10.48047/jocaaa.2024.33.05.86

Investigating the QSPR Analysis of some chemical drugs by Heinz-Quarter Mean label -Based Topological Indices.

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Abstract:

Chemical graph theory is a branch of Mathematical chemistry that uses graph theory to analyse chemical structures. This article focuses on using labeled-based topological indices to model the molecular structure of pharmaceuticals and predict their physicochemical properties without extensive laboratory procedures. The indices are essential for the QSPR Analysis of chemical drugs. Also calculate linear regression model and labeled -based topological indices of some drugs namely Norfloxacin, Lomefloxacin, cinoxacin, Entrofloxacin, Gatifloxacin, Gemifloxacin, Pefloxacin, Levofloxacin. This study looks at how these topological indices correlate with physicochemical properties such as LogP, Molar Refractivity (MR), Boiling Point (BP), Flash point (FP), Polar surface area (PSA), Complexity(C), Polarizability(P), Molecular Volume (MV). The aim of this work is to investigate the characteristics of various drugs and how they are correlate with their properties. We introduce Heinz-Quarter Mean label-based indices to characterise the structures of the chemical drugs.

Keywords:

Heinz-Quarter Mean Labeling, Labeled Topological Indices, Linear regression model, Quantitative structure property Relationships (QSPR), Correlation coefficient.

Subject Classification (MSC2020):05C92

1.Introduction:

Topological indices are numerical values used in chemical graph theory to describe the structure of a molecule by converting it into a graph. In this representation, we use hydrogen suppressed molecular graphs, where atoms are treated as vertices and chemical bonds as edges**.** These indices help to summarize complex molecular structure into simple numbers. These invariant TIs play an important role in QSPR/QSAR studies, where researchers relate molecular structure to biological activity or physical properties like boiling point, Complexity, Refractivity etc. Princess Rathinabai. G et al [1] found “Topological indices for labeled graphs”. Rasheed et al [2] estimate “The physiochemical properties of Heart attack treatment medicines by using Topological Indices”. Vinutha S.V et al [3] investigate “Cordial labeling of molecular structures and labeled topological indices of Molecular Graphs”, a QSPR Model. Gowri. J and J. Jeya Priya [4] introduced HMC Labeling of certain types of Graphs,”. S. Latha et al and S.S. Sandhya et al introduced Heinz-Quarter Mean Labeling [5]. Motivated by these works, we introduce Heinz-

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Quarter Mean labeling on some chemical drugs and to produce labeled topological indices to characterise the physiochemical properties and their correlation coefficients.

2.Chemical structures of drugs:

This section gives a description of Norfloxacin, Lomefloxacin, Cinnoxacin, Entrofloxacin, Gatifloxacin, Gemifloxacin, Pefloxacin, Levofloxacin along with their chemical structures. It also includes a Heinz-Quarter mean graph representations of these compounds and similar representations for other drugs can be produced using the same technique.

(i) Norfloxacin: [$C_{16}H_{18}FN_3O_3$]

Norfloxacin is a type of fluoroquinolone antibiotic used to treat bacterial infections, particularly Urinary Tract infections (UTIs). It works by destroying bacteria, but it does not work against viral illness such as the common cold or flu. In 2008, the European Medicines Agency issued a recommendation to limit and carefully control the use to safety and effectiveness considerations. This medication works by either killing the bacteria or by stopping their growth and multiplication within the body. Its chemical formula is $C_{16}H_{18}FN_3O_3$.The depicted structure contains 23 atoms and 25 bonds. The chemical structure and its Heinz-Quarter Mean graph are given in Fig.1.

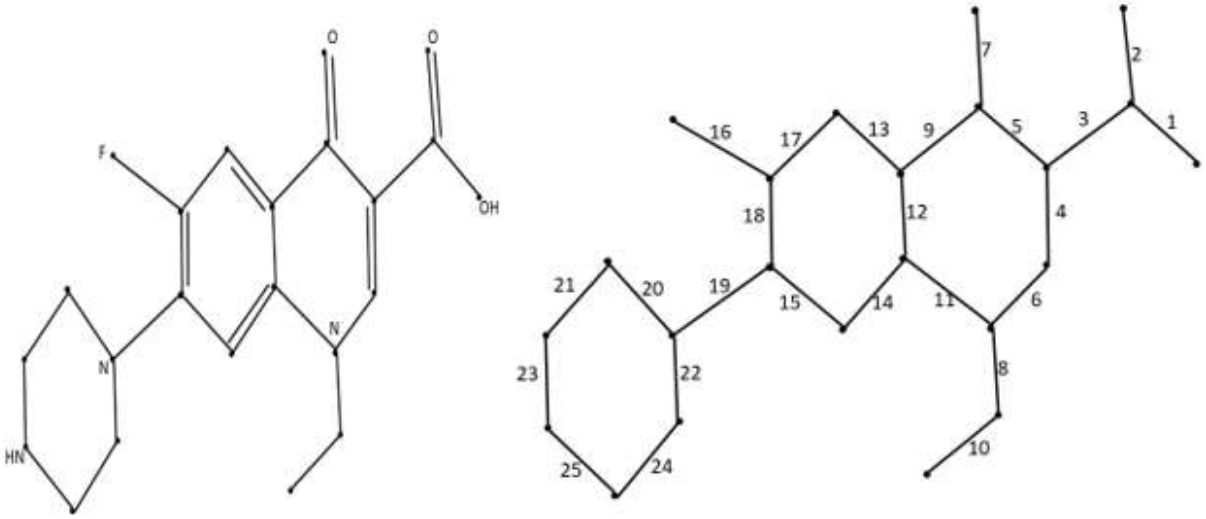

Fig.1 Chemical structure of Norfloxacin and its Heinz Mean Labeled graph

(ii).Lomefloxacin: [$C_{17}H_{19}F_2N_3O_3$]

Lomefloxacin is an antibiotic in a class of drugs called fluroquinolones. It used to manage various bacterial infections, such as bronchitis, Urinary tract infections and infections involving the skin and ears. Its chemical formula is $C_{17}H_{19}F_2N_3O_3$. It has 25 atoms and 27 bonds.

