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Research Article

Degree-Based Topological Indices and QSPR Analysis of Antituberculosis Drugs

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A topological index of graph G is a numerical quantity which describes its topology. If it is applied to molecular structure of a chemical compounds, then it reflects the theoretical properties of the chemical compounds. In this paper, well-known degree-based topological indices are applied on chemical structures of antituberculosis drugs. Chemical structure is considered as graph, where elements are taken as vertices and bounds between them are taken as edges. Furthermore, QSPR analysis of the said topological indices are discussed, and it is shown that these topological indices are highly correlated with the physical properties of antituberculosis drugs. This theocratical analysis may help the chemist and people working in pharmaceutical industry to predict properties of antituberculosis drugs without experimenting.

1. Introduction

Before discovery/invention of antibiotics, lives of humans and animals were on great threat of being infected by some bacteria. In previous century, different bacterial infections were the most common causes of death until Alexander Flemings discovered Penicillin in 1929, the first antibiotic which was introduced to the world in 1940.

Tuberculosis (TB) is a contagious infection caused by bacteria "*Mycobacterium tuberculosis*" that usually attacks lungs. It can also spread to other parts of body, like brain and spine.

A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds between atoms. *Cheminformatics* is a new subject which is a combination of chemistry, mathematics, and information science. It studies quantitative structure-activity (QSAR) and structure-property (QSPR) relationships that are used to predict the biological activities and properties of different chemical compounds. The molecular topological indices or simply the topological indices are used in chemistry. Wiener was the first who first showed that the Wiener index number is closely correlated with the boiling points of alkane molecules [18]. Later, work on quantitative structure-activity relationships showed that it is also correlated with other quantities including the parameters of its critical point [16], density, surface tension, viscosity of its liquid phase [14], and the van der Waals surface area of the molecule [10]. In the QSAR/QSPR study, physico-chemical properties and topological indices are used to predict bioactivity of the chemical compounds. In this work, it is shown that no single topological index exists that correlates with all the physical properties of chemical compounds.

A graph $G(V, E)$ with vertex set $V(G)$ and edge set $E(G)$ is connected if there exists a connection between any pair of vertices in G. The distance between two vertices u and v is denoted as $d(u, v) = d_G(u, v)$ and is defined as the length of shortest path between u and v in graph G. The number of vertices of G adjacent to a given vertex v is the "degree" of this vertex and will be denoted by $d_v(G)$ or if misunderstanding is not possible simply by d_v. The concept of degree is somewhat closely related to the concept of valence in chemistry.

Some of the degree-based topological indices which we use in this work are defined as follows.

Definition 1. *ABC* index is proposed by Estrada et al. in [7], as

$$ABC(G) = \sum_{e=uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}. \quad (1)$$

Definition 2. The Randić index is proposed by Milan Randić in [13], as

$$R(G) = \sum_{e=uv\in E(G)} \sqrt{\frac{1}{d_u d_v}}. \quad (2)$$

Definition 3. The sum connectivity index is proposed by Zhou and Trinjstic in [19], as

$$S(G) = \sum_{e=uv\in E(G)} \sqrt{\frac{1}{d_u + d_v}}. \quad (3)$$

Definition 4. The *GA* index is proposed by Vukicevic et al. in [17], as

$$GA(G) = \sum_{e=uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}. \quad (4)$$

Definition 5. The first and second Zagreb indices are proposed by Gutman and Trinajestic in [11], as

$$M_1(G) = \sum_{e=uv\in E(G)} (d_u + d_v),$$
$$M_2(G) = \sum_{e=uv\in E(G)} (d_u d_v). \quad (5)$$

Definition 6. The Harmonic index is proposed by Fajtlowicz et al. in [9], as

$$H(G) = \sum_{e=uv\in E(G)} \frac{2}{d_u + d_v}. \quad (6)$$

Definition 7. The hyper-Zagreb index is proposed by Shirdel et al. in [15], as

$$HM(G) = \sum_{e=uv\in E(G)} (d_u + d_v)^2. \quad (7)$$

Definition 8. The third Zagreb index is proposed by Fath-Tabar et al. in [1], as

$$ZG_3(G) = \sum_{e=uv\in E(G)} |d_u - d_v|. \quad (8)$$

Definition 9. The forgotten index is proposed by Furtula et al. in [8], as

$$F(G) = \sum_{e=uv\in E(G)} \left[(d_u)^2 + (d_v)^2\right]. \quad (9)$$

Definition 10. The symmetric division index is proposed in [2], as

$$SS\ D(G) = \sum_{e=uv\in E(G)} \left[\frac{P}{Q} + \frac{Q}{P}\right], \quad (10)$$

where $P = \min[d_u, d_v]$ and. $Q = \max[d_u, d_v]$.

Some of the work in this area can be seen in [3–6, 12].

2. Results and Discussion

The above defined 11 topological indices are used for the modeling of six physical properties: boiling point (BP), enthalpy of vaporization (E), flash point (F), molar refractivity (MR), molar volume (MV), and polarizability (P) of 15 antituberculosis drugs: amikacin, bedaquiline, clofazimine, delamanid, ethambutol, ethionamide, imipenem-cilastatin, isoniazid, levofloxacin, linezolid, moxifloxacin, p-aminosalicylic acid, pyrazinamide, rifampin, and terizidone.

