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RESEARCH ARTICLE

Predictive Ability of Some Neighborhood Degree-Based Topological Indices for Antituberculosis Drugs

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Abstract

Objectives: To study some newly introduced neighborhood degree-based topological indices (TIs) for chemical structures of antituberculosis drugs as predictors of various physicochemical properties of antituberculosis drugs. **Methods:** We compute neighborhood TIs of the 15 antituberculosis drugs from their chemical structures. Further we apply Quantitative Structure Property Relationship (QSPR) approach to correlate the physicochemical properties such as boiling point, flash point, enthalpy, molar refractivity, polarizability and molar volume of the drugs with the values of the TIs obtained from the structures. **Findings:** The TIs are found to have very good correlation with the properties of the drugs. Although all the considered TIs can be used to predict the physicochemical properties of the drugs, but to have better result, we consider three indices based on their correlation with each property of the drugs and established a linear regression equation to obtain the said properties of the drugs. Also, the predicted values are compared with the experimented values and found to have good predictive ability with a very low margin of error with the experimented values. **Novelty:** We have considered 16 neighborhood degree-based topological indices which are found to have better correlation with the properties of antituberculosis drugs than the degree-based TIs.

Keywords: Neighborhood degree - based topological indices; Antituberculosis drugs; QSPR/QSAR; Degree; Regression

1 Introduction

Topological index is a mathematical formula which is applied to model some molecular structures. It is used to predict various physicochemical properties of a chemical compound and they find an important place in Quantitative structure property/activity relationship(QSPR/QSAR) studies. Due to high risk involvements, financial limitations and time, it is not always possible to analyze the properties of a compound by experimenting in laboratory. QSPR[(1)] and QSAR[(2)] methods are used to correlate the physicochemical properties and the bio-activities of chemical compounds. To create effective regression models with high predictive ability for these qualities, structure-

based TIs are used. In the field of chemical graph theory there are over 3000 TIs. The TIs are obtained form the chemical structure of the compounds. TIs can be classified into some classes such as degree/valency-based indices[3], distance-based indices[4], neighborhood degree-based indices[5] , reduced reverse degree-based indices[6], status-based indices[7], spectrum-based indices[8] etc. It is not always possible to analyse the properties of a molecule by laboratory experiments due to financial limitations, time or involvement of high risk. Therefore, calculating TI is an efficient method to the limitations of such laboratory experiments. Till now many researchers have studied TIs for various chemical structures in the field of chemical graph theory. Although there are thousands of TIs but not all the TIs are useful for QSPR/QSAR analysis. It is very important to have a strong correlation of the TIs with the physichochemical properties of the chemical compounds to have a good result.

Tuberculosis (TB) is a serious disease caused by "Mycobacterium Tuberculosis" mainly effect the lungs. It is an infectious disease which makes the disease more dangerous. Although the TB germs typically attack the lungs, they can also affect the kidney, spine, and brain. Not every person who contracts the TB germs gets ill. Latent TB infection (LTBI) and TB disease are consequently two TB-related diseases. TB disease can be lethal if it is not adequately treated. For the treatment of the Tuberculosis disease the approved drugs are Amikacin, Bedaquiline, Clofazimine, Delamanid, Ethambutol, Ethionamide, Imipenem-cilastatin, Isoniazid, Levofloxacin, Linezolid, Moxifloxacin, p-Aminosalicyclic acid, Pyrazinamide, Rifampin and Terizidone. Figure 1 shows the chemical structure of the drugs.

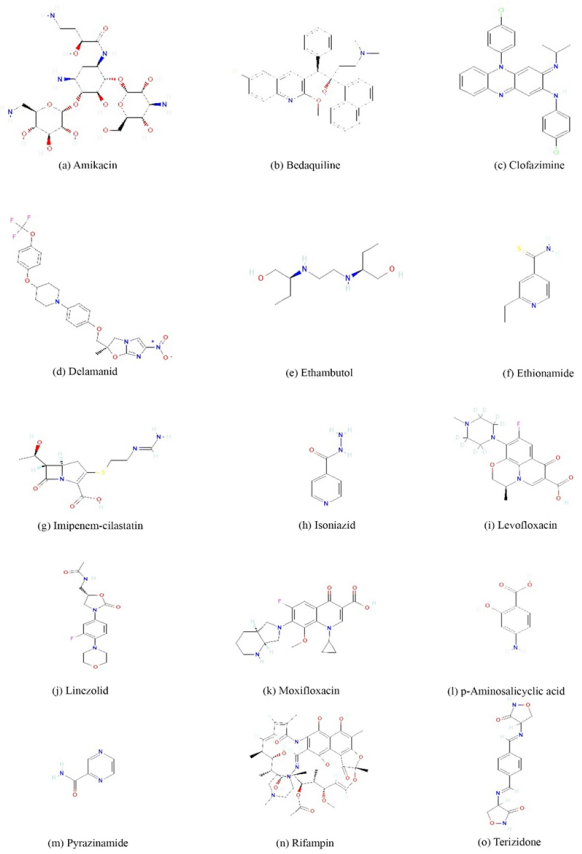

Fig 1. Chemical structure of 15 anti tuberculosis drugs[9]