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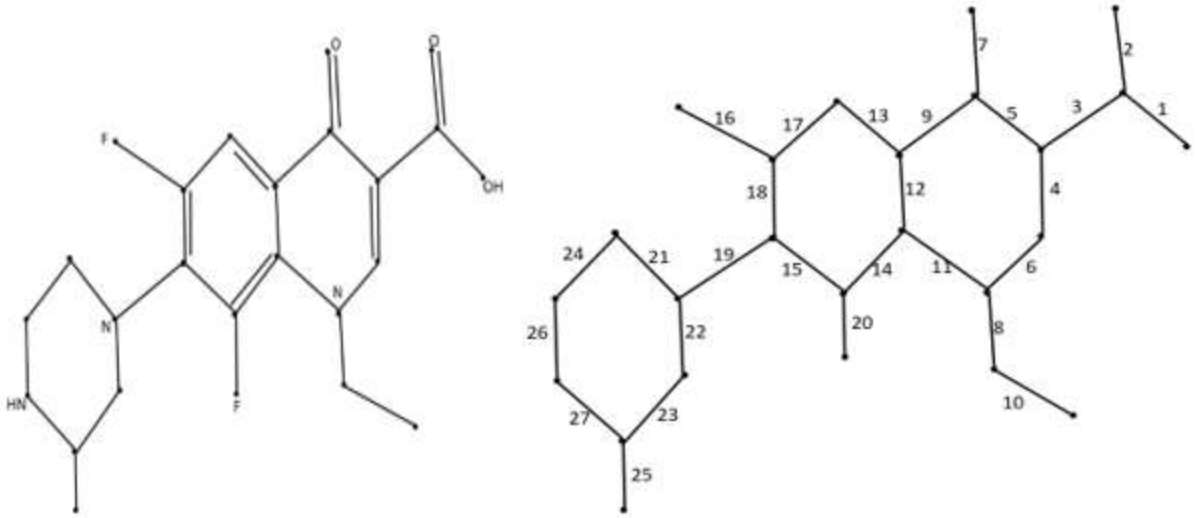

Fig.2 Chemical structure of Lomefloxacin and its Heinz Mean Labeled graph

(iii). Cinnoxacin: [$C_{12}H_{10}N_2O_5$]

Cinnoxacin is a quinolone antibiotic primarily used to treat acute or recurrent Urinary tract infections (UTIs) caused by susceptible gram-negative bacteria, such as E. coli. It works by killing bacteria or preventing their growth in the urinary system. Its chemical formula is $C_{12}H_{10}N_2O_5$.It has 19 atoms and 21 bonds**.**

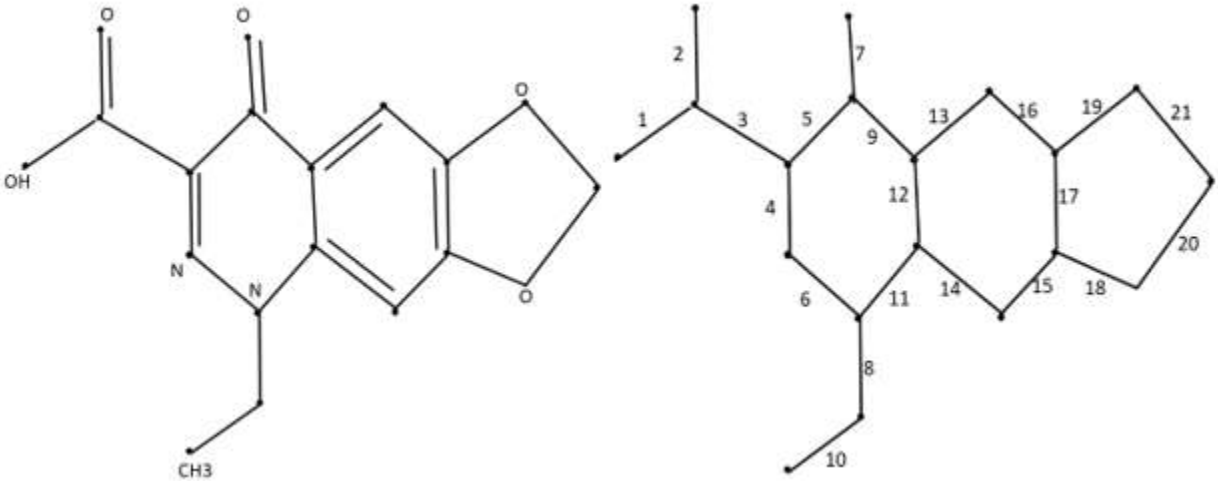

Fig.3 Chemical structure of Cinnoxacin and its Heinz Mean Labeled graph

(iv) Entrofloxacin: [$C_{19}H_{22}FN_3O_3$]

Entrofloxacin is a synthetic fluoroquinolone antibiotic widely used in veterinary medicine. It works by inhibiting bacterial DNA synthesis, which stops the growth and replication of bacteria.

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This antibiotic is commonly prescribed for dogs and cats to treat various bacterial infections. Its chemical formula is $C_{19}H_{22}FN_3O_3$.It has 26 atoms and 29 bonds.

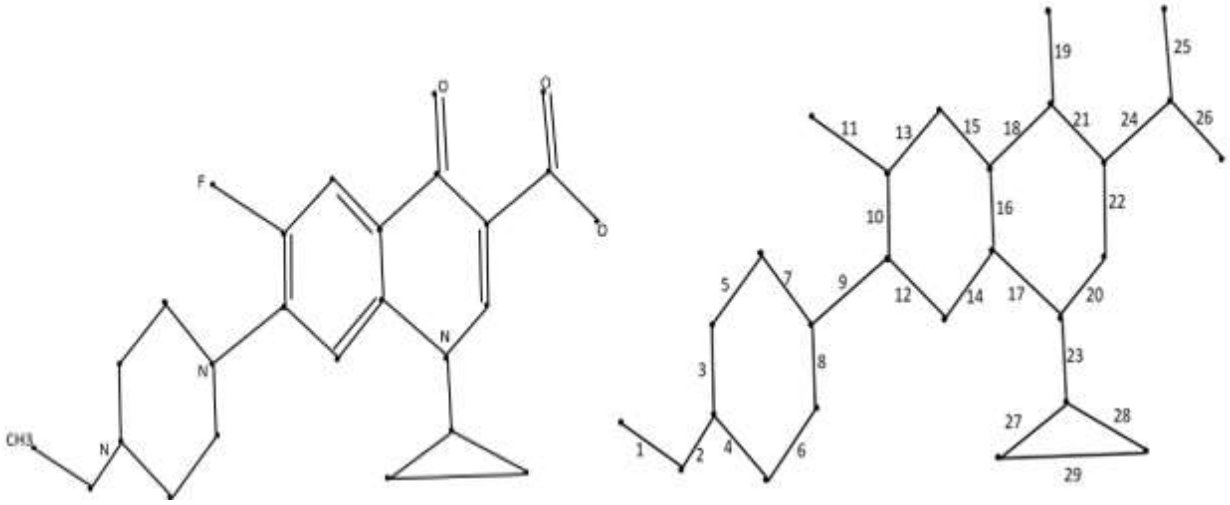

Fig.4 Chemical structure of Entrofloxacin and its Heinz Mean Labeled graph

(v) Gatifloxacin: [$C_{19}H_{22}FN_3O_4$]

Gatifloxacin is a fourth -generation fluoroquinolone antibiotic with molecular formula $C_{19}H_{22}FN_3O_4$.It is primarily used for treating bacterial eye infections, especially bacterial conjunctivitis (pink eye) by killing bacteria and stopping their growth. It is usually applied as an ophthalmic solution (eye drops) to help relieve symptoms such as redness, itching and watery or eye discharge.

