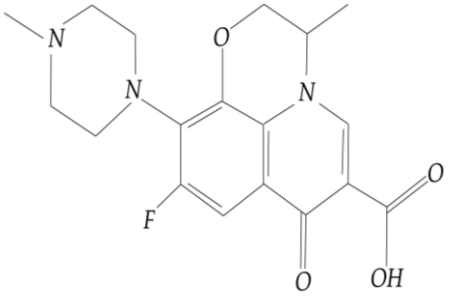
This structure has 26 atoms and 29 bonds. In the following, HMC Labeling of depicted.

$$1 \to 2 \to 3 \to 4 \to 5 \to 6 \to 7 \to 8 \to 9 \to 10 \to$$

$$11 \to 12 \to 13 \to 14 \to 15 \to 16 \to 17 \to 18 \to$$
$$19 \to 20 \to 21 \to 22 \to 23 \to 24 \to 25 \to 26$$
$$1 \to 1 \to 1 \to 1 \to 2 \to 2 \to 2 \to 2$$

$$\to 2 \to 1 \to 2 \to 2 \to 2 \to 2 \to 2 \to$$

$$2 \to 1 \to 2 \to 2 \to 2 \to 1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 1$$



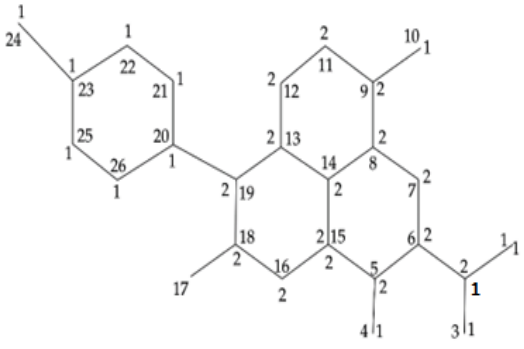
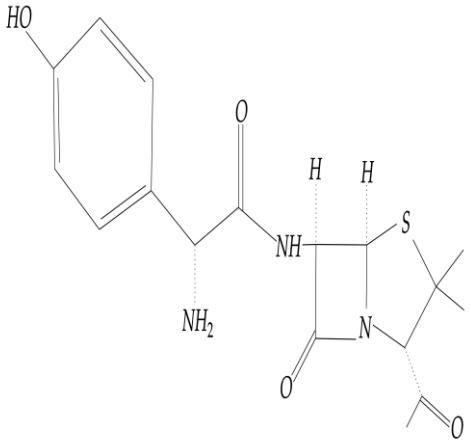


***Figure 4**: Ofloxacin's chemical composition and HMC labeling*

4.5. Amoxicillin

This structure has 28 atoms and 30 bonds. In the following, HMC labeling is depicted.

$$1 \to 2 \to 3 \to 4 \to 5 \to 6 \to 7 \to 8 \to 9 \to 10$$
$$\to 11 \to 12 \to 13 \to 14 \to 15 \to 16 \to 17 \to 18 \to 19$$
$$\to 20 \to 21 \to 22 \to 23 \to 24 \to 25 \to 26 \to 27 \to 28$$
$$1 \to 2 \to 2 \to 2 \to 2 \to 2 \to 2 \to 2 \to 2$$
$$\to 2 \to 2 \to 2 \to 2 \to 1 \to 2 \to 2 \to 1 \to 1$$
$$\to 1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 1 \to 1$$



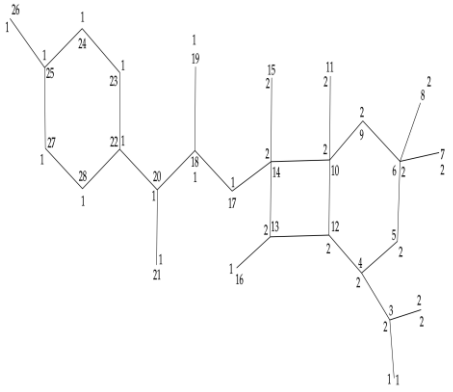


***Figure 5**: Amoxicillin chemical composition and HMC labeling*

Table 1: Calculated values of several molecular graphs' various forms of the topological indicators with labels