Recently some researchers studied on antituberculosis drugs. In 2021, Klendrova et al.[2] has studied the activity of antituberculosis drugs using TIs. In 2022, Prasant et al.[10] have computed the degree-based and neighborhood degree-based TIs of four drugs used for the cure of tuberculosis. But their correlation with the properties of the drugs is not studied which is an important part of considering of TIs as predictor variables. In 2022, Adnan et al.[9] have studied degree-based TIs for 15 antituberculosis drugs. The studied TIs are very well correlated with the properties of the drugs. But still there are more indices to be studied for the drugs which may give a better result than the degree-based TIs. In this study we have considered some

well-known neighborhood degree-based TIs and conduct a QSPR analysis to correlate the physicochemical properties of the drugs with the values of the TIs. Also, we calculate the properties of antituberculosis drugs using the regression model obtained from the analysis. The considered indices are found to have better predictive ability then the degree-based TIs considered by Adnan et al.[9] for the antituberculosis drugs.

2 Methodology

2.1 Topological Indices and Properties of the Drugs

In this analysis, we examine the prediction power of 16 neighbourhood degree-based TIs for antituberculosis drugs. To do this, we first determine their correlation with the mentioned drugs properties such as boiling point (BP), flash point (FP), enthalpy of vaporization (EV), molar refractivity (MR), polarizability (P) and molar volume MV) only take into account the indices with the strongest correlation, and then build a linear regression model specifically for them. Table 1 shows the physical properties of the drugs. The values of the properties are in °C. The data of the physical properties are taken from ChemSpider, http://www.chemspider.com/. We then compare the results to the actual values to obtain the predicted physicochemical properties. We utilise the following TIs in this work to predict ability.

Table 1. Physical properties of the drugs used for the treatment of tuberculosis

Name of medicine	Boiling point	Flash point	Enthalpy of vaporization	Molar refractivity	Polarizability	Molar volume
Amikacin	981.8	547.6	162.2	134.9	53.5	363.9
Bedaquiline	702.7	378.8	108	156.2	61.9	420.1
Clofazimine	566.9	296.7	85.1	136.2	54	366.1
Delamanid	653.7	349.1	96.3	127.7	50.6	368
Ethambutol	345.3	113.7	68.3	58.6	23.2	207
Ethionamide	247.9	103.7	46.5	49	19.4	142
Imipenemcilastatin	530.2	274.5	92.7	72.7	28.8	183.9
Isoniazid	251.97	251	-	36.9	14.6	110.2
Levofloxacin	571.5	299.4	90.1	91.1	36.1	244
Linezolid	585.5	307.9	87.5	83	32.9	259
Moxifloxacin	636	338.7	98.8	101.8	40.4	285
p-Aminosalicyclic acid	380.8	184.1	66.3	39.3	15.6	102.7
Pyrazinamide	173.3	119.1	54.1	31.9	12.6	87.7
Rifampin	937.4	561.3	153.5	213.1	84.5	611.7
Terizidone	-	-	-	76.1	30.2	198.9

In 2010, Ghorbani and Hosseinzadeh introduced the fourth atom bond connectivity index[11]. In 2011, Grovac et al. introduced the fifth geometric arithmetic index[11]. In 2013, Ghorbani and Hosseinzadeh defined the neighborhood third version of the Zagreb index[12]. In 2017, Kulli[13] introduced the fifth arithmetic geometric index. In 2017 Kulli[14] introduced the fifth hyper-first and second zagreb index. In 2019, Mondal et al.[15] defined the nighborhood second Zagreb index. In 2019, Mondal et al.[15] defined the modified neighborhood forgotten topological index. In 2019, Verma et al.[16] defined the neighborhood second modified Zagreb index. In 2019, Verma and Mondal[16] introduced the neighborhood harmonic index. In 2019, Verma and Mondal[16] defined the neighborhood inverse sum index. Mondal et al.[17] defined the five ND indices namely first NDe index ND_1, second NDe index ND_2, third NDe index ND_3, fourth NDe index ND_4 and fifth NDe index ND_5 in 2021.

2.2 Computational Method

Recently in 2022, Chamua et al.[18] have used a matlab programme to evaluate neighbourhood degree-based TIs. The pseudocode of the program is presented in Figure 2. We used the same M-program to compute more TIs. The TIs of 15 drugs are shown in Tables 2 and 3.