2.1. Regression Models. The following equation is used to correlate the various physical properties of various drugs used for the treatment of tuberculosis with some topological indices. We have used the following linear regression model:

$$P = A + b[TI], \quad (11)$$

where P is physical property of drug, A is constant, b is regression coefficient, and TI is topological index. Constant A and regression coefficient b is calculated from SPSS software for seven physical properties and eleven degree-based topological indices of molecular structure of fourteen drugs. Using equation (11), following are the linear regression model for the defined degree-based topological indices:

(1) Regression models for atom bond connectivity index: $ABC(G)$

Boiling point = $142.94 + 19.699[ABC(G)]$

Enthalpy = $38.04 + 2.605[ABC(G)]$

Flash point = $67.648 + 11.254[ABC(G)]$

Molar refraction = $1.797 + 4.588[ABC(G)]$

Molar volume = $8.698 + 12.686[ABC(G)]$

Polarizability = $0.685 + 1.82[ABC(G)]$

(2) Regression models for Randić index: $R(G)$

Boiling point = $124.752 + 33.178[R(G)]$

Enthalpy = $35.127 + 4.424[R(G)]$

Flash point = $59.012 + 18.814[R(G)]$

Molar refraction = $-2.76 + 7.757[R(G)]$

Molar volume = $-5.066 + 21.541[R(G)]$

Polarizability = $-1.122 + 3.077[R(G)]$

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

Name of medicine	Boiling point	Melting point	Flash point	Enthalpy of vaporization	Molar refractivity	Polarizability	Surface tension	Molar volume
Amikacin	981.8	203.5	547.6	162.2	134.9	53.5	103.3	363.9
Bedaquiline	702.7	176	378.8	108	156.2	61.9	52.6	420.1
Clofazimine	566.9	210	296.7	85.1	136.2	54	47.1	366.1
Delamanid	653.7	193	349.1	96.3	127.7	50.6	50	368
Ethambutol	345.3	89	113.7	68.3	58.6	23.2	38.1	207
Ethionamide	247.9	163	103.7	46.5	49	19.4	39.8	142
Imipenem-cilastatin	530.2		274.5	92.7	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	90.1	91.1	36.1	70.3	244
Linezolid	585.5	177	307.9	87.5	83	32.9	47.7	259
Moxifloxacin	636	270	338.7	98.8	101.8	40.4	60.6	285
p-Aminosalicylic aci	380.8	145	184.1	66.3	39.3	15.6	83.4	102.7
Pyrazinamide	173.3	190	119.1	54.1	31.9	12.6	60.7	87.7
Rifampin	937.4	183	561.3	153.5	213.1	84.5	48	611.7
Terizidone		175			76.1	30.2	62.5	198.9

Physical properties are taken from ChemSpider.

(3) . Regression models for sum-connectivity index. $S(G)$

Boiling point = $133.839 + 31.497[S(G)]$

Enthalpy = $36.755 + 4.169[S(G)]$

Flash point = $63.724 + 17.895[S(G)]$

Molar refraction = $-0.81 + 7.373[S(G)]$

Molar volume = $1.064 + 20.419[S(G)]$

Polarizability = $-0.348 + 2.925[S(G)]$

(4) Regression models for geometric-arithmetic index ($GA(G)$)

Boiling point = $197.225 + 14.102[GA(G)]$

Enthalpy = $45.041 + 1.89[GA(G)]$

Flash point = $97.24 + 8.114[GA(G)]$

Molar refraction = $21.849 + 3.067[GA(G)]$

Molar volume = $60.81 + 8.621[GA(G)]$

Polarizability = $8.648 + 1.216[GA(G)]$

(5) Regression models for first Zagreb index: $M_1(G)$

Boiling point = $159.511 + 2.802[M_1(G)]$

Enthalpy = $40.359 + 0.37[M_1(G)]$

Flash point = $75.639 + 1.611[M_1(G)]$

Molar refraction = $4.118 + 0.664[M_1(G)]$

Molar volume = $15.714 + 1.3[M_1(G)]$

Polarizability = $1.606 + 0.264[M_1(G)]$

(6) Regression models for second Zagreb index: $M_2(G)$

Boiling point = $176.377 + 2.294[M_2(G)]$

Enthalpy = $42.366 + 0.304[M_2(G)]$

Flash point = $85.303 + 1.32[M_2(G)]$

Molar refraction = $11.967 + 0.52[M_2(G)]$

Molar volume = $37.688 + 1.431[M_2(G)]$

Polarizability = $4.716 + 0.206[M_2(G)]$

(7) Regression models for harmonic index: $H(G)$

Boiling point = $124.25 + 34.754[H(G)]$

Enthalpy = $35.279 + 4.616[H(G)]$

Flash point = $59.249 + 19.664[H(G)]$

Molar refraction = $-3.359 + 8.161[H(G)]$

Molar volume = $-6.627 + 22.655[H(G)]$

Polarizability = $-1.359 + 3.237[H(G)]$

(8) Regression models for hyper-Zagreb index: $HM(G)$

Boiling point = $175.29 + 0.538[HM(G)]$

Enthalpy = $42.25 + 0.071[HM(G)]$

Flash point = $84.694 + 0.31[HM(G)]$

Molar refraction = $10.754 + 0.123[HM(G)]$

Molar volume = $34.659 + 0.34[HM(G)]$

Polarizability = $4.237 + 0.049[HM(G)]$

(9) Regression models for third Zagreb index: $ZG_3(G)$.