Compound's Name	SQI(G)	SI(G)	PI(G)	NLI(G)
Ciprofloxacin	320	198	386	72.143
Sparfloxacin	388	238	473	84.675
Clofazimine	446	270	545	98.207
Ofloxacin	382	228	482	79.932
Amoxicillin	412	245	516	83.842

Compound's Name	SOLI(G)	FI(G)	CSQI(G)	CSI(G)
Ciprofloxacin	143.063	828	4	2.475
Sparfloxacin	174.730	1076	4.217	2.587
Clofazimine	194.444	1158	4.055	2.455
Ofloxacin	166.053	1054	4.341	2.591
Amoxicillin	183.920	1310	4.578	2.722

Compound's Name	CPI(G)	CNLI(G)	CSOLI(G)	CFI(G)
Ciprofloxacin	4.825	0.902	1.788	10.35
Sparfloxacin	4.75	0.920	1.899	11.696
Clofazimine	4.955	0.893	1.768	10.527
Ofloxacin	5.477	0.908	1.887	11.977
Amoxicillin	5.733	0.932	2.044	14.556

Table 2: Properties of various molecular structures from a physico-chemical perspective

Component's Name	Polar Surface	Polarizability	Molar Volume	Boiling Point

Ciprofloxacin	72.88	33.11	226.8 +/- 3.0	581.8
Sparfloxacin	98.9	39.35	392.4	640.4 +/- 55.0
Clofazimine	40	51.52	473.4	566.9 +/- 50.0
Ofloxacin	73.3	36.69	244.0 +/-5.0	571.5
Amoxicillin	158	35.52	419.5	743.2

5. Regression

Regression models are used to fit the curves. Therefore, in this study, we will investigate linear, quadratic, cubic, logarithmic, as well as exponential regression models. The correlation's squared coefficients, the test of F-ratio, and the degree of importance may all be shown in the regression model's table (sig). Topological indices truly conclude the physicochemical feature's particular variable of dependence when F-ratio tests are bigger than once for efficient models and significance values are less than 0.05. The maximum is the regression model's best predictor or measure of fit.

5.1. Main Results

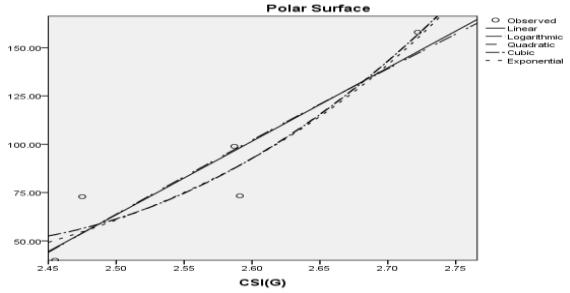
The data in Tables 1 and 2 were used in conjunction with the SPSS statistical package to produce the cubic, logarithmic, linear, and quadratic as well as Models of exponential regression. The square of the correlation coefficient between several topological indices and the physicochemical characteristics of the antibiotics Ciprofloxacin, Sparfloxacin, Clofazimine, Ofloxacin, and Amoxicillin, which are used to treat bacterial infections, is shown in Tables 3, 4, 5 and 6. Here is a list of a few of the top indicators of the topological index regression models for that particular physicochemical characteristic. The polar surface regression models with CSI(G), CPI(G), CNLI(G), CSOLI(G), and CFI(G) with the cubic, quadratic, linear, and logarithmic, and exponential regression models are clearly displayed in Table 3A. The Polarizability Models of Regression with NLI(G) are shown in Table 4A. The Molar Volume regression models with SI(G) and NLI(G) are shown in Table 5A. The regression models for boiling point with CPI(G), CNLI(G), CSOLI(G), and CFI(G) are shown in Table 6A.