Algorithm 1 Computational Technique

Input: The Graph G
Output: Computation of neighborhood degree sum for each vertex in G.
Intialization: G←the graph, n←no. of vertices, A←adjacency matrix of G.
Store the sum of each column of A in a new matrix S.
loop $i = 1$ *to* n
    $y \leftarrow 0$.
    loop $j = 1$ *to* n
        if $A(i,j) = 1$ **then**
            Store $y + S(1,j)$ *in* y.
        end if
    end loop
    Store y in a variable $y(i)$.
end loop
Retrive neighborhood degree sum for each vertex from $y(i) = 1, \ldots, n$.
Calculate the function $f(u,v)$, where$f$ is any vertex neighborhood degree sum-based TI.

Fig 2. Computational Technique

Table 2. Topological indices of the drugs

Name of medicine	$M_1'(G)$	$M_2^*(G)$	$F_N^*(G)$	$M_2^{nm}(G)$	$NH(G)$	$NI(G)$	$ABC_4(G)$	$GA_5(G)$
Amikacin	494	1472	3138	1.64	7.63	118.59	40.94	1495.45
Bedaquiline	482	1493	3118	1.55	7.55	117.79	40.51	1509.22
Clofazimine	428	1285	2628	1.32	6.74	105.72	36.76	1292.19
Delamanid	482	1399	2856	1.39	7.50	119.15	41.74	1406.19
Ethambutol	112	244	524	0.89	3.19	26.83	12.67	248.42
Ethionamide	110	280	588	0.54	2.31	26.72	10.81	283.46
Imipenemcilastatin	204	550	1158	1.04	4.29	49.66	19.72	557.14
Isoniazid	96	234	496	0.53	2.19	23.24	9.82	237.44
Levofloxacin	360	1152	2412	0.94	4.95	87.60	28.54	1165.26
Linezolid	288	819	1698	1.01	4.93	70.63	25.74	826.40
Moxifloxacin	414	1340	2796	1.08	5.62	100.93	32.50	1354.24
p-Aminosalicyclic acid	116	307	658	0.47	2.17	27.93	10.78	312.41
Pyrazinamide	86	207	436	0.44	1.94	20.94	8.88	209.3
Rifampin	760	2350	499.4	2.22	11.09	182.96	61.57	2385.53
Terizidone	256	680	1408	0.90	4.56	62.84	23.77	685.92

Table 3. Topological indices of the drugs

Name of medicine	$AG_5(G)$	$N_1(G)$	$ND_2(G)$	$ND_3(G)$	$ND_4(G)$	$ND_5(G)$	$HM_1G_5(G)$	$HM_2G_5(G)$
Amikacin	1495.49	241.93	12.53	18836	7.88	93.44	6082	60444
Bedaquiline	1509.22	238.24	12.32	20220	7.65	86.1	6104	71119
Clofazimine	1292.19	212.71	11.09	16324	6.79	75.98	5198	53403
Delamanid	1406.19	239.64	12.51	16752	7.55	86.14	5654	50601
Ethambutol	248.42	54.81	4.52	2300	3.29	28.83	1012	5416
Ethionamide	283.46	54.21	3.54	3036	2.36	23.59	1148	8300
Imipenemcilastatin	557.14	100.63	6.48	6526	4.36	42.33	2258	19956
Isoniazid	237.44	47.23	3.29	2452	2.23	21.52	964	6490
Levofloxacin	1165.26	177.55	8.41	15868	5.05	61.93	4716	55844
Linezolid	826.40	142.61	7.96	9868	4.99	54.23	3336	30205
Moxifloxacin	1354.24	204.37	9.54	18534	5.73	70.26	5476	65178
p-Aminosalicyclic acid	312.41	56.92	3.44	3496	2.22	23.87	1272	9949
Pyrazinamide	209.72	42.44	2.95	2116	1.97	18.98	850	5437
Rifampin	2385.53	372.72	18.55	31700	11.41	138.76	9694	109518
Terizidone	685.92	126.82	7.39	7456	4.61	49.97	2768	20376