Boiling point = $188.731 + 14.187[ZG_3(G)]$

Enthalpy = $45.595 + 1.819[ZG_3(G)]$

Flash point = $96.444 + 7.998[ZG_3(G)]$

Molar refraction = $18.618 + 3.077[ZG_3(G)]$

Molar volume = $49.304 + 8.748[ZG_3(G)]$

Polarizability = $7.358 + 1.221[ZG_3(G)]$

(10) Regression models for forgotten index: $F(G)$

Boiling point = $174.862 + 1.017[F(G)]$

Enthalpy = $42.93 + 0.134[F(G)]$

Flash point = $81.722 + 0.593[F(G)]$

Molar refraction = $10.095 + 0.235[F(G)]$

Molar volume = $32.425 + 0.648[F(G)]$

Table 2: Various drugs and topological indices values.

Name of medicine	ABC(G)	R(G)	S(G)	GA(G)	M1(G)	M2(G)	H(G)	HM(G)	ZG3(G)	F(G)	SSD(G)
Amikacin	30.266	18.85	19.24	40.18	191	247	17.83	1046	38	542	101.33
Bedaquiline	28.46	17.61	18.41	38.95	190	197	17.08	959	29	501	90
Clofazimine	27.06	16.68	17.47	18.97	186	216	16.16	901	29	469	85.16
Delamanid	30.38	18.29	19.15	40.43	204	234	17.53	1004	42	536	99.41
Ethambutol	10.6	8.19	7.64	14.53	60	60	7.9	252	12	132	34
Ethionamide	7.95	5.23	5.22	10.57	50	54	5	234	10	124	26
Imipenem-cilastatin	15.88	9.87	10.07	21.03	108	130	9.33	550	18	290	53.33
Isoniazid	8.02	5.21	5.21	10.55	50	55	4.966	234	8	156	26.33
Levofloxacin	20.75	12.37	13.05	27.99	146	186	11.83	754	22	394	67.66
Linezolid	19.43	11.95	12.4	26.08	130	152	11.46	640	42	336	62.66
Moxifloxacin	24.1	14.4	15.29	16.97	172	215	13.866	894	24	464	77.33
p-Aminosalicylic acid	8.13	5.1	5.1	10.38	52	58	4.76	252	12	136	28
Pyrazinamide	6.54	4.3	4.3	4.84	55	43	4.13	182	6	96	21
Rifampin	44.87	27.32	28.14	59.19	309	374	25.78	1593	55	855	151.5
Terizidone	18.66	11.54	11.99	11.74	124	144	11.13	604	20	316	50.33

Table 3: Correlation coefficients.

Topological index	Correlation coefficients of boiling point	Correlation coefficients of enthalpy	Correlation coefficients of flash point	Correlation coefficients of molar refraction	Correlation coefficients of molar volume	Correlation coefficients of polarizability
ABC(G)	0.921	0.866	0.903	0.980	0.973	0.980
R(G)	0.921	0.872	0.896	0.984	0.981	0.984
S(G)	0.919	0.864	0.897	0.983	0.978	0.984
GA(G)	0.894	0.865	0.883	0.909	0.917	0.908
M1(G)	0.899	0.840	0.887	0.974	0.965	0.974
M2(G)	0.921	0.869	0.910	0.953	0.943	0.954
H(G)	0.918	0.865	0.891	0.985	0.982	0.985
HM(G)	0.925	0.872	0.914	0.971	0.959	0.971
ZG3(G)	0.877	0.796	0.849	0.872	0.890	0.872
F(G)	0.917	0.868	0.917	0.970	0.959	0.970
SSD(G)	0.925	0.879	0.912	0.978	0.974	0.978