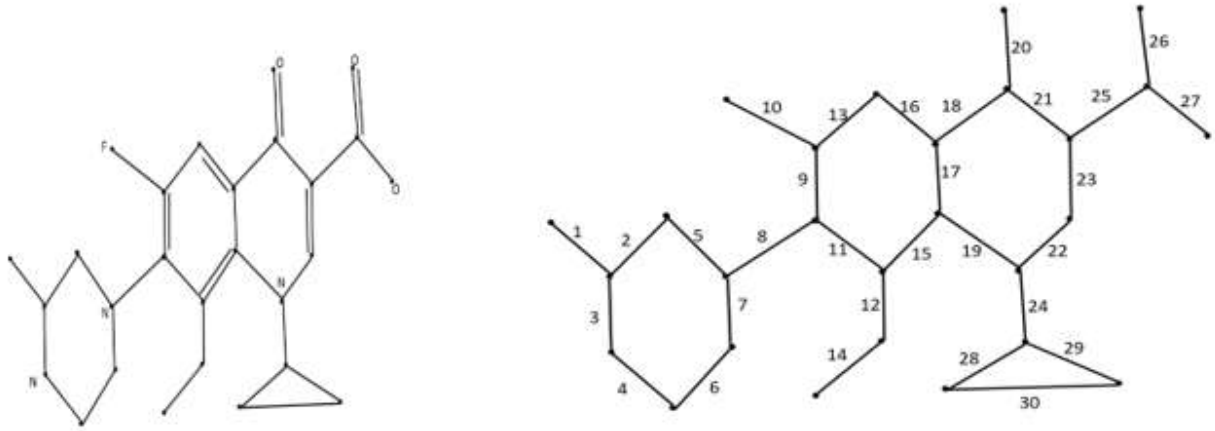

Fig.5 Chemical structure of Gatifloxacin and its Heinz Mean Labeled graph

(vi) Gemifloxacin: [$C_{18}H_{20}FN_5O_4$]

Gemifloxacin is a fluoroquinolone antibiotic that treats bacterial infections, with a particular focus on pneumonia and bronchitis. It also used for infections of the urinary tract, tonsils, sinus, nose, throat, skin and soft tissues and lungs. Its chemical formula is $C_{18}H_{20}FN_5O_4$.It has 28 atoms and 31 bonds.

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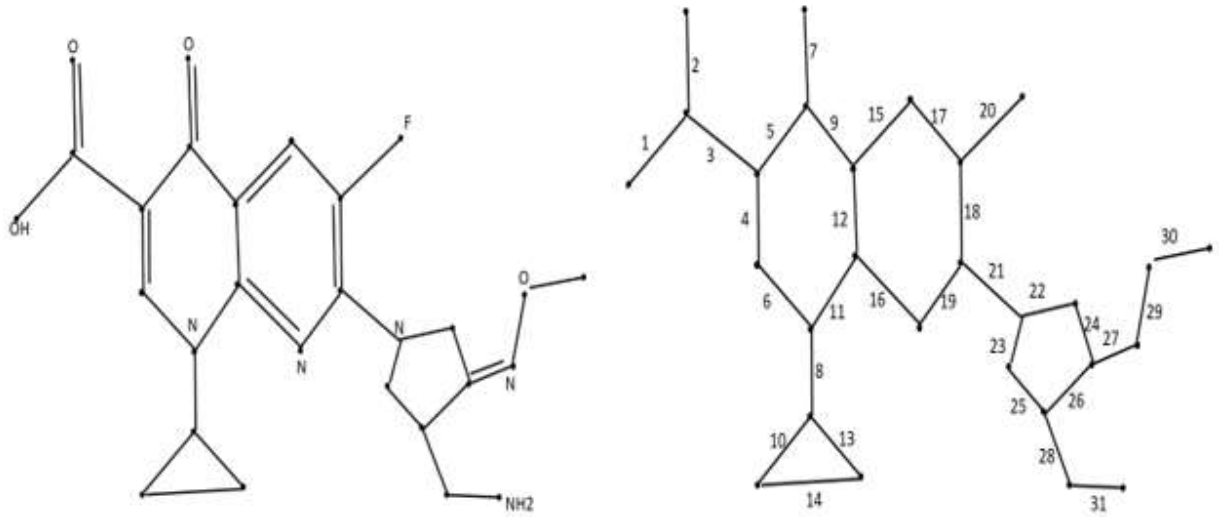

Fig.6 Chemical structure of Gemifloxacin and its Heinz Mean Labeled graph

(vii)Pefloxacin: [$C_{17}H_{20}FN_3O_3$]

Pefloxacin is a fluoroquinolone antibiotic with broad-spectrum activity, commonly used to treat severe bacterial infections such as those affecting the urinary tract (UTIs), respiratory system (like pneumonia), gastrointestinal tract (such as typhoid fever), skin and soft tissues infections. Its chemical formula is $C_{17}H_{20}FN_3O_3$.It has 24 atoms and 26 bonds.

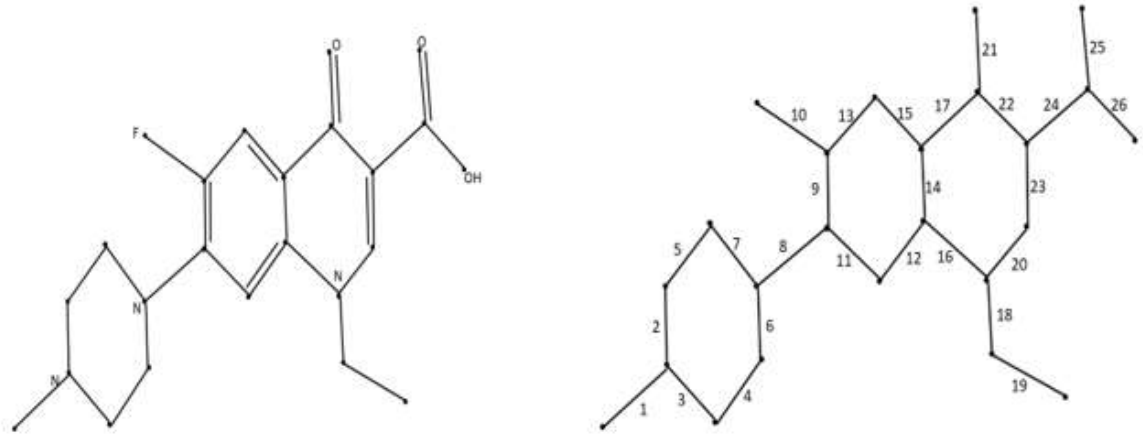

Fig.7 Chemical structure of Pefloxacin and its Heinz Mean Labeled graph

(viii)Levofloxacin: [$C_{18}H_{20}FN_3O_4$]

Levofloxacin is a broad-spectrum fluoroquinolone antibiotic commonly prescribed for treating bacterial infections such as pneumonia, bronchitis, urinary tract infections, skin infections and prostatitis. Its chemical formula is $C_{18}H_{20}FN_3O_4$. It has 26 atoms and 29 bonds.