3 Results and Discussion

3.1 Analysis

The obtained correlation coefficient of TIs of the drugs with their properties are shown in Table 4. The six physicochemical characteristics of the drugs are strongly correlate with each of the TIs. They may all be used to build a linear regression model to predict the physicochemical properties of the drugs. However, in order to generate our projected property for the linear regression model, we choose the top 3 indices for each property of the drugs based on the highest correlation coefficient of the indices with the drugs. Examining the correlation of the indices with the physical properties of the drugs, we see that $ND_5(G)$ index has the highest correlation(r=0.9249) followed by the indices $ND_4(G)$ with correlation r=0.9215 and $M_2^{nm}(G)$ with correlation r=0.9212 respectively with the boiling point of the drugs. For Flash point of the drugs $ND_5(G)$ index gives the strongest correlation r=0.9123 followed by $M_1^{'}(G)$ index with correlation r=0.9024 and $F_N^*(G)$ index with correlation r=0.9021 respectively. $M_2^{nm}(G)$ has the highest correlation r=0.8963 with the enthalpy of the drugs along with $ND_5(G)$ index with correlation r=0.8821 and $ND_4(G)$ with correlation r=0.8767 respectively as the second and third strongest among the defined indices. For molar refraction $NH(G)$ index has the highest correlation (r=0.9891) followed by $ND_4(G)$ with correlation r=0.9889 and $ND_2(G)$ index with correlation r=0.9872. For polarizability $NH(G)$ gives the strongest correlation(r=0.9891) and $ND_4(G)$ with correlation r=0.9889, $ND_5(G)$ with correlation r=0.9872 being the second and third highest correlated index respectively. Lastly, for molar volume we get $ND_4(G)$ index as the highest correlated index with correlation r=0.9843 and $NH(G)$ being the second highest and $ND_2(G)$ being the third highest with correlation coefficients r=0.9840 and 0.9805 respectively. So we consider $M_2^{nm}(G)$, $M_1^{'}(G)$, $F_N^*(G)$, $NH(G)$, $ND_2(G)$, $ND_4(G)$ and $ND_5(G)$ index to construct the linear regression model to obtain the physical properties of the antituberculosis drugs.

Table 4. Correlation coefficient (C.C.) of topological indices with physicochemical properties

Topological index	C.C. of BP	C.C. of FP	C.C. of EV	C.C. of MR	C.C. of P	C.C. of MV
$M_1^{'}(G)$	0.914	0.902	0.857	0.978	0.978	0.968
$M_2^*(G)$	0.906	0.897	0.847	0.971	0.971	0.959
$F_N^*(G)$	0.910	0.902	0.857	0.971	0.971	0.959
$M_2^{nm}(G)$	0.921	0.889	0.896	0.976	0.976	0.977
$NH(G)$	0.918	0.896	0.870	0.989	0.989	0.984
$NI(G)$	0.911	0.898	0.850	0.978	0.978	0.967
$ABC_4(G)$	0.904	0.888	0.837	0.979	0.979	0.968
$GA_5(G)$	0.914	0.898	0.856	0.984	0.984	0.976
$AG_5(G)$	0.907	0.898	0.850	0.971	0.971	0.959
$ND_1(G)$	0.912	0.900	0.854	0.978	0.978	0.967
$ND_2(G)$	0.918	0.899	0.865	0.987	0.987	0.981
$ND_3(G)$	0.896	0.889	0.839	0.962	0.962	0.985
$ND_4(G)$	0.922	0.900	0.877	0.989	0.989	0.984
$ND_5(G)$	0.925	0.912	0.882	0.983	0.983	0.976
$HM_1G_5(G)$	0.908	0.900	0.852	0.971	0.971	0.959
$HM_2G_5(G)$	0.878	0.873	0.822	0.951	0.951	0.937

3.2 Regression Model

Regression equation for $M_1'(G)$ index
Flash point = $0.6245[M_1'(G)] + 96.989$
Regression equation for $F_N^*(G)$ index
Flash point = $0.0925[F_N^*(G)] + 113$

Regression equation for $M_2^{nm}(G)$ index
Boiling point = $436.55[M_2^{nm}(G)] + 70.979$
Enthalpy = $59.909[M_2^{nm}(G)] + 26.018$

Regression equation for $ND_2(G)$
Molar refraction = $11.251[ND_2(G)] + 0.5089$
Polarizability = $4.4627[ND_2(G)] + 0.176$
Molar volume = $31.119[ND_2(G)] + 5.0386$

Regression equation for $ND_4(G)$ index
Boiling point = $80.495[ND_4(G)] + 118.46$
Enthalpy = $10.817[ND_4(G)] + 33.756$

Molar refraction = $18.931[ND_4(G)] - 4.6442$
Polarizability = $7.5089[ND_4(G)] - 1.8671$
Molar volume = $52.475[ND_4(G)] - 9.8098$

Regression equation for $ND_5(G)$
Boiling point = $6.3752[ND_5(G)] + 164.78$
Flash point = $3.6736[ND_5(G)] + 77.957$
Enthalpy = $0.8571[ND_5(G)] + 39.994$

Regression equation for $NH(G)$
Molar refraction = $19.369[NH(G)] - 5.1169$
Polarizability = $7.6826[NH(G)] - 2.0544$
Molar volume = $53.659[NH(G)] - 10.966$