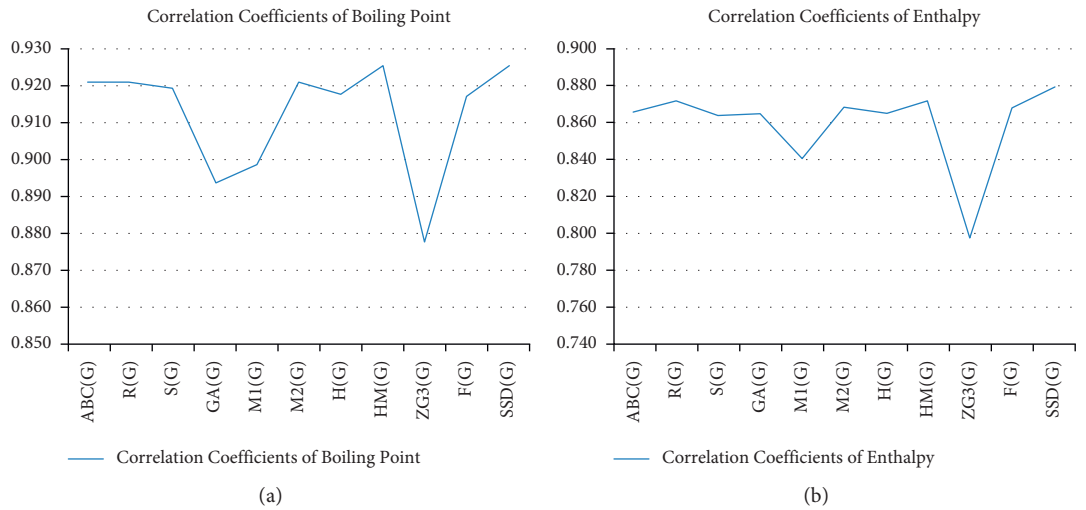

Figure 1: Continued.

Figure 1: Physical properties and topological indices. (a) Boiling Point on TI. (b) Enthalpy on TI. (c) Flash point on TI. (d) Molar Refraction on TI. (e) Molar Volume on TI. (f) Polarizability on TI.

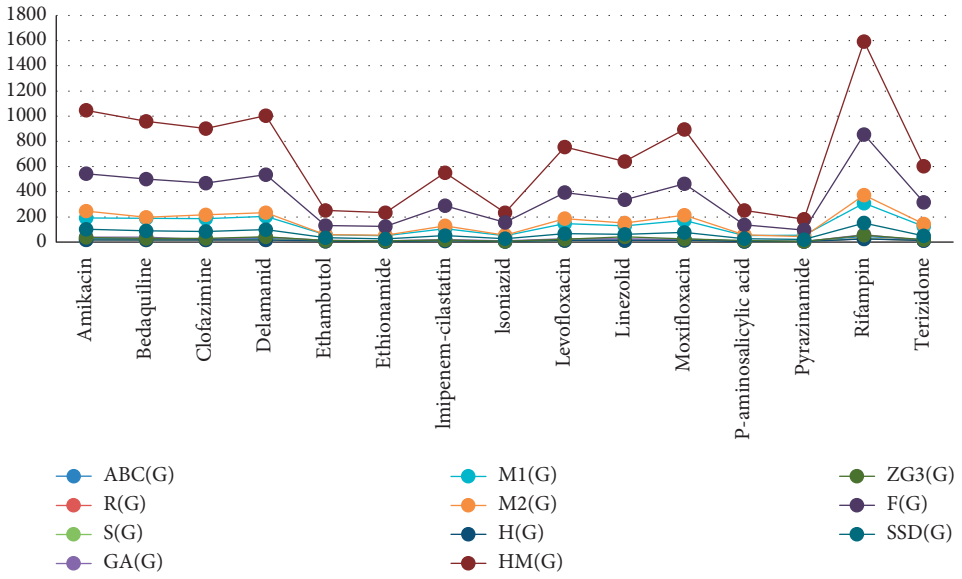

Figure 2: Medicine with topological indices.

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

Physical property	N	A	b	r	$r2$	F	p	Indicator
Boiling point	14	142.940	19.699	0.921	0.848	67.034	≤0.0001	Significant
Enthalpy	13	38.040	2.605	0.866	0.750	33.027	≤0.0001	Significant
Flash point	14	67.648	11.254	0.903	0.816	53.137	≤0.0001	Significant
Molar refraction	14	1.797	4.588	0.980	0.961	320.196	≤0.0001	Significant
Molar volume	15	8.698	12.686	0.973	0.947	233.580	≤0.0001	Significant
Polarizability	15	0.685	1.820	0.980	0.961	322.025	≤0.0001	Significant

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

Physical property	N	A	b	r	$r2$	F	p	Indicator
Boiling point	14	124.752	33.178	0.921	0.848	66.986	≤0.0001	Significant
Enthalpy	13	35.127	4.424	0.872	0.760	34.889	≤0.0001	Significant
Flash point	14	59.012	18.814	0.896	0.804	49.123	≤0.0001	Significant
Molar refraction	14	−2.760	7.757	0.984	0.968	398.969	≤0.0001	Significant
Molar volume	15	−5.066	21.541	0.981	0.963	338.102	≤0.0001	Significant
Polarizability	15	−1.122	3.077	0.984	0.969	401.220	≤0.0001	Significant

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

Physical property	N	A	b	r	$r2$	F	p	Indicator
Boiling point	14	133.839	31.497	0.919	0.845	65.492	≤0.0001	Significant
Enthalpy	13	36.755	4.169	0.864	0.747	32.410	≤0.0001	Significant
Flash point	14	63.724	17.895	0.897	0.804	49.215	≤0.0001	Significant
Molar refraction	14	−0.810	7.373	0.983	0.967	382.171	≤0.0001	Significant
Molar volume	15	1.064	20.419	0.978	0.956	285.344	≤0.0001	Significant
Polarizability	15	−0.348	2.925	0.984	0.967	384.473	≤0.0001	Significant

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

Physical property	N	A	b	r	$r2$	F	p	Indicator
Boiling point	14	197.225	14.102	0.894	0.799	47.624	≤0.0001	Significant
Enthalpy	13	45.041	1.890	0.865	0.748	32.691	≤0.0001	Significant
Flash point	14	97.240	8.114	0.883	0.779	42.398	≤0.0001	Significant
Molar refraction	14	21.849	3.067	0.909	0.826	61.559	≤0.0001	Significant
Molar volume	15	60.810	8.621	0.917	0.841	68.909	≤0.0001	Significant
Polarizability	15	8.648	1.216	0.908	0.825	61.422	≤0.0001	Significant

Table 8: Statistical parameters for the linear QSPR model for $M_1(G)$.

