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Rehan-Lanel Indices for Evaluating the Pharmacological Properties of Anti-tuberculosis Drugs

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Abstract

Tuberculosis (TB) is still a major health concern across the world, mostly because Mycobacterium tuberculosis may change and become resistant to numerous medicines. Knowing how the molecular structure of anti-TB medications affects their physicochemical qualities might assist make better drugs. We examined twelve frequently utilized anti-tuberculosis medications, including amikacin, bedaquiline, clofazimine, delamanid, ethambutol, and others. We used ideas from chemical graph theory to characterize their molecular architectures. The first to fourth Rehan-Lanel (RL) and Revan Rehan-Lanel (RRL) topological indices were found using these structures. After we figured out these numbers, we looked at how they are connected to other physicochemical qualities, such as the boiling point, melting point, molar volume, molar refraction, polarizability, surface tension, and flash point. The results indicated that some indices are significantly correlated with these qualities. The RL_1 and RRL_1 indices exhibited more robust correlations with factors such as molar volume and boiling point. These findings indicate that RL-based indices may serve as effective descriptors for evaluating certain physicochemical properties of anti-tuberculosis medications and might facilitate early predictions without only depending on comprehensive laboratory data.

Keywords: Chemical graph theory, topological indices, quantitative structure–activity relationship (QSAR), anti-tuberculosis pharmaceuticals, molecular modelling.

Introduction

The presence of *Mycobacterium tuberculosis*, a bacterium that is acknowledged for its ability to affect a variety of organs, including the brain and spine, in addition to the lungs, is the primary reason why Tuberculosis (*TB*) remains a significant global health issue. This disease can lead to severe health consequences. The pathogen's adaptability and persistent nature require the development of innovative strategies in the areas of diagnosis, treatment, and prevention. "Cheminformatics is an interdisciplinary field that combines mathematics, computer science, and chemistry to better understand chemical compounds and their behaviour". It plays an important role in studies involving quantitative structure–activity relationships (*QSAR*) and quantitative structure–property relationships (*QSPR*), which help scientists predict the biological activities and properties of chemical substances. These methods are valuable because they speed up the discovery and development of new therapeutic drugs.

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This study explores how molecular graph theory and cheminformatics can be applied to better understand and predict the biological behaviour of compounds related to tuberculosis treatment. The main goal is to identify new compounds with promising anti-tuberculosis potential using *QSAR* and *QSPR* models, thereby contributing to global efforts to combat this persistent disease. "In chemical graph theory, topological indices are widely used because they convert molecular structural information into numerical values that can be analysed mathematically".

Specifically, these indices dive into molecular graphs, where they express topological structures of molecules by numerical descriptors. Topological indices are utilized to examine chemical properties of pharmaceuticals while boosting *QSAR/QSPR*s studies. "Degree-based topological indices, which have been investigated for their linkage between varieties of chemical compound attributes, show a significant demand over different ranges of topological indices" [6, 7, 9].

Harold Wiener came up with the idea of topological indices while investigating paraffins in 1947. This led to the creation of the Wiener index. This index, "which is often called the route number [1, 11], is one of the most researched molecular topological indices in chemical graph theory since it has unique theoretical features and may be used in a lot of different ways". Milan Randic [12] subsequently came up with the first real degree-based topological index. "It was first termed the branching index, then the connectedness index, and today most people call it the Randic index". The first and second Zagreb indices were introduced by I. Gutman and N. Trinajstic in 1972. They are found by adding up the squares of the degrees of the vertices in a graph. Since then, numerous scholars have examined and used these indexes a lot.

In 2009, Vukicevic and Furtula [20] proposed the geometrical-arithmetic index, "adding to the growing list of topological indices. This index provides further insight into the geometric and arithmetic properties of molecular graphs, expanding the toolkit available for analysing molecular structures". In 2015, Furtula and Gutman [4] restudied another index related to the total of the cubed degrees of the vertices of a network, calling it the "Forgotten topological index" or "F-index". In [5], Gunawardhana and Lanel introduced the Rehan-Lanel indices. In this study, we use the first, second, third and fourth Rehan Lanel indices and the first four Revan Rehan-Lanel indices for modelling physical properties of some tuberculosis drugs.