Fig 3. Regression Model

3.3 Statistical Parameter

In this section we obtain the regression parameters. N is the number of observations, c is constant or Y-intercept, m is slope, r is correlation coefficient, r^2 is coefficient of determination or the percentage of the variance in the dependent variable that a linear model accounts for, SE is standard error and SF is significance F. The standard error of the regression determined the accuracy of the regression coefficient. Significant F is used to examine the reliability of the result. If Significant F is smaller then 0.05, then the model is considered to be significant and if Significant F is greater than 0.05 then the model is insignificant and so can be considered useful. In Tables 5, 6, 7, 8, 9, 10 and 11 we obtained the statistical parameters for linear QSPR model for the obtained top 3 indices for different physical properties.

Table 5. Statistical parameters for the linear QSPR model for $M_1'(G)$

Physical property	*N*	*C*	m	*r*	r^2	*SE*	*SF*	Indicator
Flash point	14	96.989	0.6245	0.9024	0.8143	0.0861	1E-05	Significant

Table 6. Statistical parameters for the linear QSPR model for $F_N^*(G)$

Physical property	*N*	*C*	*m*	*r*	r^2	*SE*	*SF*	Indicator
Flash point	14	113	0.0925	0.9021	0.8137	0.0128	1E-05	Significant

Table 7. Statistical parameters for the linear QSPR model for $M_2^{nm}(G)$

Physical property	*N*	*C*	*m*	*r*	r^2	*SE*	*SF*	Indicator
Boiling point	14	70.979	436.55	0.9212	0.8486	53.2323	3E-06	Significant
Enthalpy	13	26.018	59.909	0.8963	0.8031	8.9391	3.677E-05	Significant

Table 8. Statistical parameters for the linear QSPR model for $ND_2(G)$

Physical property	*N*	*C*	*m*	*r*	r^2	*SE*	*SF*	*Indicator*
Molar refraction	15	0.5089	11.251	0.9872	0.9745	0.5047	9.6227E-12	Significant
Polarizability	15	0.176	4.4627	0.9872	0.9746	0.1997	9.3035E-12	Significant
Molar Volume	15	5.0386	31.119	0.9805	0.9613	1.7307	1.4488E-10	Significant

Table 9. Statistical parameters for the linear QSPR model for $ND_4(G)$

Physical property	N	C	m	r	r^2	SE	SF	Indicator
Boiling point	14	118.46	80.495	0.9215	0.8492	9.7913	2.8412E-06	Significant
Enthalpy	13	33.756	10.817	0.8767	0.7686	1.7895	8.3704E-12	Significant
Molar refraction	15	-4.6442	18.931	0.9889	0.9778	0.7906	3.8781E-12	Significant
Polarizability	15	-1.8671	7.5089	0.9889	0.9779	0.3129	3.7754E-12	Significant
Molar volume	15	-9.8098	52.475	0.9843	0.9688	2.6101	3.5557E-11	Significant

Table 10. Statistical parameters for the linear QSPR model for$ND_5(G)$

Physical property	N	C	m	r	r^2	SE	SF	Indicator
Boiling point	14	164.78	6.3752	0.9249	0.8554	0.7556	2.2023E-06	Significant
Flash point	14	77.957	3.6736	0.9123	0.8323	0.4760	5.4217E-06	Significant
Enthalpy	13	39.994	0.8571	0.8821	0.7781	0.1382	6.6172E-05	Significant

Table 11. Statistical parameters for the linear QSPR model for $NH(G)$

Physical property	N	C	m	r	r^2	SE	SF	Indicator
Molar refractivity	15	-5.1169	19.369	0.9891	0.9783	0.7996	3E-12	Significant
Polarizability	15	-2.0544	7.6826	0.9891	0.9784	0.3165	3.2643E-12	Significant
Molar volume	15	-10.966	53.659	0.9840	0.9682	2.6952	4.0219E-11	Significant

3.4 Computation and Comparison of the Properties of the Drugs

The linear regression model is applied in this part to evaluate the drug properties. We acquire three values for each of the drug properties because we select the three TIs having the strongest connections to those properties. In addition, we contrast the outcomes with the drugs experimented properties. In Tables 12, 13 and 14, we show the comparison of each property of the drugs. Here we take the predicted values obtained from the highest correlated index. In [9] Adnan et al. have studied the physical properties of the antituberculosis drugs using the degree-based TIs. As compared to the results obtained by the degree-based TIs our considered neighborhood degree-based TIs found to have better correlation with the properties of the drugs which leads to a better predictive model. The correlation with the BP is same and the correlation of the FP is only slightly lower. Other than BP and FP other properties have better correlation with neighborhood degree-based TIs. See Figure 8 for the comparison of the correlation obtained by degree-based and neighborhood degree-based TIs.