Table 3: Regression models connecting labeled topological indexes to the physical characteristic (Polar surface) of a particular chemical structure.

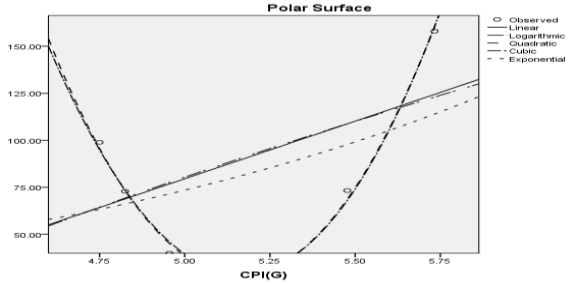
Descriptors of Molecules	Equation	R Square	F-Statistics	p-value
CSI(G)	Linear	0.856	17.805	0.024
	Logarithmic	0.85	16.978	0.026
	Quadratic	0.893	8.359	0.107
	Cubic	0.894	8.411	0.106
	Exponential	0.813	13.038	0.036
CPI(G)	Linear	0.362	1.701	0.283
	Logarithmic	0.344	1.571	0.299
	Quadratic	0.992	122.738	0.008
	Cubic	0.989	87.811	0.011
	Exponential	0.267	1.094	0.373
CNLI(G)	Linear	0.939	46.045	0.007
	Logarithmic	0.937	44.565	0.007
	Quadratic	0.941	47.568	0.006
	Cubic	0.962	25.658	0.038
	Exponential	0.943	49.453	0.006
CSOLI(G)	Linear	0.899	26.753	0.014
	Logarithmic	0.893	25.031	0.015
	Quadratic	0.917	11.018	0.083
	Cubic	0.917	11.06	0.083
	Exponential	0.835	15.21	0.03
CFI(G)	Linear	0.84	15.712	0.029
	Logarithmic	0.827	14.323	0.032
	Quadratic	0.852	5.767	0.148
	Cubic	0.852	5.766	0.148
	Exponential	0.714	7.499	0.071

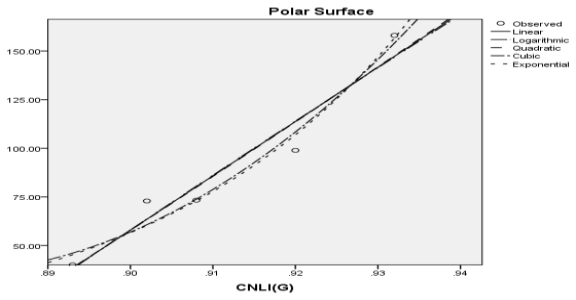
Table 3A: Regression model of CSI(G), CPI(G), CNLI(G) & CSOLI(G) with Polar Surface (dependent variable).

I.V	Equation		Linear	Log	Quad	Cubic	Exp
CSI(G)	Synopsis of the model	R-Squ	0.856	0.85	0.893	0.894	0.813
		F	17.806	16.978	8.359	8.411	13.038
		DF1	1	1	2	2	1
		DF2	3	3	2	2	1
		Sig.	0.024	0.026	0.107	0.106	0.036
	Prediction of Parameters	Cons.	-886.6	-832.2	5393.8	1544.2	0.002
		B1	380.08	977.94	-4487	0	4.214
		B2			941.6	-800.2	
		B3				225.21	