Definition 1.1. Let a graph G consists of a set of vertices $V(G)$ and a set of edges $E(G)$. "The first Rehan-Lanel index, the second Rehan-Lanel index, the third Rehan-Lanel index, and the fourth Rehan-Lanel index" [5] are defined as follows,

i. $RL_1(G) = \sum_{uv \in E(G)} (d_G^2(u) + d_G^2(v) + d_G(u)d_G(v))$
ii. $RL_2(G) = \sum_{uv \in E(G)} (d_G^2(u) + d_G^2(v) - d_G(u)d_G(v))$
iii. $RL_3(G) = \sum_{uv \in E(G)} (d_G(u) - d_G(v) + d_G(u)d_G(v))$
iv. $RL_4(G) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)|\, d_G(u)d_G(v)$

Throughout the paper G is a connected graph that is finite, simple, and has vertex and edge sets denoted by $V(G)$ and $E(G)$. $d_G(u)$ is the degree of a vertex u, and it is determined by the

number of vertices that are adjacent to it. In the context of the graph G, let $\Delta(G)$ indicate the greatest (lowest) degree among the vertices of G correspondingly. In the graph G, the Revan vertex degree of u is defined as the expression $r_G(u) = \Delta(G) + \delta(G) - d_G(u)$. Within this context, the Revan edge that connects the Revan vertices u and v is denoted by the symbol uv.

Kulli introduced the first and second Revan indices based on the Zagreb indices in [14], "more details and applications of Revan indices can be found in [2, 3, 15, 16, 17, 18, 19]". In 2024, Gunawardhana and Lanel proposed the first, second, third and fourth Rehan-Lanel indices [5] of a graph G as follows.

Definition 1.2. The first, second, third, and fourth Revan Rehan-Lanel indices of a graph G are defined by,

i. $RRL_1(G) = \sum_{uv \in E(G)} (r_G^2(u) + r(v) + r(u) r_G(v))$
ii. $RRL_2(G) = \sum_{uv \in E(G)} (r_G^2(u) + r(v) - r(u) r_G(v))$
iii. $RRL_3(G) = \sum_{uv \in E(G)} (r_G(u) - r_G(v) + r_G(u) r_G(v))$
iv. $RRL_4(G) = \sum_{uv \in E(G)} (|r_G(u) - r(v)| r_G(u) r_G(v))$

This study investigates the quantitative relationships between the molecular structures of twelve anti-tuberculosis drugs and their physicochemical properties by using the above Rehan Lanel (RL) and Revan RL topological indices. Specifically, the study aims to compute these indices from chemical graphs and assess their effectiveness as descriptors for modelling key physical properties, such as boiling point, melting point, flash point, molar refraction, polarizability, surface tension, and molar volume. Also, we establish predictive models that can provide insights into the physicochemical behaviour of anti-tuberculosis drugs based on their molecular topology.

Methodology

This study utilized chemical graphs to illustrate the molecular structures of twelve anti-TB medications. A point is an atom, while a line is a link between atoms. The medicines were "amikacin, bedaquiline, clofazimine, delamanid, ethambutol, ethionamide, imipenem-cilastatin, isoniazid, levofloxacin, linezolid, moxifloxacin, and p-aminosalicylic acid". When counting the edges, double bonds were counted as two edges. We utilized these chemical graphs to find the first, second, third, and fourth Rehan Lanel (*RL*) indices and the first, second, third, and fourth Revan Rehan–Lanel indices for each medication in a systematic way. We used these eight topological indices as molecular descriptors to generate informed estimations about the compounds' boiling point (*BP*), melting point (*MP*), flash point (*FP*), molar refraction (*MR*), polarizability (*PL*), surface tension (*ST*), and molar volume (*MV*).

To explore the relationship between topological descriptors and physicochemical properties, statistical techniques such as correlation analysis and regression modelling were employed. Correlation coefficients were calculated for each pair of physicochemical property and topological index in order to evaluate the strength of their association. For the regression analysis, the following linear model was applied:

$$P = a + b[TI]$$

where P represents the physical property of the drug, a is a constant, b is the regression coefficient, and TI denotes the topological index. The parameters a and b were estimated using R software, based on seven physicochemical properties and eight degree-based topological indices derived from the molecular structures of twelve drugs. This method allowed the development of linear regression models that link degree-based topological indices with physicochemical properties, providing a quantitative framework for predicting and better understanding the behaviour of anti-tuberculosis drugs.

Results and Discussion

In this section, we present a quantitative framework for predicting physicochemical properties, namely, boiling point (BP), melting point (MP), flash point (FP), molar refraction (MR), polarizability (PL), surface tension (ST), and molar volume (MV). The values of physicochemical properties of twelve tuberculosis medicines are presented in Table 1. These values were extracted from ChemSpider.

Table1: Physical properties of various tuberculosis drugs

Name of medicine	*BP*	*MP*	*FP*	*MR*	*PL*	*ST*	*MV*
Amikacin	981.8	203.5	547.6	134.9	53.5	103.3	363.9
Bedaquiline	702.7	176	378.8	156.2	61.9	52.6	420.1
Clofazimine	566.9	210	296.7	136.2	54	47.1	366.1
Delamanid	653.7	193	349.1	127.7	50.6	50	368
Ethambutol	345.6	89	113.7	58.6	23.2	38.1	207
Ethionamide	247.9	163	103.7	49	19.4	39.8	142
Imipenem	530.2	190	274.5	72.7	28.8	71	183.9
Isoniazid	251.97	172	251	36.9	14.6	57.8	110.2
Levofloxacin	571.5	224	299.4	91.1	36.1	70.3	244
Linezolid	585.5	177	307.9	83	32.9	47.7	259
Moxifloxacin	636	270	338.7	101.8	40.4	60.7	285
p-Aminosalicylic	380.8	145	184.1	39.3	15.6	83.4	102.7

Resource: Physical properties are obtained from ChemSpider.