Physical property	N	A	b	r	$r2$	F	p	Indicator
Boiling point	14	159.511	2.802	0.899	0.808	50.411	≤0.0001	Significant
Enthalpy	13	40.359	0.370	0.840	0.706	26.417	≤0.0001	Significant
Flash point	14	75.639	1.611	0.887	0.787	44.458	≤0.0001	Significant
Molar refraction	14	4.118	0.664	0.974	0.949	241.578	≤0.0001	Significant
Molar volume	15	15.714	1.833	0.965	0.931	175.131	≤0.0001	Significant
Polarizability	15	1.606	0.264	0.974	0.949	242.643	≤0.0001	Significant

Table 9: Statistical parameters for the linear QSPR model for $M_2(G)$.

Physical property	N	A	b	r	$r2$	F	p	Indicator
Boiling point	14	176.377	2.294	0.921	0.848	67.069	≤0.0001	Significant
Enthalpy	13	42.366	0.304	0.869	0.755	33.832	≤0.0001	Significant
Flash point	14	85.303	1.320	0.910	0.827	57.458	≤0.0001	Significant
Molar refraction	14	11.967	0.520	0.953	0.909	130.015	≤0.0001	Significant
Molar volume	15	37.688	1.431	0.943	0.889	104.388	≤0.0001	Significant
Polarizability	15	4.716	0.206	0.954	0.909	130.608	≤0.0001	Significant

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

Physical property	N	A	b	r	$r2$	F	p	Indicator
Boiling point	14	124.250	34.754	0.918	0.842	0.842	≤0.0001	Significant
Enthalpy	13	35.279	4.616	0.865	0.748	32.682	≤0.0001	Significant
Flash point	14	59.249	19.664	0.891	0.795	46.457	≤0.0001	Significant
Molar refraction	14	−3.359	8.161	0.985	0.970	422.174	≤0.0001	Significant
Molar volume	15	−6.627	22.655	0.982	0.964	347.348	≤0.0001	Significant
Polarizability	15	−1.359	3.237	0.985	0.970	424.568	≤0.0001	Significant

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

Physical property	N	A	b	r	$r2$	F	p	Indicator
Boiling point	14	175.290	0.538	0.925	0.857	71.653	≤0.0001	Significant
Enthalpy	13	42.250	0.071	0.872	0.761	34.961	≤0.0001	Significant
Flash point	14	84.694	0.310	0.914	0.835	60.823	≤0.0001	Significant
Molar refraction	14	10.754	0.123	0.971	0.943	213.272	≤0.0001	Significant
Molar volume	15	34.659	0.340	0.959	0.919	148.407	≤0.0001	Significant
Polarizability	15	4.237	0.049	0.971	0.943	214.463	≤0.0001	Significant

Table 12: Statistical parameters for the linear QSPR model for $ZG_3(G)$.

Physical property	N	A	b	r	$r2$	F	p	Indicator
Boiling point	14	188.731	14.187	0.877	0.770	40.068	≤0.0001	Significant
Enthalpy	13	45.595	1.819	0.796	0.634	19.044	≤0.0012	Significant
Flash point	14	96.444	7.998	0.849	0.721	30.987	≤0.0001	Significant
Molar refraction	14	18.618	3.077	0.872	0.761	41.284	≤0.0001	Significant
Molar volume	15	49.304	8.748	0.890	0.793	49.736	≤0.0001	Significant
Polarizability	15	7.358	1.221	0.872	0.761	41.320	≤0.0001	Significant

Table 13: Statistical parameters for the linear QSPR model for $F(G)$.

Physical property	N	A	b	r	$r2$	F	p	Indicator
Boiling point	14	174.862	1.017	0.917	0.841	63.583	≤0.0001	Significant
Enthalpy	13	42.930	0.134	0.868	0.753	33.540	≤0.0001	Significant
Flash point	14	81.722	0.593	0.917	0.842	63.799	≤0.0001	Significant
Molar refraction	14	10.095	0.235	0.970	0.940	204.155	≤0.0001	Significant
Molar volume	15	32.425	0.648	0.959	0.920	150.473	≤0.0001	Significant
Polarizability	15	3.976	0.093	0.970	0.940	205.151	≤0.0001	Significant

Table 14: Standard error of estimate.