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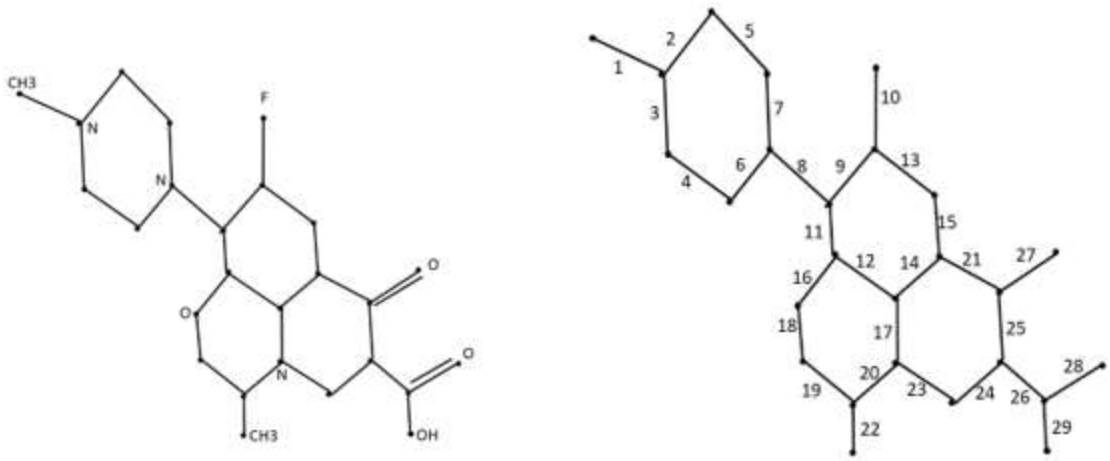

Fig.8 Chemical structure of levofloxacin and its Heinz Mean Labeled graph

3.Basic definitions:

3.1. Incident of a vertex

In [3], Labeled incident of a vertex "x" is defined as the sum of edge labels that incident to that vertex and is denoted by $L_i(x) = \sum_{\forall x \, \epsilon V(G)} f(xy)$

3.2. Heinz-Quarter Mean Labeling

A graph G = (V, E) having p vertices and q edges. Let f: V(G)→{1,2,….q+1}be an injective function. For a vertex labeling f, the induced edge labeling f (e = uv) is defined by

$f(e = uv) = \left\lfloor \frac{\sqrt[4]{f(u)f(v)}\left(\sqrt{f(u)}+\sqrt{f(v)}\right)}{2} \right\rfloor$ or $\left\lfloor \frac{\sqrt[4]{f(u)f(v)}\left(\sqrt{f(u)}+\sqrt{f(v)}\right)}{2} \right\rfloor$ .Then f is called Heinz-Quarter mean labeling .A graph which admits Heinz-Quarter mean labeling is called Heinz-Quarter mean graph

The notations used in this section are listed in Table-1.

Table:1 Heinz-Quarter Mean Labeled topological indices

Topological Descriptors	Formulae
• HQM labeled Incident vertex of G	$L_i(x) = \sum_{\forall x \, \epsilon V(G)} f(xy)$
• HQM labeled square Index of G	$SQI(G) = \sum_{\forall x \epsilon V(G)} L_i(x)^2$
• HQM labeled product index of G	$PI(G) = \sum_{\forall xy \epsilon E(G)} L_i(x) \quad L_i(y)$

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- HQM labeled sum index of G $SI(G) = \sum_{\forall xy \epsilon E(G)} L_i(x) \quad + L_i(y)$
- HQM Nirmala Index of G $NLI(G) = \sum_{\forall xy \epsilon E(G)} \sqrt{L_i(x) + L_i(y)}$
- HQM Somber Index of G $SOLI(G) = \sum_{\forall xy \epsilon E(G)} \sqrt{L_i(x)^2 + L_i(y)^2}$
- HQM Forgotten Index of G $FI(G) = \sum_{\forall xy \epsilon E(G)} L_i(x)^2 + L_i(y)^2$
- HQM labeled cluster square Index of G $CSQI(G) = \frac{SQI(G)}{\sum_{\forall x \epsilon V(G)} L_i(x)}$
- HQM labeled cluster sum Index of G $CSI(G) = \frac{SI(G)}{\sum_{\forall x \epsilon V(G)} L_i(x)}$

4.Regression Model:

In this article, TIs of some chemical drugs are calculated. The computed TIs for the respective drugs are listed in Table:2. Some urinary tract infections medicines are used in this analysis. Regression analysis is conducted as part of this study. A QSPR modeling study is carried out using nine topological indices derived from drug structures. The physio chemical properties of chemical drugs are listed in Table:3. The regression model is applied to determine the linear regression values for each topological Indices.

$Y = \gamma + \delta X$

Here the dependent variable Y and the independent variable as X and it has two coefficients γ and δ. δ represents the slope value and γ represents the constant value.

This article uses several statistical parameters. A parameter is a useful measure in statistics that helps describe the characteristics of a specific population**.**

Y - represents the Physical-chemical properties of chemical drugs

X – denotes the topological indices of drugs

R – Pearson Correlation coefficient

F – represents the Fisher's statistic

N – sample population (Here the value of N is 8, because 8 chemical drugs are used)

The correlation coefficient R expresses how strongly changes in one variable are linked to changes in another. The correlation coefficient lies between -1 and +1, indicating the strength and direction of the relationship between two variables.

If R value is closer to 1 then very strong positive correlation (It occurs when both variables change in the same direction)

If R value is closer to -1 then very strong negative correlation (It occurs when variables change in the opposite direction).

If R value is 0 then weak or no correlation.

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The probability value (P-value) is less than or equal to 0.05 then the result is statistically significant.

The probability value (P-value) is greater than 0.05 then the result is Insignificant. Also a higher value of F corresponds to a lower p-value, indicating that the result is statistically significant. In this article the correlation of all physio chemical properties are good, except Polar surface area, Boiling Point and LogP.

Table 2. The derived values of Labeled Topological Indices of some chemical drugs.