Regression models for the selected indices:

1. BP = 96.086+0.286 [$RL_1(G)$]
   MP =136.215+0.025 [$RL_1(G)$]
   FP = 39.99+0.1611 [$RL_1(G)$]
   MR = 4.547+0.059 [$RL_1(G)$]
   PL = 1.769+0.024 [$RL_1(G)$]
2. BP = 94.285+0.705 [$RL_2(G)$]
   MP =143.001+0.051 [$RL_2(G)$]
   FP = 77.882+0.338 [$RL_2(G)$]
   MR = 3.871+0.148 [$RL_2(G)$]
   PL = 1.678+0.356 [$RL_2(G)$]
4. BP = 71.035+0.4311 [$RL_4(G)$]
   MP = 346.450+0.425[$RL_4(G)$]
   FP = 59.990+0.461 [$RL_4(G)$]
   MR = 4.547+0.059 [$RL_4(G)$]
   PL = 1.769+0.024 [$RL_4(G)$]
5. BP = 101.699+0.663 [$RRL_1(G)$]
   MP = 148.589+0.054 [$RRL_1(G)$]
   FP = 61.516+0.342[RRL_1(G)]
   MR = 16.238 + 0.113[RRL_1(G)]
   PL = 6.414+0.045[RRL_1(G)]

3. BP = 84.285+0.405 [$RL_3(G)$]
   MP = 103.041+0.451 [$RL_3(G)$]
   FP = 67.852+0.438 [$RL_3(G)$]
   MP = 2.679+0.158 [$RL_3(G)$]
   PL = 1.238+0.460 [$RL_3(G)$]

6. BP = 192.593+0.911 [$RRL_2(G)$]
   MP = 161.817+0.059 [$RRL_2(G)$]
   FP =109.105+0.469 [$RRL_2(G)$]
   MR =19.383 +0.188 [$RRL_2(G)$]
   PL = 7.673+0.007 [$RRL_2(G)$]

7. BP = 123.575+1.782 [$RRL_3(G)$]
   MP =154.506+0.128 [$RRL_3(G)$
   FP = 70.661+0.929 [$RRL_3(G)$]
   MR = 18.725 + 0.309 [$RRL_3(G)$]
   PL = 7.404+0.122 [$RRL_3(G)$]

8. BP = 126.796+1.299 [$RRL_4(G)$]
   MP =155.580+0.091[$RRL_4(G)$]
   FP = 75.861+0.666 [$RRL_4(G)$]
   MR = 17.796 + 0.230 [$RRL_4(G)$]
   PL = 7.036+0.091 [RRL_4(G)]

The computed RL indices of each anti-tuberculosis drugs are presented in Table 2.

Table 2: Values of *RL* indices of each anti-tuberculosis medicine

Medicine	RL_1	RL_2	RL_3	RL_4	RRL_1	RRL_2	RRL_3	RRL_4
Amikacin	2294	802	518	716	1348	674	476	636
Bedaquiline	2335	971	579	482	835	771	363	474
Clofazimine	1517	647	357	390	703	342	208	300
Delamanid	2449	1017	603	604	859	478	290	414
Ethambutol	1000	468	192	336	625	345	215	316
Ethionamide	827	345	201	204	347	225	121	164
Imipenem	1276	536	302	384	586	306	208	274
Isoniazid	687	218	184	146	255	137	91	116
Levofloxacin	1752	736	462	462	662	366	232	312
Linezolid	1625	691	381	470	650	366	228	320
Moxifloxacin	2062	852	518	480	757	417	263	360
p-Aminosalicylic	732	280	202	128	282	130	100	118

In Table 3, we present the correlation coefficients between values of nine degree-based Rehan-Lanel topological indices and six physical properties of medicines. The main drawback of our study is the lack of satisfactory correlate findings among degree-based topological index, and the melting point and surface tension of anti-tuberculosis drug. But the correlations values between RL indices and MP are high compared to the correlations between other degree-based indices and MP of these anti-TB drugs. However, the theoretical analysis of our study could strengthen the prediction of anti-tuberculosis medicinal attributes with zero involvement of laboratory experimentation.