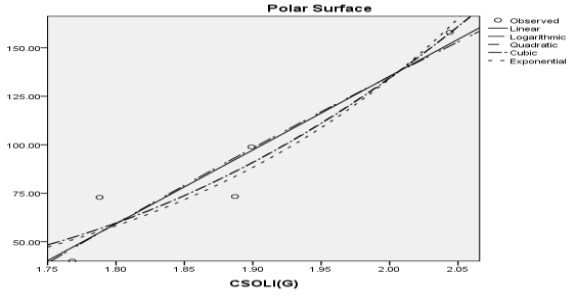


I.V	Equation		Linear	Log	Quad	Cubic	Exp
CPI(G)	Synopsis of the model	R-Squ	0.362	0.344	0.992	0.989	0.267
		F	1.701	1.571	122.7	87.811	1.094
		DF1	1	1	2	2	1
		DF2	3	3	2	2	3
		Sig.	0.283	0.299	0.008	0.011	0.373
	Prediction of Parameters	Cons.	-226.4	-420.7	10710.4	7026.0	3.695
		B1	61.194	311.4	-4140.6	-2032.0	0.598
		B2			401.259	0	
		B3				25.391	





I.V	Equation		Linear	Log	Quad	Cubic	Exp
CSOLI(G)	Synopsis of the model	R-Squ	0.899	0.893	0.917	0.917	0.835
		F	26.573	25.031	11.018	11.06	15.21
		DF1	1	1	2	2	1
		DF2	3	3	2	2	3
		Sig.	0.014	0.015	0.083	0.083	0.03
	Prediction of Parameters	Cons.	-625.32	-364.14	1576.1	357.87	0.032
		B1	380.32	720.45	-1938.1	0	4.17
		B2			608.65	-417.3	
		B3				180.75	



I.V	Equation		Linear	Log	Quad	Cubic	Exp
CFI(G)	Synopsis of the model	R-Squ	0.84	0.827	0.852	0.852	0.714
		F	15.712	14.323	5.767	5.766	7.499
		DF1	1	1	2	2	1
		DF2	3	3	2	2	3
		Sig.	0.029	0.032	0.148	0.148	0.071
	Prediction of Parame-	Cons.	-194.6	-634.6	166.48	51.24	4.113
		B1	23.96	293.75	-1938.1	-6.229	0.251
		B2			2.357	0	
		B3				0.064	

I.V	Equation		Linear	Log	Quad	Cubic	Exp
CNLI(G)	Synopsis of the model	R-Squ	0.939	0.937	0.941	0.962	0.943
		F	46.045	44.565	47.568	25.658	49.453
		DF1	1	1	1	2	1
		DF2	3	3	3	2	3
		Sig.	0.007	0.007	0.006	0.038	0.006
	Prediction of Parameters	Cons.	-2453.8	326.09	-1181.6	18847.6	2.08E-11
		B1	2790.8	2544.6	0	-32222.8	31.815
		B2			1530.1	0	
		B3				14005.3	

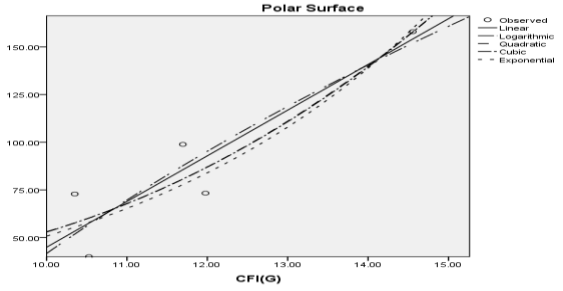


Table 4: Regression models relating certain molecular structures' physicochemical properties (polarizability) with labeled topological indices.

Descriptors of Molecules	Equation	R Square	F-Statistics	p-value
NLI(G)	Linear	0.889	24.056	0.016
	Logarithmic	0.858	18.114	0.024
	Quadratic	0.965	27.572	0.035
	Cubic	0.966	28.126	0.034
	Exponential	0.905	28.6	0.013

Table 4A: Regression model of NLI(G) with Polarizability

Dependent Variable	The independent variable	Equation		Linear	Logarithmic	Quadratic	Cubic	Exponential	Curve fit Pic
Polarizability	NLI(G)	Synopsis of the Model	R Squared	0.889	0.858	0.965	0.966	0.905	
			F	24.056	18.114	27.572	28.126	28.6	
			DF1	1	1	2	2	1	
			DF2	3	3	2	2	3	
			Sig.	0.016	0.024	0.035	0.034	0.013	
		Predictions of Parameters	Constants	-20.971	-226.002	143.876	56.184	9.218	
			B1	0.719	59.969	-3.168	0	0.017	
			B2			0.023	-0.015		
			B3				0		

Table 5: Regression models relating certain molecular structures' physicochemical properties (Molar volume) with labeled topological indices.