Molecular Descriptors								
Name of the drugs	SQI(G)	SI(G)	PI(G)	NLI(G)	SQLI(G)	FI(G)	CSQI(G)	CSI(G)
Norfloxacin	25,810	1563	29986	188.86	1129.42	64,007	39.71	2.40
Lomefloxacin	33,064	1825	37,694	211.70	1325.73	82,879	43.73	2.41
Cinnoxacin	15,960	1141	19,181	147.83	823.72	40,741	34.54	2.47
Entrofloxacin	42,452	2190	51,399	238.93	1591.95	1,13,666	48.80	2.52
Gatifloxacin	46,858	2340	57,113	386.20	1698.66	1,25,602	50.38	2.52
Gemifloxacin	48,426	2398	56,920	260.51	1732.80	1,22,476	48.82	2.42
Pefloxacin	30,144	1735	35,654	201.77	1268.65	81,151	42.88	2.47
Levofloxacin	42,118	2194	50,545	239.80	1600.82	1,14,602	48.41	2.52

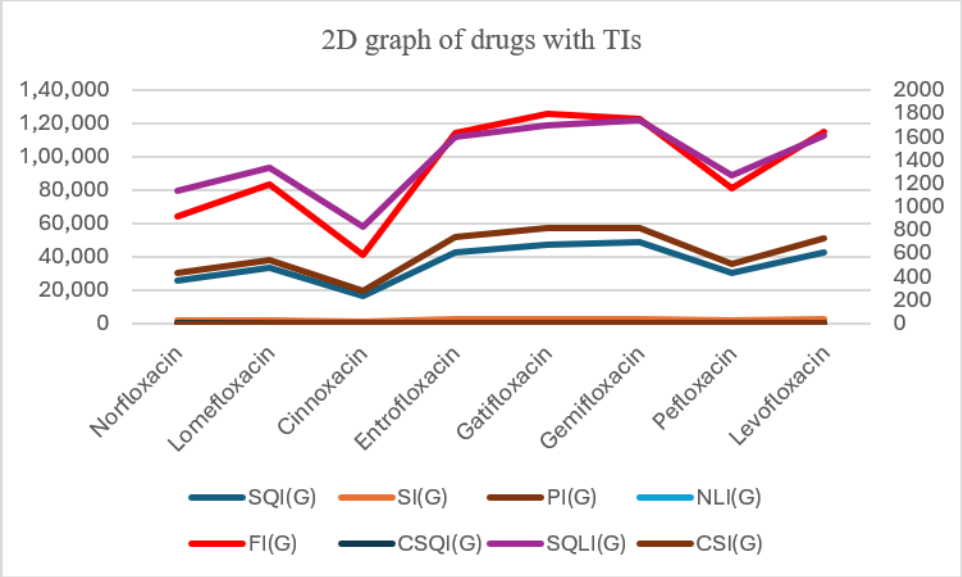

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Table:3. Physio chemical values of drugs

Name of the drugs	Molar Refractivity	Polarizability	Molecular Volume	Complexity	Polar surface area	LogP	Boiling point	Flash point
Norfloxacin	85.48	32.26	319.33	519	72.9	-1.03	695.6	289.9
Lomefloxacin	90.11	34.72	351.35	585	72.9	-0.3	542.7	282
Cinnoxacin	73.6	24.72	262.22	385	88.4	1.5	517.2	266.6
Entrofloxacin	97.98	37.53	359.40	613	64.1	0.58	560.5	292.8
Gatifloxacin	98.82	38.29	375.4	653	82.11	2.6	607.8	321.4
Gemifloxacin	99.74	39.02	389.4	725	121.4	2.3	638.9	340.2
Pefloxacin	90.77	34.4	333.36	545	64.1	0.27	529.1	273.8
Levofloxacin	94.94	36.69	361.36	634	73.32	2.1	572	299.4

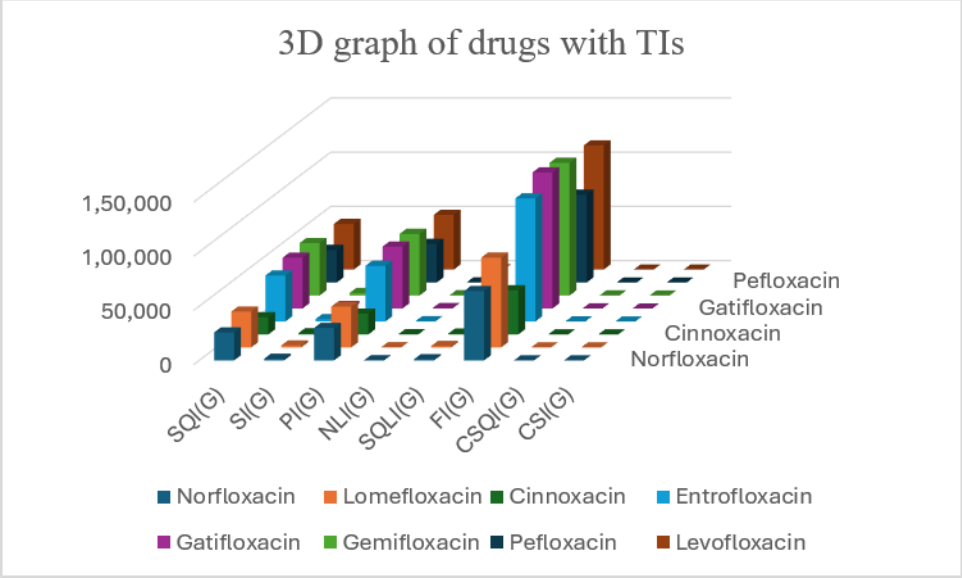

Table:4. Regression model between Molar Refractivity and Labeled Topological Indices

Topological indices	Γ	δ	R	R^2	F-value	P-value	Measure
SQI(G)	64.76	0.0008	0.9712	0.9431	99.53	$5.869 X10^{-5}$	Significant
SI(G)	53.74	0.0196	0.9777	0.9559	129.91	$2.734 X 10^{-5}$	Significant

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PI(G)	65.59	0.0007	0.9653	0.9318	81.95	0.000101	Significant
NLI(G)	69.59	0.0932	0.7531	0.5672	7.862	0.0310	Significant
SOLI(G)	53.79	0.0270	**0.9791**	0.9585	138.71	$2.26 X10^{-5}$	Significant
FI(G)	65.86	0.0003	0.9676	0.9362	87.97	$8.34 X10^{-5}$	Significant
CSQI(G)	22.10	1.5526	0.9783	0.9571	133.72	$2.52 X10^{-5}$	Significant
CSI(G)	-36.35	51.8124	0.3039	0.0924	0.6106	0.4643	Insignificant

We note from Table 4:

- The index SI(G) is the strongest model with an R^2 of 0.9559, meaning it explains 95.59% of the changes in Molar refractivity. The P-value is $2.734 X 10^{-5}$, which is below the common significance level of 0.05. Then the regression model is significant.
- The index SOLI(G) is the strongest model with an R^2 of 0.9585, meaning it explains 95.85% of the changes in Molar refractivity. The P-value is $2.26 X10^{-5}$, which is below the common significance level of 0.05. Then the regression model is significant.
- The index CSQLI(G) is the strongest model with an R^2 of 0.957, meaning it explains 95.7% of the changes in Molar refractivity. The P-value is $2.52 X10^{-5}$, which is below the common significance level of 0.05. Then the regression model is significant.
- The index SQI(G) is the strongest model with an R^2 of 0.943, meaning it explains 94.3% of the changes in Molar refractivity. The P-value is $5.869 X10^{-5}$,which is below the common significance level of 0.05. Then the regression model is significant.
- The index PI(G) is the strongest model with an R^2 of 0.932, meaning it explains 93.2% of the changes in Molar refractivity. The P-value is 0.000101, which is below the common significance level of 0.05. Then the regression model is significant.
- The index FI(G) is the strongest model with an R^2 of 0.9362, meaning it explains 93.6% of the changes in Molar refractivity. The P-value is $8.34 X10^{-5}$, which is below the common significance level of 0.05. Then the regression model is significant.
- The index NI(G) have P-value 0.0310 which is less than 0.05. Then the regression model in NI(G) significant.
- The index CSI(G) have P-value 0.4643 which is greater than 0.05. Then the regression model in CSI(G) is Insignificant.

Table:5 Regression model between Molecular Volume and Labeled Topological Indices

Topological indices	Γ	δ	R	R^2	F-value	P-value	Measure
SQI(G)	223.45	0.0034	0.9653	0.931	82.07	0.000101	Significant
SI(G)	173.98	0.0884	**0.9699**	0.9407	95.1147	$6.68 X10^{-5}$	Significant
PI(G)	228.54	0.0027	0.9485	0.8996	53.77	0.000329	Significant

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NLI(G)	246.64	0.4152	0.7380	0.5446	7.1804	0.0366	Significant
SQLI(G)	174.48	0.1214	0.9696	0.9401	94.21	6.86 $X10^{-5}$	Significant
FI(G)	230.41	0.0012	0.9452	0.8934	50.28	0.000395	Significant
CSQI(G)	36.85	6.8771	0.9530	0.9082	59.34	0.000251	Significant
CSI(G)	45.78	120.9096	0.1560	0.0243	0.1496	0.7123	Insignificant

In this table SI(G) has the P-value 6.68 $X10^{-5}$ which is closest to zero. So the result is highly significant.

Table:6 Regression model between Polarizability and Labeled Topological Indices

Topological indices	Γ	δ	R	R^2	F-value	P-value	Measure
SQI(G)	20.85	0.0004	0.9551	0.9122	62.43	0.000218	Significant
SI(G)	15.07	0.0102	0.9641	0.9295	79.12	0.000112	Significant
PI(G)	21.36	0.0003	0.9437	0.8904	48.78	0.000429	Significant
NLI(G)	23.52	0.0477	0.7298	0.5326	6.8384	0.039851	Significant
SOLI(G)	15.09	0.0140	**0.9655**	0.9322	82.6063	9.96X 10^{-5}	Significant
FI(G)	21.50	0.0001	0.9460	0.8949	51.13	0.000377	Significant
CSQI(G)	-1.346	0.8072	0.9628	0.9270	76.0759	0.000126	Significant
CSI(G)	-15.488	20.3514	0.2260	0.0511	0.3228	0.5905	Insignificant

In this table, the index SOLI(G) has highest correlation value and its P-value is almost zero. so it has strong correlation between topological indices and Polarizability.

Table:7 Regression model between Complexity and Labeled Topological Indices

Topological indices	Γ	δ	R	R^2	F-value	P-value	Measure
SQI(G)	270.71	0.0088	0.9691	0.9391	92.57	7.21 $X10^{-5}$	Significant
SI(G)	143.90	0.2280	**0.9712**	0.9432	99.69	**5.84 $X10^{-5}$**	Significant
PI(G)	284.06	0.0071	0.9516	0.9055	57.50	0.000274	Significant
NLI(G)	340.73	1.0307	0.7114	0.5061	6.1476	0.047842	Insignificant

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SQLI(G)	145.85	0.3126	0.9694	0.9398	93.70	6.97 $X10^{-5}$	Significant
FI(G)	290.28	0.0031	0.9438	0.8908	48.94	0.000425	Significant
CSQI(G)	-194.91	17.4049	0.9364	0.8768	42.68	0.000614	Significant
CSI(G)	-60.26	260.571	0.1305	0.0170	0.10395	0.7580	Insignificant

In table:7, SI(G) has highest correlation coefficient value 0.9712 and R^2 value 0.9432 means 94.32% of changes in complexity also the P-value is **$5.84 X10^{-5}$** which is closed to zero and less than 0.05. Therefore the regression model is significant for SI(G).

Table:8 Regression model between Flash point and Labeled Topological Indices

Topological indices	Γ	Δ	R	R^2	F-value	P-value	Measure
SQI(G)	230.50	0.0018	**0.8467**	0.7169	15.1966	0.008	Significant
SI(G)	205.57	0.0469	0.8336	0.6948	13.6622	0.010133	Significant
PI(G)	232.77	0.0015	0.8385	0.7030	14.20334	0.009303	Significant
NLI(G)	236.16	0.2542	0.7322	0.5361	6.934527	0.038885	Significant
SOLI(G)	206.83	0.0637	0.8242	0.6792	12.7055	0.011863	Significant
FI(G)	236.05	0.0006	0.8050	0.6481	11.0488	0.015926	Significant
CSQI(G)	146.55	3.3412	0.7500	0.5625	7.715653	0.032094	Significant
CSI(G)	251.52	17.9402	0.0375	0.0014	0.008445	0.929772	Insignificant

In this table, SQI(G) has lowest P-value. so the correlation coefficient between Flash point and Labeled topological indices are significant. CSI(G) have P-value 0.92977 which is greater than 0.05. Then the result is insignificant.

Table:9 Regression model between Boiling point and Labeled Topological Indices

Topological indices	Γ	Δ	R	R^2	F-value	P-value	Measure
SQI(G)	529.22	0.0015	0.2812	0.0791	0.5151	0.4999	Insignificant
SI(G)	506.49	0.0398	0.2850	0.0812	0.5305	0.4938	Insignificant
PI(G)	533.30	0.0012	0.2665	0.0710	0.4589	0.5234	Insignificant
NLI(G)	527.22	0.2378	0.2761	0.0762	0.4952	0.5080	Insignificant

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SOLI(G)	509.68	0.0525	0.2738	0.0750	0.4863	0.5117	Insignificant
FI(G)	541.25	0.0004	0.2268	0.0514	0.3253	0.5891	Insignificant
CSQI(G)	481.54	2.2714	0.2056	0.0423	0.2647	0.6253	Insignificant
CSI(G)	1749.17	-472.862	0.3984	0.1587	1.1319	0.3283	Insignificant

From Table:9, all the P-values are greater than 0.05 which gives insignificant results

(not statistically significant). This means there is no statistically significant linear relationship between these topological indices and the boiling point.