Table 3: Correlations of RL indices with physical properties

Topological Index	BP	MP	FP	MR	PL	ST	MV
RL_1	0.8865	0.5547	0.8160	0.8996	0.8997	0.1891	0.9054
RL_2	0.7702	0.4749	0.6735	0.8722	0.8723	-0.0042	0.9047
RL_3	0.8485	0.6106	0.8019	0.8780	0.8781	0.1915	0.8724
RL_4	0.9228	0.4612	0.8245	0.8136	0.8137	0.2787	0.8350
RRL_1	0.9418	0.3629	0.8433	0.8158	0.8160	0.3929	0.8264
RRL_2	0.8376	0.2555	0.7470	0.8771	0.8770	0.1778	0.8840
RRL_3	0.9360	0.3168	0.8464	0.8249	0.8250	0.3892	0.8301
RRL_4	0.9260	0.3040	0.8260	0.8996	0.8997	0.1891	0.9054

Table 4: Statistical parameters for the linear QSPR model for $RL_1(G)$

Physical Property	a	b	r	r^2	F	p	Indicator
BP	96.0863	0.2862	0.8865	0.7636	36.53	≤ 0.05	Significant
MP	125.5309	0.0381	0.5547	0.2423	4.518	≥ 0.05	Not significant
FP	52.3739	0.1518	0.8160	0.6325	19.93	≤ 0.05	Significant
MR	2.4210	0.0570	0.8996	0.7903	42.45	≤ 0.05	Significant
PL	0.9386	0.0226	0.8997	0.7905	42.5	≤ 0.05	Significant
ST	51.5033	0.0056	0.1891	0.0000	0.371	≥ 0.05	Not significant
MV	19.4	0.1519	0.9054	0.8018	45.49	≤ 0.05	Significant

Table 5: Statistical parameters for the linear QSPR model for $RL_2(G)$

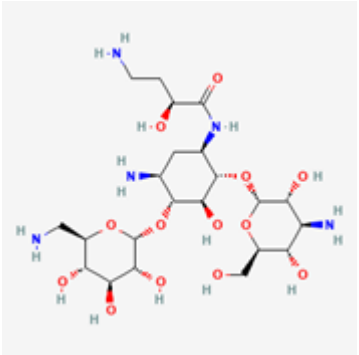
Physical Property	a	b	r	r^2	F	p	Indicator
BP	133.6127	0.6427	0.7702	0.6274	19.52	≤ 0.05	Significant
MP	129.55808	0.08698	0.4749	0.1988	3.729	≥ 0.05	Not significant
FP	84.813	0.321	0.6735	0.4471	9.894	≥ 0.05	Significant
MR	3.7098	0.1379	0.8722	0.7693	37.68	≤ 0.05	Significant
PL	1.45323	0.05468	0.8723	0.7693	37.69	≤ 0.05	Significant
ST	58.2589	0.0030	-0.0042	-0.09812	0.01712	≥ 0.05	Not Significant
MV	19.8264	0.3721	0.9047	0.8036	46	≤ 0.05	Significant

Table 6: Statistical parameters for the linear QSPR model for $RL_3(G)$

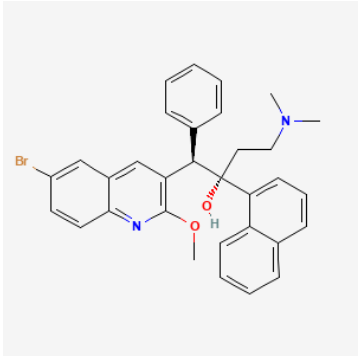
Physical Property	a	b	r	r^2	F	p	Indicator
BP	120.321	1.123	0.8485	0.6907	25.57	≤ 0.05	Significant
MP	120.4017	0.1717	0.6106	0.3147	6.05	≥ 0.05	Significant
FP	59.2430	0.6116	0.8019	0.6074	18.02	≤ 0.05	Significant
MR	5.5945	0.2282	0.8780	0.7479	33.63	≤ 0.05	Significant
PL	2.19579	0.09051	0.8781	0.7481	33.68	≤ 0.05	Significant
ST	51.50008	0.02319	0.1915	-0.05965	0.3808	≥ 0.05	Not significant
MV	30.7206	0.6001	0.8724	0.7372	31.86	≤ 0.05	Significant

Table 7: Statistical parameters for the linear QSPR model for $RL_4(G)$

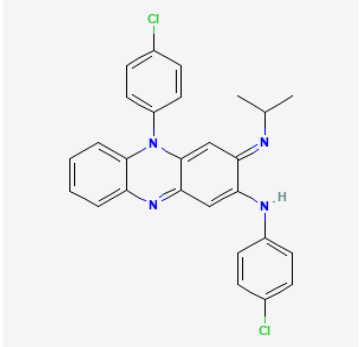
Physical Property	a	b	r	r^2	F	p	Indicator
BP	102.51	1.09	0.9228	0.8381	57.95	≤ 0.05	Significant
MP	138.2794	0.1152	0.4612	0.135	2.716	≥ 0.05	Not Significant
FP	62.8549	0.5604	0.8245	0.6478	21.23	≤ 0.05	Significant
MR	15.1976	0.1885	0.8136	0.6282	19.59	≤ 0.05	Significant
PL	6.00529	0.07475	0.8137	0.6284	19.6	≤ 0.05	Significant
ST	48.10429	0.03008	0.2787	-0.01454	0.8424	≥ 0.05	Not significant
MV	49.4826	0.5119	0.8350	0.6669	23.03	≤ 0.05	Significant