Topological index	Std. error of the estimate for boiling point	Std. error of the estimate for enthalpy	Std. error of the estimate for molar refraction	Std. error of the estimate for flash point	Std. error of the estimate for molar volume	Std. error of the estimate for polarizability
ABC(G)	98.80842	17.71587	10.53701	63.40101	34.10937	4.16784
R(G)	98.83840	17.35274	9.47621	65.44951	28.58485	3.74830
S(G)	99.78636	17.84127	9.67553	65.40054	31.00944	3.82645
GA(G)	113.75977	17.78385	22.27504	69.37762	59.18170	8.84300
M1(G)	111.19073	19.21715	12.05471	68.10000	39.05016	4.77125
M2(G)	98.78608	17.55617	16.08332	61.39726	49.43571	6.36590
H(G)	100.68522	17.78575	9.22010	66.92575	28.21576	3.64692
HM(G)	96.04169	17.33909	12.78650	59.96174	42.15912	5.05818
ZG3(G)	121.73452	21.44588	26.10552	78.04393	67.62305	10.35071
F(G)	76.32456	11.75776	17.41567	93.39236	73.68525	6.90532
SSD(G)	96.18479	16.88420	11.19841	60.73508	33.75294	4.43398

Table 15: Comparison of actual and computed values for boiling point from regression models.

Name of drug	Boiling point of drug	Boiling point computed from regression model for ABC index	Boiling point computed from regression model for R(G) index	Boiling point computed from regression model for S(G) index	Boiling point computed from regression model for GA(G) index	Boiling point computed from regression model for M1(G) index	Boiling point computed from regression model for M2(G) index	Boiling point computed from regression model H(G) index	Boiling point computed from regression of HM(G) index	Boiling point computed from regression model for ZG3(G) index	Boiling point computed from regression model of F(G) index	Boiling point computed from regression model of SSD(G) index
Amikacin	981.8	739.16	750.16	739.84	763.82	694.65	743.07	743.91	738.32	727.82	726.12	751.10
Bedaquiline	702.7	703.58	709.02	713.70	746.48	691.85	628.36	717.84	691.49	600.14	684.42	683.56
Clofazimine	566.9	676.00	678.16	684.09	464.73	680.64	671.95	685.87	660.27	600.14	651.87	654.70
Delamanid	653.7	741.41	731.58	737.01	767.35	731.08	713.25	733.48	715.72	784.57	720.01	739.65
Ethambutol	345.3	351.75	396.48	374.48	402.12	327.62	314.04	398.80	310.94	358.97	309.12	349.71
Ethionamide	247.9	299.55	298.27	298.25	346.28	299.60	300.27	298.02	301.25	330.60	300.98	302.02
Imipenem-cilastatin	530.2	455.77	452.22	451.02	493.78	462.10	474.64	448.50	471.34	444.09	469.81	464.95
Isoniazid	251.97	300.93	297.61	297.94	346.00	299.60	302.56	296.84	301.25	302.22	333.53	303.98
Levofloxacin	571.5	551.70	535.16	544.88	591.93	568.57	603.12	535.39	581.15	500.84	575.59	550.37
Linezolid	585.5	525.70	521.23	524.40	564.99	523.74	525.11	522.53	519.79	784.57	516.60	520.57
Moxifloxacin	636	617.69	602.52	615.43	436.53	641.42	669.66	606.14	656.51	529.21	646.78	608.02
p-Aminosalicylic acid	380.8	303.10	293.96	294.47	343.60	305.20	309.45	289.68	310.94	358.97	313.18	313.94
Pyrazinamide	173.3	271.77	267.42	269.28	265.48	313.61	275.03	267.78	273.26	273.85	272.50	272.21

Table 16: Comparison of actual values computed values for enthalpy from regression models.

Name of drug	Boiling point of drug	Boiling point computed from regression model for ABC index	Boiling point computed from regression model for R(G) index	Boiling point computed from regression model for S(G) index	Boiling point computed from regression model for GA(G) index	Boiling point computed from regression model for M1(G) index	Boiling point computed from regression model for M2(G) index	Boiling point computed from regression model H(G) index	Boiling point computed from regression of HM(G) index	Boiling point computed from regression model for ZG3(G) index	Boiling point computed from regression model of F(G) index	Boiling point computed from regression model of SSD(G) index
Amikacin	981.8	739.16	750.16	739.84	763.82	694.65	743.07	743.91	738.32	727.82	726.12	751.10
Bedaquiline	702.7	703.58	709.02	713.70	746.48	691.85	628.36	717.84	691.49	600.14	684.42	683.56
Clofazimine	566.9	676.00	678.16	684.09	464.73	680.64	671.95	685.87	660.27	600.14	651.87	654.70
Delamanid	653.7	741.41	731.58	737.01	767.35	731.08	713.25	733.48	715.72	784.57	720.01	739.65
Ethambutol	345.3	351.75	396.48	374.48	402.12	327.62	314.04	398.80	310.94	358.97	309.12	349.71
Ethionamide	247.9	299.55	298.27	298.25	346.28	299.60	300.27	298.02	301.25	330.60	300.98	302.02
Imipenem-cilastatin	530.2	455.77	452.22	451.02	493.78	462.10	474.64	448.50	471.34	444.09	469.81	464.95
Isoniazid	251.97	300.93	297.61	297.94	346.00	299.60	302.56	296.84	301.25	302.22	333.53	303.98
Levofloxacin	571.5	551.70	535.16	544.88	591.93	568.57	603.12	535.39	581.15	500.84	575.59	550.37
Linezolid	585.5	525.70	521.23	524.40	564.99	523.74	525.11	522.53	519.79	784.57	516.60	520.57
Moxifloxacin	636	617.69	602.52	615.43	436.53	641.42	669.66	606.14	656.51	529.21	646.78	608.02
p-Aminosalicylic acid	380.8	303.10	293.96	294.47	343.60	305.20	309.45	289.68	310.94	358.97	313.18	313.94
Pyrazinamide	173.3	271.77	267.42	269.28	265.48	313.61	275.03	267.78	273.26	273.85	272.50	272.21

Table 17: Comparison of actual values computed values for Flash point from regression models.