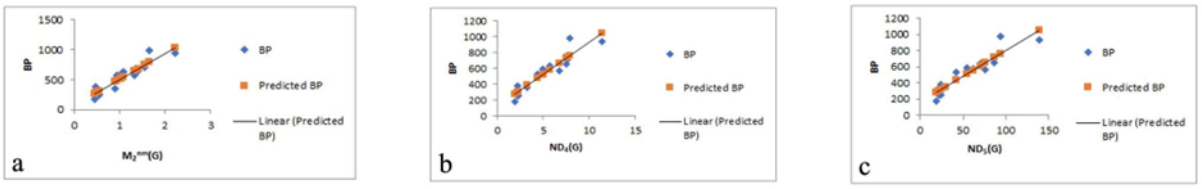

Fig 4. Line fit plot of boiling point and a) $M_2^{nm}(G)$, b) $ND_4(G)$, c) $ND_5(G)$

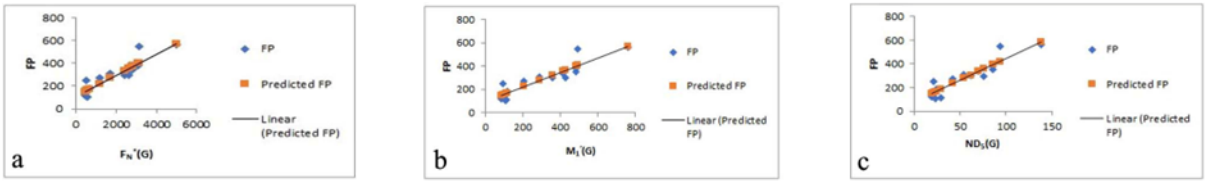

Fig 5. Line fit plot of flash point and a) $F_N^*(G)$, b) $M_1'(G)$, c) $ND_5(G)$

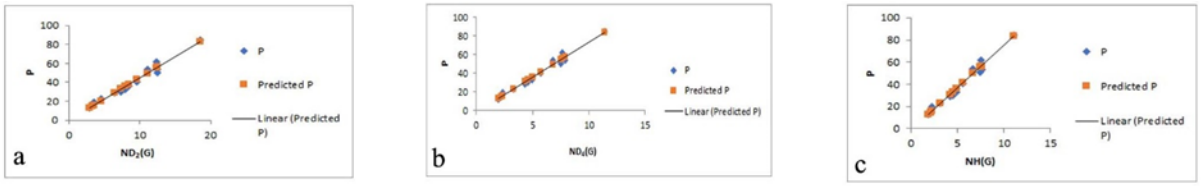

Fig 6. Line fit plot of polarizability and a) $ND_2(G)$, b) $ND_4(G)$, c) $NH(G)$

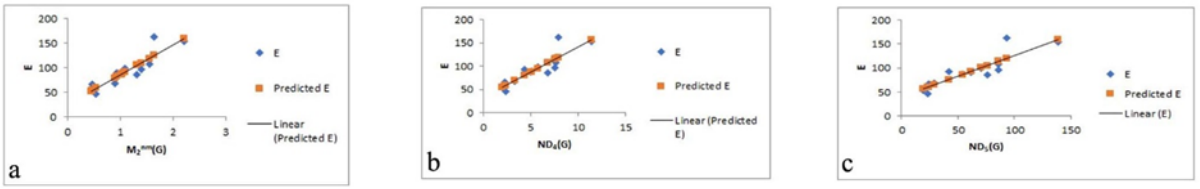

Fig 7. Line fit plot of enthalpy and a) $M_2^{nm}(G)$, b) $ND_4(G)$, c) $ND_5(G)$

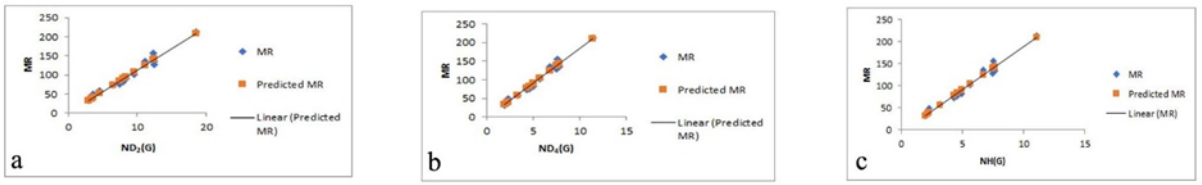

Fig 8. Line fit plot of molar refractivity and a) $ND_2(G)$, b) $ND_4(G)$, c) $NH(G)$