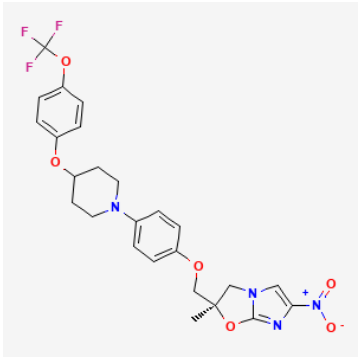
(a) Amikacin



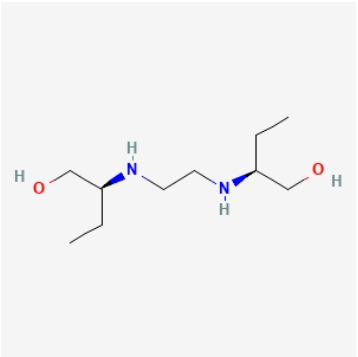
(b) Bedaquiline



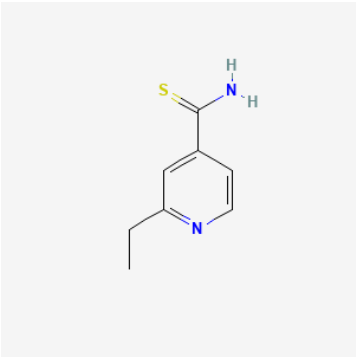
(c) Clofazimine



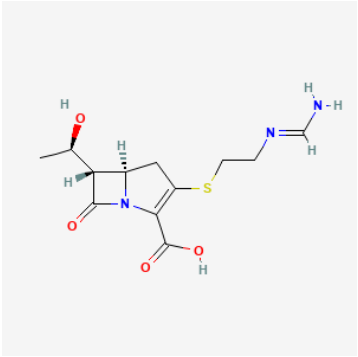
(d) Delamanid



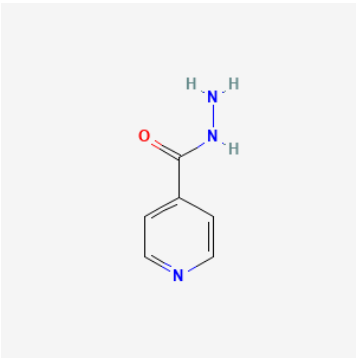
(e) Ethambutol



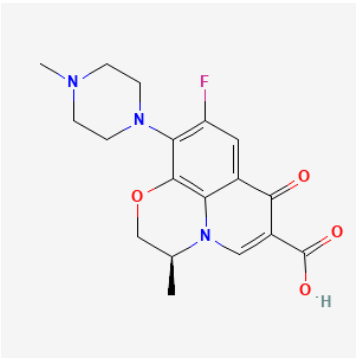
(f) Ethionamide



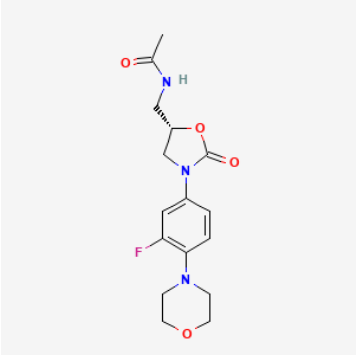
(g) Imipenem



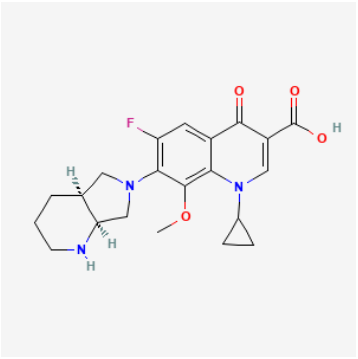
(h) Isoniazid



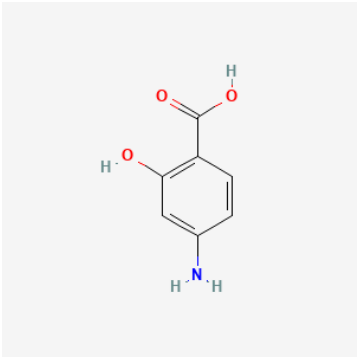
(i) Levofloxacin



(j) Linezolid



(k) Moxifloxacin



(l) P-Aminosalicyclic

Figure 1: Chemical Structures of Medicines
Resource: Chemical structures are taken from PubChem