Table:10 Regression model between Polar surface Area and Labeled Topological Indices

Topological Indices	Γ	Δ	R	R^2	F-value	P-value	Measure
SQI(G)	63.59	0.0005	0.2780	0.0773	0.5024	0.5050	Insignificant
SI(G)	59.43	0.0106	0.2486	0.0618	0.3951	0.5528	Insignificant
PI(G)	65.06	0.0004	0.2595	0.0673	0.4331	0.5349	Insignificant
NLI(G)	69.37	0.0449	0.1700	0.0289	0.1786	0.6873	Insignificant
SOLI(G)	60.68	0.0138	0.2341	0.0548	0.3477	0.5769	Insignificant
FI(G)	68.07	0.0001	0.2096	0.0439	0.2756	0.6184	Insignificant
CSQI(G)	63.39	0.3698	0.1090	0.0119	0.0722	0.7972	Insignificant
CSI(G)	371.41	-118.20	0.3245	0.1053	0.70605	0.43296	Insignificant

From Table:10, all the P-values is greater than 0.05 which gives insignificant results (not statistically significant). This means there is no statistically significant linear relationship between these labelled topological indices and Polar surface area.

Table:11 Regression model between LogP and Labeled Topological Indices

Topological Indices	Γ	Δ	R	R^2	F-value	P-value	Measure
SQI(G)	-1.2290	6.27×10^{-5}	0.5372	0.2886	2.4338	0.1698	Insignificant
SI(G)	-1.9975	0.00156	0.5145	0.2647	2.1595	0.1921	Insignificant
PI(G)	-1.2861	5.41×10^{-5}	0.5652	0.3194	2.8164	0.14432	Insignificant
NLI(G)	-1.5711	0.0110	0.5866	0.3441	3.1474	0.1264	Insignificant

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SOLI(G)	-1.9770	0.002134	0.5123	0.2625	2.1351	0.19427	Insignificant
FI(G)	-1.2433	2.41×10^{-5}	0.5618	0.3156	2.7671	0.1473	Insignificant
CSQI(G)	-4.1423	0.1152	0.4798	0.2302	1.7947	0.228868	Insignificant
CSI(G)	-35.101	14.6390	0.5676	0.3222	2.8521	0.14222	Insignificant

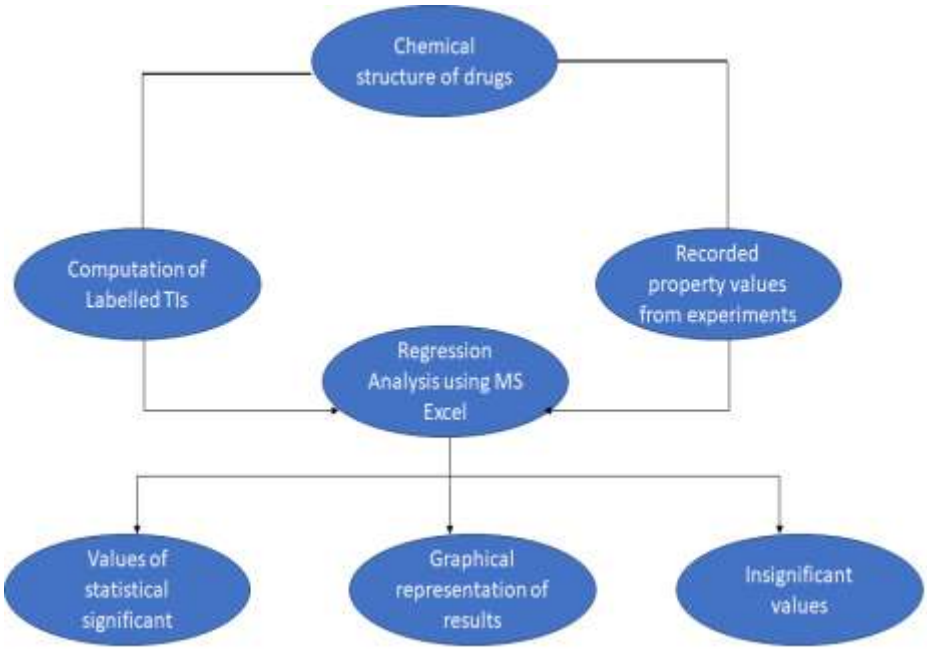
From Table:11, all the P-values is greater than 0.05 which gives insignificant results (not statistically significant). This means there is no statistically significant linear relationship between these labelled topological indices and Polar surface area.

5.Methods used to calculate the results:

This paper outlines two significant calculation techniques in the field of pharmaceuticals.

(i) Labeled Topological indices
(ii) Statistical Analysis

The computation of topological indices involves vertex incidence under Heinz-Quarter mean labeling, and the results are obtained using a calculator. The experimental data for drugs used to treat urinary tract infections are sourced from PubChem. We apply a linear regression model to evaluate both experimental and predicted data. Statistical computations and line graph plotting are carried out using MS Excel.Figure-1 shows the detailed steps involved in estimating the properties of chemical drugs.



6.Analysis of correlation coefficients:

The following table shows the comparison of correlation coefficients with TIs.

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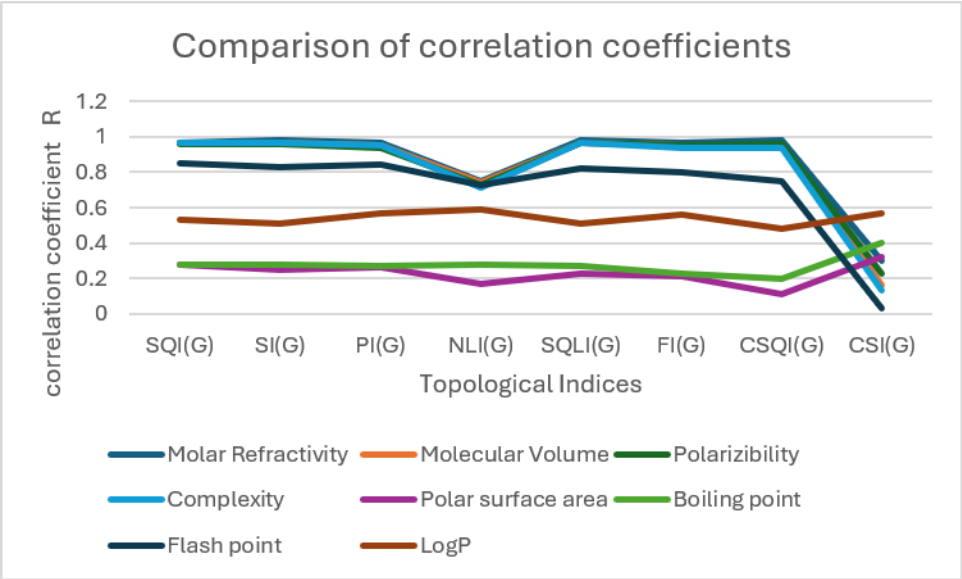
Topological Indices Vs physiochemical property	SQI(G)	SI(G)	PI(G)	NLI(G)	SOLI(G)	FI(G)	CSQI(G)	CSI(G)
Molar Refractivity	0.9712	0.9777	0.9653	0.7531	**0.9791**	0.9676	0.9783	0.3039
Molecular Volume	0.9653	**0.9699**	0.9485	0.7380	0.9696	0.9452	0.9530	0.1560
Polarizability	0.9551	0.9641	0.9437	0.7298	**0.9655**	0.9460	0.9628	0.2260
Complexity	0.9691	**0.9712**	0.9516	0.7114	0.9694	0.9438	0.9364	0.1305
Polar Surface Area	0.2780	0.2486	0.2595	0.1700	0.2341	0.2096	0.1090	0.3245
Boiling Point	0.2812	0.2850	0.2665	0.2761	0.2738	0.2268	0.2056	0.3984
Flash point	**0.8467**	0.8336	0.8385	0.7322	0.8242	0.8050	0.7500	0.0375
LogP	0.5372	0.5145	0.5652	0.5866	0.5123	0.5618	0.4798	0.5676