Descriptors of Molecules	Equation	R Square	F-Statistics	p-value
SI(G)	Linear	0.821	13.766	0.034
	Logarithmic	0.812	12.949	0.037
	Quadratic	0.824	4.687	0.176
	Cubic	0.824	4.687	0.176
	Exponential	0.804	12.327	0.039
NLI(G)	Linear	0.775	10.308	0.049
	Logarithmic	0.789	11.228	0.044
	Quadratic	0.808	4.204	0.192
	Cubic	0.81	4.25	0.19
	Exponential	0.739	8.51	0.062
SOLI(G)	Linear	0.849	16.914	0.026

	Logarithmic	0.83	14.648	0.031
	Quadratic	0.884	7.612	0.116
	Cubic	0.882	7.478	0.118
	Exponential	0.846	16.509	0.027

Table 5A: Regression model of SI(G), NLI(G) & SOLI(G) with Molar Volume

Dependent Variable	The independent variable	Equation		Linear	Logarithmic	Quadratic	Cubic	Exponential	Curve fit Pic
Molar Volume	SI(G)	Synopsis of the Model	R Squared	0.821	0.812	0.824	0.824	0.804	
			F	13.766	12.949	4.687	4.687	12.327	
			DF1	1	1	2	2	1	
			DF2	3	3	2	2	3	
			Sig.	0.034	0.037	0.176	0.176	0.039	
		Predictions of Parameters	Constants	-544.072	-4413.094	-58.944	-124.403	22.64	
			B1	3.797	872.919	-0.405	0	0.011	
			B2			0.009	0.009		
			B3				-2.92E-06		
	NLI(G)	Synopsis of the Model	R Squared	0.775	0.789	0.808	0.81	0.739	
			F	10.308	11.228	4.204	4.25	8.51	
			DF1	1	1	2	2	1	
			DF2	3	3	2	2	3	
			Sig.	0.049	0.044	0.192	0.19	0.062	
		Predictions of Parameters	Constants	-503.299	-3516.992	-2162.847	-1659.161	26.462	
			B1	10.202	874.581	49.335	30.675	0.03	
			B2			-0.228	0		
			B3				-0.001		
	SOLI(G)	Synopsis of the Model	R Squared	0.849	0.83	0.884	0.882	0.846	
			F	16.914	14.648	7.612	7.478	16.509	
			DF1	1	1	2	2	1	
			DF2	3	3	2	2	3	
			Sig.	0.026	0.031	0.116	0.118	0.027	
		Predictions of Parameters	Constants	-542.814	-4042.87	1226.387	600.393	22.209	
			B1	5.185	854.101	-16.118	-5.16	0.016	
			B2			0.063	0		
			B3				0		

Table 6: Regression models relating some molecular structures' boiling point and other physicochemical properties to labeled topological indices.