Table 8: Statistical parameters for the linear QSPR model for $RRL_1(G)$

Physical Property	*a*	*b*	*r*	r^2	*F*	*p*	Indicator
BP	101.699	0.663	0.9418	0.8733	76.79	≤ 0.05	Significant
MP	148.5894	0.0543	0.3629	0.04638	1.535	≥ 0.05	Not significant
FP	61.5156	0.3423	0.8433	0.6822	24.61	≤ 0.05	Significant
MR	16.2382	0.1129	0.8158	0.6321	19.9	≤ 0.05	Significant
PL	6.41391	0.04476	0.8160	0.6324	19.93	≤ 0.05	Significant

ST	43.45153	0.02532	0.3929	0.06982	1.826	≥ 0.05	Not significant
MV	54.8992	0.3026	0.8264	0.6513	21.55	≤ 0.05	Significant

Table 9: Statistical parameters for the linear QSPR model for $RRL_2(G)$

Physical Property	a	b	r	r^2	F	p	Indicator
BP	192.5930	0.9114	0.8376	0.6694	23.28	≥ 0.05	Significant
MP	161.8171	0.0594	0.2555	-0.0267	0.714	≥ 0.05	Not significant
FP	109.1046	0.4687	0.7470	0.5138	12.62	≥ 0.05	Significant
MR	19.3832	0.1876	0.8771	0.7463	33.35	≥ 0.05	Significant
PL	7.6728	0.0074	0.8770	0.746	33.31	≥ 0.05	Significant
ST	53.4127	0.01772	0.1778	-0.0652	0.3266	≥ 0.05	Not significant
MV	64.3124	0.5004	0.8840	0.7597	35.77	≤ 0.05	significant

Table 10: Statistical parameters for the linear QSPR model for $RRL_3(G)$

Physical Property	a	b	r	r^2	F	p	Indicator
BP	123.575	1.782	0.9360	0.8611	69.21	≤ 0.05	Significant
MP	154.5057	0.1282	0.3168	0.0116	1.129	≥ 0.05	Not significant
FP	70.661	0.9293	0.8464	0.688	25.26	≤ 0.05	Significant
MR	18.7251	0.3087	0.8249	0.6485	21.29	≤ 0.05	Significant
PL	7.4038	0.1224	0.8250	0.6487	21.31	≤ 0.05	Significant
ST	44.3367	0.0679	0.3892	0.0667	1.786	≥ 0.05	Not significant
MV	62.8455	0.8221	0.8301	0.658	22.17	≤ 0.05	Significant

Table 11: Statistical parameters for the linear QSPR model for $RRL_4(G)$

Physical Property	a	b	r	r^2	F	p	Indicator
BP	126.796	1.299	0.9260	0.8407	59.07	≤ 0.05	Significant
MP	155.5807	0.0908	0.3040	0.0031	1.034	≥ 0.05	Not significant
FP	75.8613	0.6664	0.8260	0.6462	21.09	≤ 0.05	Significant
MR	17.7958	0.2297	0.8996	0.6634	22.68	≤ 0.05	Significant
PL	7.03622	0.0911	0.8997	0.6636	22.7	≤ 0.05	Significant
ST	46.7676	0.0422	0.1891	0.0186	1.209	≥ 0.05	Not significant
MV	57.6812	0.6203	0.9054	0.658	22.17	≤ 0.05	Significant