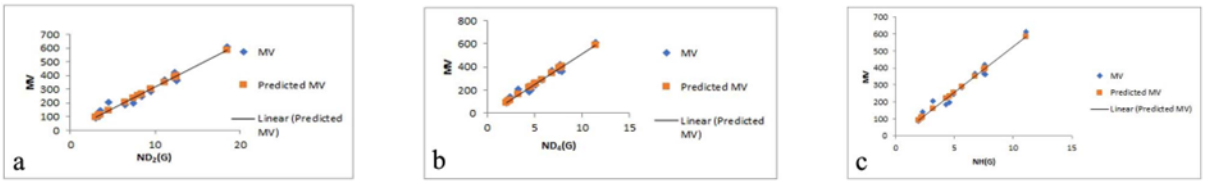

Fig 9. Line fit plot of molar volume and a) $ND_2(G)$, b) $ND_4(G)$, c) $NH(G)$

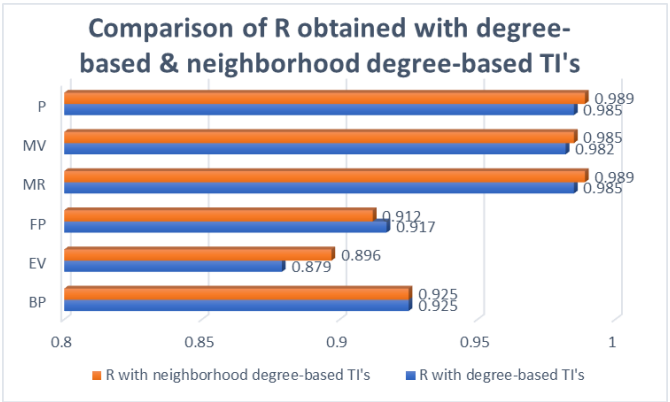

Fig 10. Comparison of the correlations obtained by degree-based and neighborhood degree-based indices

Table 12. Comparison between the obtained values and actual values of the drugs

Name of medicine	BP of drug	BP obtained from $ND_5(G)$	BP obtained from $ND_4(G)$	BP obtained from $M_2^{nm}(G)$	FP of drug	FP obtained from $ND_5(G)$	FP obtained from $M_1'(G)$	FP obtained from $F_N^*(G)$
Amikacin	981.8	760.45	752.76	787.47	547.6	421.2	405.49	403.25
Bedaquiline	702.7	713.7	734.32	748.04	378.8	394.26	397.99	401.4
Clofazimine	566.9	649.15	664.89	645.74	296.7	357.07	364.27	356.08
Delamanid	653.7	713.95	726.12	679.69	349.1	394.41	397.99	377.17
Ethambutol	345.3	348.59	383.54	462.06	113.7	183.88	166.93	161.46
Ethionamide	247.9	315.14	308.66	307.62	103.7	164.6	165.68	167.38
Imipenemcilastatin	530.2	434.66	469.13	526.36	274.5	233.47	224.39	220.11
Isoniazid	251.97	301.96	298.2	301.56	251	157	156.94	158.87
Levofloxacin	571.5	559.58	524.63	479.58	299.4	305.46	321.81	336.1
Linezolid	585.5	510.49	520.02	511.88	307.9	277.17	276.84	270.1
Moxifloxacin	636	612.71	579.39	544.20	338.7	336.07	355.53	371.62
p-Aminosalicyclic acid	380.8	316.93	297.17	275.07	184.1	165.63	169.43	173.86
Pyrazinamide	173.3	285.75	277.09	264.83	119.1	147.67	150.7	153.32
Rifampin	937.4	1049.39	1036.54	1038.39	561.3	587.7	571.6	574.92

Table 13. Comparison between the obtained values and actual values of the drugs

Name of medicine	E of drug	E obtained from $M_2^{nm}(G)$	E obtained from $ND_5(G)$	Eobtained from $ND_4(G)$	MR of drug	MR obtaind from $NH(G)$	MRobtained from $ND_4(G)$	MR obtained from $ND_2(G)$
Amikacin	162.2	124.34	120.08	118.99	134.9	142.69	144.53	141.57
Bedaquiline	108	118.93	113.9	116.52	156.2	148.19	140.2	139.1
Clofazimine	85.1	104.89	105.11	107.19	136.2	125.42	123.87	125.3
Delamanid	96.3	109.55	113.83	115.41	127.7	140.09	138.27	141.24
Ethambutol	68.3	79.68	64.71	69.38	58.6	56.7	57.7	51.38
Ethionamide	46.5	58.49	60.21	59.32	49	39.69	40.09	40.37
Imipenemcilastatin	92.7	88.51	76.28	80.88	72.7	78.02	77.83	73.37
Isoniazid	-	-	-	-	36.9	37.25	37.63	37.48
Levofloxacin	90.1	82.09	93.07	88.34	91.1	90.78	90.88	95.14
Linezolid	87.5	86.52	86.47	87.72	83	90.45	89.8	90.04
Moxifloxacin	98.8	90.96	100.22	95.7	101.8	103.73	103.76	107.88
p-Aminosalicyclic acid	66.3	54.03	60.45	57.77	39.3	36.94	37.38	39.2
Pyrazinamide	54.1	52.62	56.26	55.07	31.9	32.55	32.66	33.66
Rifampin	153.5	158.78	158.93	157.13	213.1	209.76	211.27	209.21
Terizidone	-	-	-	-	76.1	83.25	82.65	83.61