Descriptors of Molecules	Equation	R Square	F-Statistics	p-value
CPI(G)	**Linear**	0.299	1.278	0.34
	Logarithmic	0.282	1.178	0.357
	Quadratic	0.965	27.315	0.035
	Cubic	0.971	33.011	0.029
	Exponential	0.275	1.14	0.364
CNLI(G)	**Linear**	0.854	17.618	0.025
	Logarithmic	0.85	17.026	0.026
	Quadratic	0.859	18.236	0.024
	Cubic	0.987	78.433	0.013
	Exponential	0.867	19.841	0.022
CSOLI(G)	**Linear**	0.824	14.01	0.033
	Logarithmic	0.811	12.88	0.037
	Quadratic	0.908	9.896	0.092
	Cubic	0.908	9.886	0.092
	Exponential	0.82	13.663	0.034
CFI(G)	**Linear**	0.808	12.663	0.038
	Logarithmic	0.786	11.014	0.045
	Quadratic	0.858	6.066	0.142
	Cubic	0.86	6.119	0.14
	Exponential	0.795	11.6	0.042

Table 6A: Regression model of CPI(G) & CNLI(G) with Boiling Point

Dependent Variable	The independent variable	Equation		Linear	Logarithmic	Quadratic	Cubic	Exponential	Curve fit Pic
Boiling Point	CPI(G)	Synopsis of the Model	R Squared	0.299	0.282	0.965	0.971	0.275	
			F	1.278	1.178	27.315	33.011	1.14	
			DF1	1	1	2	2	1	
			DF2	3	3	2	2	3	
			Sig.	0.34	0.357	0.035	0.029	0.364	
		Predictions of Parameters	Constants	136.566	-159.738	19157.943	6609.92	302.16	
			B1	94.055	477.126	-7213.81	0	0.139	
			B2			697.866	-681.193		
			B3				87.666		
	CNLI(G)	Synopsis of the Model	R Squared	0.854	0.85	0.859	0.987	0.867	
			F	17.618	17.026	18.236	78.433	19.481	
			DF1	1	1	1	2	1	
			DF2	3	3	3	2	3	
			Sig.	0.025	0.026	0.024	0.013	0.022	
		Predictions of Parameters	Constants	-3482.536	1003.44	-1432.296	81933.317	1.077	
			B1	4504.167	4100.511	0	-135895.7	6.972	
			B2			2473.238	0		
			B3				56159.267		
	CSOLI(G)	Synopsis of the Model	R Squared	0.824	0.811	0.908	0.908	0.82	
			F	14.01	12.88	9.896	9.886	13.663	
			DF1	1	1	2	2	1	
			DF2	3	3	2	2	3	
			Sig.	0.033	0.037	0.092	0.092	0.034	
		Predictions of Parameters	Constants	-535.123	-109.18	7624.733	4911.424	104.874	
			B1	615.749	1161.522	-7977.721	-3688.883	0.944	
			B2			2256.043	0		
			B3				394.923		
	CFI(G)	Synopsis of the Model	R Squared	0.808	0.786	0.858	0.86	0.795	
			F	12.663	11.014	6.066	6.119	11.6	
			DF1	1	1	2	2	1	
			DF2	3	3	2	2	3	
			Sig.	0.038	0.045	0.142	0.14	0.042	
		Predictions of Parameters	Constants	150.618	-572.139	1369.949	737.102	301.606	
			B1	39.771	484.478	-159	0	0.061	
			B2			7.96	-5.232		
			B3				0.361		

CONCLUSION

The molecular structure was analyzed in this paper using regression models. The molecular descriptors of those structures, found as Ciprofloxacin, Sparfloxacin, Clofazimine, Ofloxacin, and Amoxicillin, are mentioned in the paper. The Components' computation results were then compiled after that. The QSPR study discovered that molecule-level characteristics [13] (topological indexes) are the best tools for predicting the physicochemical characteristics of drugs used in pharmacology, medicine, and other fields. The correlation between two variables, such as molecular descriptor and physical qualities, can be studied using regression models. The most accurate predictors of Polar Surface & Boiling Point are molecular identifiers like CPI(G), CNLI(G), CSOLI(G), and CFI(G). Likewise molecular descriptors NLI(G) is the best predictor for Polarizability and Molar Volume. Also SI(G) and SOLI(G) significantly predict Molar Volume and CSI(G) significantly predict Polar Surface.

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