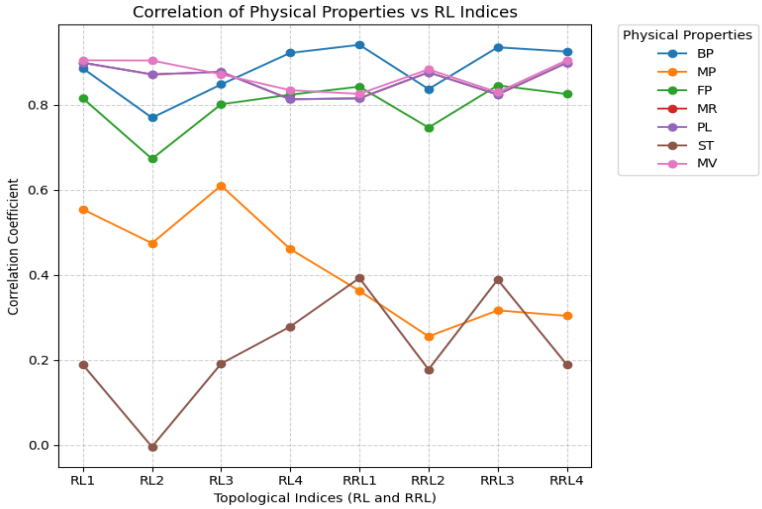


Figure 2: Correlation of Physical properties and topological indices

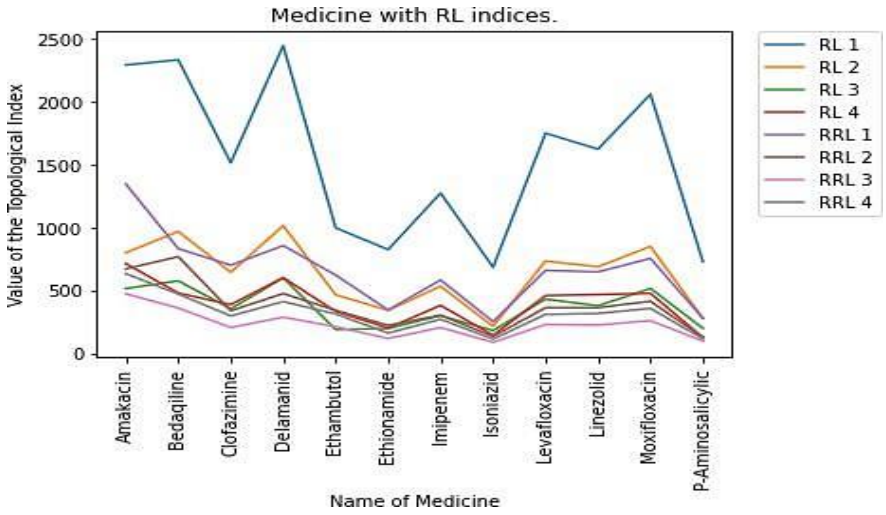


Figure 3: Comparison of topological indices with medicines

This part has been about figuring out the Regression parameters. $N, a, b, and\ r$ stand for the sample size, the constant or intercept of y, the slope, and the correlation coefficient, respectively. r^2 shows how much the response variable changes, as shown by the linear model. The $p-$value of each term tests the null hypothesis, which says that the coefficients are all zero. On the other hand, a larger (not important) p-value means that changes in the predictor are not connected to changes in the responder. Let's say we're running a test where the null hypothesis says that all the regression coefficients are equal to zero. This test first looks at the models without any explanatory variables. Then, it looks at how the model improves with additive coefficients by giving a F value as the result. Somehow, in this scenario, the model is unable to provide precise predictions. The Tables 4-11 shows the statistical parameters of linear QSPR models for a range of topological indices. Each model gives a significant result, where the p value is lower or equal to the significance level (0.05).

Conclusion

Tuberculosis (*TB*) is a bacterial disease caused by the Mycobacterium tuberculosis germs. This makes the lungs perform less properly and puts people's lives at danger by spreading to other parts of the body, such the brain and spine.

A molecular descriptor is a math formula that works on any graph that explains how a molecule is built. One number, in particular, stands for a chemical structure. Graph theory calls this number a topological descriptor, which may be linked to a molecular element to make a molecular index, notably a topological index (*TI).* The topology of the graph is used to make a topology index, which is what happens when a molecular graph is changed. We might be able to learn more about the physical and chemical characteristics of molecules by finding these indices. When you calculate these topological indices, you may see arithmetic numbers and learn more about some of the molecule's physical and chemical features. You transform a molecular graph into a number that shows how the graph is put up to generate a topological index. Topological indices are particularly significant in mathematical chemistry, especially when it comes to quantitative structure-activity relationships (*QSAR*) and quantitative structure-property relationships (*QSPR*).

Upon examining correlation coefficients horizontally for physical properties under consideration, we see that RL_1 (*G*) gives highest correlation coefficient for MV ($r = 0.9054$), MR ($r = 0.8996$) and polarizability ($r = 0.8997$). RL_2 (*G*) gives the highest correlation coefficient for MV ($r = 0.9054$). RL_3 (G) gives the highest correlation coefficient for the MR (r = 0.8780), polarizability ($r = 0.8781$). RL_4 (*G*) gives the highest correlation coefficient for BP ($r = 0.9228$). RRL_1 (*G)* gives the highest correlation coefficient for BP ($r = 0.9418$). RRL_2 (*G*) gives the highest correlation coefficient for MR ($r = 0.8771$) and polarizability ($r = 0.8770$). RRL_3 (*G*) gives the highest correlation coefficient for BP ($r = 0.9360$). RRL_4 (*G*) gives highest correlation coefficient for BP ($r = 0.9260$) and MV($r = 0.9054$). When we look vertically, BP has also good correlation with RRL_1 (G) i.e. $r = 0.9418$), and RRL_3 (*G*) ($r = 0.9360$) respectively. FP has good correlation with RRL_4 (*G*) i.e. $r = 0.8464$. MR has also good correlation with RL_1 (*G*) and RL_1 (*G*), i.e., $r = 0.8996$ both. Polarizability has also good correlation with $RL_1(G)$ and $RRL_4(G)$ i.e., ($r = 0.8997$) for both. MV has also good correlation with $RL_1(G)$, $RL_2(G)$ and RRL_4 (*G*), i.e., $r = 0.9054, 0.9047$ and $r = 0.9054$ respectively.