Name of drug	Boiling point of drug	Boiling point computed from regression model for ABC index	Boiling point computed from regression model for R(G) index	Boiling point computed from regression model for S(G) index	Boiling point computed from regression model for GA(G) index	Boiling point computed from regression model for M1(G) index	Boiling point computed from regression model for M2(G) index	Boiling point computed from regression model H(G) index	Boiling point computed from regression of HM(G) index	Boiling point computed from regression model for ZG3(G) index	Boiling point computed from regression model of F(G) index	Boiling point computed from regression model of SSD(G) index
Amikacin	981.8	739.16	750.16	739.84	763.82	694.65	743.07	743.91	738.32	727.82	726.12	751.10
Bedaquiline	702.7	703.58	709.02	713.70	746.48	691.85	628.36	717.84	691.49	600.14	684.42	683.56
Clofazimine	566.9	676.00	678.16	684.09	464.73	680.64	671.95	685.87	660.27	600.14	651.87	654.70
Delamanid	653.7	741.41	731.58	737.01	767.35	731.08	713.25	733.48	715.72	784.57	720.01	739.65
Ethambutol	345.3	351.75	396.48	374.48	402.12	327.62	314.04	398.80	310.94	358.97	309.12	349.71
Ethionamide	247.9	299.55	298.27	298.25	346.28	299.60	300.27	298.02	301.25	330.60	300.98	302.02
Imipenem-cilastatin	530.2	455.77	452.22	451.02	493.78	462.10	474.64	448.50	471.34	444.09	469.81	464.95
Isoniazid	251.97	300.93	297.61	297.94	346.00	299.60	302.56	296.84	301.25	302.22	333.53	303.98
Levofloxacin	571.5	551.70	535.16	544.88	591.93	568.57	603.12	535.39	581.15	500.84	575.59	550.37
Linezolid	585.5	525.70	521.23	524.40	564.99	523.74	525.11	522.53	519.79	784.57	516.60	520.57
Moxifloxacin	636	617.69	602.52	615.43	436.53	641.42	669.66	606.14	656.51	529.21	646.78	608.02
p-Aminosalicylic acid	380.8	303.10	293.96	294.47	343.60	305.20	309.45	289.68	310.94	358.97	313.18	313.94
Pyrazinamide	173.3	271.77	267.42	269.28	265.48	313.61	275.03	267.78	273.26	273.85	272.50	272.21

Table 18: Comparison of actual values computed values for molar refraction from regression models.

Name of drug	Molar refraction of drug	Molar refraction computed from regression model for ABC index	Molar refraction computed from regression model for R(G) index	Molar refraction computed from regression model for S(G) index	Molar refraction computed from regression model for GA(G) index	Molar refraction computed from regression model for M1(G) index	Molar refraction computed from regression model for M2(G) index	Molar refraction computed from regression model H(G) index	Molar refraction computed from regression of HM(G) index	Molar refraction computed from regression model for ZG3(G)	Molar refraction computed from regression model of F(G) index	Molar refraction computed from regression model of SSD(G)
Amikacin	134.9	140.67	143.46	141.05	145.08	131.02	140.32	142.16	139.93	135.54	137.52	143.79
Bedaquiline	156.2	132.38	133.84	134.93	141.30	130.35	114.34	136.04	129.19	107.85	127.88	128.26
Clofazimine	136.2	125.96	126.63	128.00	80.03	127.70	124.21	128.53	122.02	107.85	120.36	121.63
Delamanid	127.7	141.19	139.12	140.38	145.84	139.65	133.57	139.71	134.74	147.85	136.11	141.16
Ethambutol	58.6	50.43	60.77	55.52	66.41	43.98	43.15	61.12	41.87	55.54	41.13	51.49
Ethionamide	49	38.27	37.81	37.68	54.27	37.34	40.03	37.45	39.65	49.39	39.25	40.52
Imipenem-cilastatin	72.7	74.66	73.80	73.44	86.35	75.87	79.52	72.79	78.68	74.00	78.27	77.99
Isoniazid	36.9	38.60	37.65	37.60	54.20	37.34	40.55	37.17	39.65	43.23	46.77	40.97
Levofloxacin	91.1	97.01	93.20	95.41	107.69	101.12	108.62	93.19	103.87	86.31	102.72	97.63
Linezolid	83	90.95	89.94	90.62	101.83	90.49	90.96	90.17	89.79	147.85	89.09	90.78
Moxifloxacin	101.8	112.38	108.94	111.92	73.89	118.39	123.69	109.81	121.16	92.46	119.18	110.89
p-Aminosalicylic acid	39.3	39.10	36.80	36.79	53.68	38.67	42.11	35.49	41.87	55.54	42.07	43.26
Pyrazinamide	31.9	31.80	30.60	30.89	36.69	40.66	34.31	30.35	33.23	37.08	32.66	33.67
Rifampin	213.1	207.68	209.17	206.67	203.38	209.42	206.32	207.04	207.48	187.85	211.10	212.57

Table 19: Comparison of actual values computed values for molar volume from regression models.