- The indices CSQI(G), SI(G) and SOLI(G) shows high correlation coefficient with Molar refractivity, complexity and Polarizability respectively. These specific topological indices are excellent predictors for these physical properties.
- The index CSI(G) shows the lowest correlation across all properties particularly Flash point, Molecular volume and Complexity. It means CSI(G) is the least effective index in this specific study.
- Properties like Polar surface area, Boiling point and LogP shows very low correlation values (less than 0.6) across all indices, which gives the above topological indices are poor predictors for these properties.



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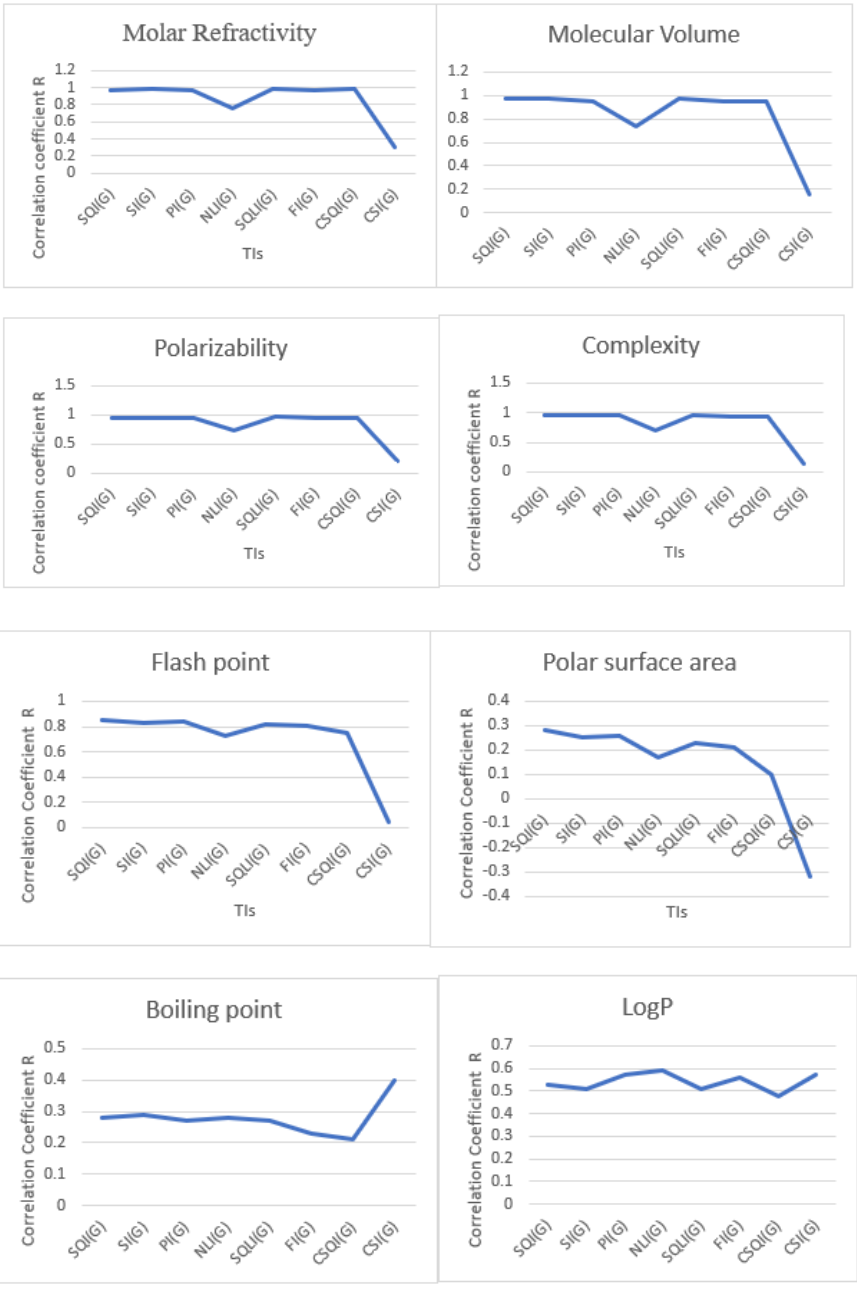
7.Graphical representation of correlation coefficients:



8.Conclusion:

This article we investigate drugs used in Urinary tract infection treatment through Heinz-Quarter Mean labelled -based topological indices and how they are correlate with physical chemical properties. In this study, most topological indices show significant regression models for predicting Molar Refractivity, Molecular Volume, Polarizability, Complexity and Flash point but not for boiling point, LogP and Polar Surface Area. Based on our study,

- R = 0.9791 indicates that Molar Refractivity strongly correlate with SOLI(G) ($R^2 = 0.9585$)

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- Molecular Volume has high correlation for SI(G) for R = 0.9699.
- Polarizability has high correlation for R = 0.9655 for SOLI(G).
- Complexity correlates well with SI(G) for R = 0.9712.
- Flashpoint with correlation coefficient R = 0.8467 has strong positive correlation.
- Boiling Point with R ranges from 0.2056 to 0.3984 is weak positive correlation.
- Polar Surface Area has correlation coefficient values from 0.1090 to 0.3245 is weak positive correlation.
- Log P ranges from 0.4798 to 0.5866 is moderate positive correlation.

Over all our result confirm that topological indices are significant tools for mapping QSPR studies. This work facilitates more to drug discovery and optimization within the chemical and pharmaceutical industries. In a similar way, we try to study the properties of other drugs with the help of Heinz-Quarter labeled indices and variety of regression models.

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