Research indicates that this theoretical approach may aid chemists and professionals in the pharmaceutical industry in forecasting the characteristics of anti-tuberculosis drugs without empirical testing. It is possible that different combinations of these drugs might be used to treat different diseases, depending on the range of the topological indices obtained in this study. We have calculated the correlation coefficient for several topological indicators in this study. This discovery will aid chemists in designing innovative pharmaceuticals by amalgamating substances that have a strong positive correlation.

More research into the link between the molecular structure of pharmaceuticals and their physical qualities might help us figure out how well new treatments will work and how safe they will be. Researchers may be able to learn more about how drugs could behave by looking at how new topological indices are connected to other physicochemical qualities including solubility, bioavailability, and stability. This can also assist find good drug candidates early on in development, which might save time and money in drug research. Also, numerical methods may be used to find the optimum link between a topological index and the physical characteristic it describes. These kinds of methods could assist make predictions about physicochemical characteristics better without having to depend just on experimental data.

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References

[1] Ahmad, I., Ahmad Chaudhry, M., Hussain, M., & Mahmood, T. (2021). Topological Descriptors on Some Families of Graphs. *Journal of Chemistry*, *2021*, 1–12. https://doi.org/10.1155/2021/6018893

[2] Ashraf, R. & Akhter, S. (2019), Revan Indices and Revan Polynomials of Silicon Carbide Graphs, *International Journal Of Engineering Research & Technology (IJERT)*, 08(09).

[3] Baig, A.Q., Naeem, M. & Gao, W.(2018) Revan and hyper-Revan indices of Octahedral and icosahedral networks. *Appl. Math. Nonlinear Sci.* 3, 33–40, https://doi.org/10.21042/amns.2018.1.00004.

[4] Furtula, B. & Gutman, I. (2015), A forgotten topological index, *Journal of Mathematical Chemistry*, 53, pp. 1184–1190.

[5] Gunawardhana, D.C. & Lanel, G.H.J., (2024), Rehan-Lanel Indices of Graphs, *arXiv* preprint arXiv:2402.08248.

[6] Gutman, I. & Polansky, O. (1986). *Mathematical Concepts in Organic Chemistry*. Berlin, Boston: De Gruyter. https://doi.org/10.1515/9783112570180

[7] Gutman, I., (2003), QSPR/QSAR Studies by Molecular Descriptors by Mircea V. Diudea, *Journal of Chemical Information and Computer Sciences*, **43**(5):1720-1721.

[8] Gutman, I., (2013), Degree-based topological indices, *Croatica Chemica Acta*, **86**(4), pp. 351-361.

[9] Pal, M., Samantha, S., & Pal, A. (2019), Handbook of Research on Advanced Applications of Graph Theory in Modern Society, *IGI Global*.

[10] Wiener, H., (1947), Structural determination of paraffin boiling points, *Journal of the American Chemical Society*, **69**(1), pp. 17-20.

[11] Nikoli´c, S. & Trinajsti´c, N., (1995), The Wiener index: Development and applications, *Croatica Chemica Acta*, **68**(1), pp. 105-129.

[12] Randic, M., (1975), Characterization of molecular branching, *Journal of the American Chemical Society*, **97**(23), pp. 6609-6615.

[13] Khalifeh, M.H., Yousefi-Azari, H. & Ashrafi, A.R., (2008), The hyper-Wiener index of graph operations. Comput. Math. Appl., **56**(5), pp. 0898-1221.

[14] Kulli, V. R. (2017). Revan Indices of Oxide and Honeycomb Networks. *International Journal of Mathematics And Its Applications*, *5*(4 - E), 663–667. Retrieved from https://ijmaa.in/index.php/ijmaa/article/view/1324

[15] Kulli, V.R., (2017), On the Product Connectivity Revan Index of Certain Nanotubes, *Journal of Computer and Mathematical Sciences*. 08. pp. 562-567

[16] Kulli, V.R., (2018), F-Revan Index and F-Revan Polynomial of Some Families of Benzenoid Systems, *Journal of Global Research in Mathematical Archives*, 5(11).

[17] Kulli, V.R. & Gutman, I., (2022), Revan Sombor Index, *Journal of Mathematics and Informatics*, 22, pp. 23-27.

[18] Kulli, V.R., (2022), Revan Sombor Indices and Their Exponentials For Certain Nanotubes, *International Journal of Engineering Sciences and Research Technology*., 11, pp. 22-31.

[19] Kulli, V. R., Méndez-Bermúdez, J. A., Rodríguez, J. M., & Sigarreta, J. M. (2023). Revan Sombor indices: Analytical and statistical study. *Mathematical biosciences and engineering : MBE*, *20*(2), 1801–1819. https://doi.org/10.3934/mbe.2023082

[20] Vukicevic, D. & Furtula, B. (2009) Topological Index Based on the Ratios of Geometrical and Arithmetical Means of End-Vertex Degrees of Edges. *Journal of Mathematical Chemistry*, **46**, 1369-1376. http://dx.doi.org/10.1007/s10910-009-9520-x