Table 14. Comparison between the obtained values and actual values of the drugs

Name of medicine	P of drug	P obtained from $NH(G)$	P obtained from $ND_4(G)$	P obtained from $ND_2(G)$	MV of drug	MV obtained from $ND_4(G)$	MV obtained from $NH(G)$	MV obtained from $ND_2(G)$
Amikacin	53.5	56.57	57.3	56.12	363.9	403.69	398.51	395.1
Bedaquiline	61.9	55.98	55.58	55.15	420.1	391.67	394.3	388.73
Clofazimine	54	49.72	49.11	49.68	366.1	346.41	350.68	350.2
Delamanid	50.6	55.54	54.82	56	368	386.33	391.3	394.28
Ethambutol	23.2	22.46	22.86	20.35	207	162.99	160.28	145.73
Ethionamide	19.4	15.72	15.86	15.99	142	114.18	113.17	115.3
Imipenemcilastatin	28.8	30.92	30.84	29.08	183.9	218.79	219.36	206.56
Isoniazid	14.6	14.75	14.9	14.84	110.2	107.37	106.4	107.3
Levofloxacin	36.1	35.98	36.02	37.71	244	254.97	254.7	266.77
Linezolid	32.9	35.85	35.59	35.69	259	251.97	253.79	252.66
Moxifloxacin	40.4	41.12	41.13	42.76	285	290.67	290.58	301.98
p-Aminosalicyclic acid	15.6	14.63	14.8	15.52	102.7	106.69	105.54	112.04
Pyrazinamide	12.6	12.88	12.93	13.33	87.7	93.6	93.37	96.74
Rifampin	84.5	83.16	83.77	82.96	611.7	588.69	584.33	582.27
Terizidone	30.2	33	32.76	33.14	198.9	232.16	233.84	234.89

4 Conclusion

In this work we have considered 15 antituberculosis drugs and 16 neighborhood degree-based TIs for the analyses. Since there are over 3000 TIs, so one must find the TI that describe very well about the properties of a chemical compound. Earlier the properties of antituberculosis drugs have been predicted using degree-based TIs from their chemical structures, however our considered indices have given a better result compared to that existing in the literature. We take 8 physical properties of the drugs for the study: boiling point, melting point, flash point, enthalpy of vaporization, molar refractivity, polarizability, surface tension and molar volume. However, only 6 of them are found to be significantly associated, and for melting point and surface tension none of the considered indices were found to have good correlation (i.e., $r < 0.6$) to model the linear regression. So, in our study, we drop these two properties. For all the aforementioned drugs, we first evaluate the 16 TIs and compute their correlations. They may all be taken into account for the regression models because they are all highly correlated. We have chosen 3 indices with the highest correlation for each of the properties separately and construct the regression models for them. Also, we have computed the values and compared the computed values with the known properties of the drugs. This study shows that a theoretical analysis might aid chemists and other pharmaceutical industry personnel in predicting the characteristics of new drugs. Future research might look for TIs that correlate well with the physical properties like melting point and surface tension. These neighborhood degree-based indices can take into consideration for creating a predictive model for the properties of different chemical structures. This TIs will help the chemist to design new medications. Additionally, it is of low cost and time effective. It can be challenging to decide which TIs need to be taken into account for a chemical graph due to the number of TIs in the literature of chemical graph theory. As a result, it is still difficult for researchers to select an appropriate TI that can be used to predict properties of chemical compounds because it would take a lot of time to examine it for such a vast number of TIs. We may broadly divide the CC (Carbon Carbon) bonds in chemical compounds into two categories viz. internal CC bonds and terminal or external CC bonds. These categories won't play equal role in essence of a chemical property. It is observed that it is mostly the external CC bonds which have greater contributions, but there are some exceptions. For example, in [19] 3-methylheptane and 4-methylheptane there is a terminal CC bond that has smaller weight than an internal CC bond. Knowing the desirable qualities of a descriptor, such as giving larger weights to terminal bonds rather than to interior bonds, is helpful in the construction of novel molecular descriptors. So, finding the explanation for better correlation or poor performance of a TI in case of a chemical property, is always an interesting but challenging task.

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