Name of drug	Molar volume of drug	Molar volume computed from regression model for ABC index	Molar volume computed from regression model for R(G) index	Molar volume computed from regression model for S(G) index	Molar volume computed from regression model for GA(G) index	Molar volume computed from regression model for M1(G) index	Molar volume computed from regression model for M2(G) index	Molar volume computed from regression model H(G) index	Molar volume computed from regression of HM(G) Index	Molar volume computed from regression model for ZG3(G)	Molar volume computed from regression model of F(G) index	Molar volume computed from regression model of SSD(G)
Amikacin	363.9	392.65	400.98	393.92	407.20	365.72	391.20	397.31	389.95	381.74	383.54	401.74
Bedaquiline	420.1	369.74	374.27	376.97	396.60	363.89	319.64	380.32	360.40	303.01	356.98	358.65
Clofazimine	366.1	351.98	354.23	357.78	224.35	356.56	346.84	359.48	340.70	303.01	336.25	340.25
Delamanid	368	394.10	388.92	392.08	409.36	389.54	372.60	390.51	375.69	416.73	379.65	394.44
Ethambutol	207	143.17	171.35	157.06	186.07	125.66	123.56	172.35	120.26	154.28	117.94	145.71
Ethionamide	142	109.55	107.59	107.65	151.93	107.34	114.97	106.65	114.14	136.79	112.75	115.29
Imipenem-cilastatin	183.9	210.15	207.54	206.68	242.11	213.62	223.75	204.74	221.48	206.77	220.29	219.21
Isoniazid	110.2	110.44	107.16	107.44	151.76	107.34	116.41	105.88	114.14	119.29	133.48	116.54
Levofloxacin	244	271.93	261.39	267.53	302.11	283.26	303.90	261.38	290.77	241.77	287.66	273.70
Linezolid	259	255.19	252.35	254.25	285.65	253.94	255.24	253.00	252.05	416.73	250.09	254.69
Moxifloxacin	285	314.43	305.12	313.26	207.11	330.90	345.40	307.51	338.32	259.26	333.01	310.48
p-Aminosalicylic acid	102.7	111.84	104.79	105.20	150.30	111.00	120.70	101.21	120.26	154.28	120.53	122.89
Pyrazinamide	87.7	91.66	87.56	88.86	102.54	116.50	99.23	86.94	96.48	101.79	94.61	96.28
Rifampin	611.7	577.92	583.43	575.64	571.09	581.96	572.97	577.42	575.75	530.46	586.30	592.51

Table 20: Comparison of actual values computed values for polarizability from regression models.

Name of drug	Molar volume of drug	Molar volume computed from regression model for ABC index	Molar volume computed from regression model for *R(G)* index	Molar volume computed from regression model for *S(G)* index	Molar volume computed from regression model for *GA(G)* index	Molar volume computed from regression model for *M1(G)* index	Molar volume computed from regression model for M2(G) index	Molar volume computed from regression model H(G) index	Molar volume computed from regression of HM(G) index	Molar volume computed from regression model for ZG3(G)	Molar volume computed from regression model of F(G) index	Molar volume computed from regression model of SSD(G)
Amikacin	363.9	392.65	400.98	393.92	407.20	365.72	391.20	397.31	389.95	381.74	383.54	401.74
Bedaquiline	420.1	369.74	374.27	376.97	396.60	363.89	319.64	380.32	360.40	303.01	356.98	358.65
Clofazimine	366.1	351.98	354.23	357.78	224.35	356.56	346.84	359.48	340.70	303.01	336.25	340.25
Delamanid	368	394.10	388.92	392.08	409.36	389.54	372.60	390.51	375.69	416.73	379.65	394.44
Ethambutol	207	143.17	171.35	157.06	186.07	125.66	123.56	172.35	120.26	154.28	117.94	145.71
Ethionamide	142	109.55	107.59	107.65	151.93	107.34	114.97	106.65	114.14	136.79	112.75	115.29
Imipenem-cilastatin	183.9	210.15	207.54	206.68	242.11	213.62	223.75	204.74	221.48	206.77	220.29	219.21
Isoniazid	110.2	110.44	107.16	107.44	151.76	107.34	116.41	105.88	114.14	119.29	133.48	116.54
Levofloxacin	244	271.93	261.39	267.53	302.11	283.26	303.90	261.38	290.77	241.77	287.66	273.70
Linezolid	259	255.19	252.35	254.25	285.65	253.94	255.24	253.00	252.05	416.73	250.09	254.69
Moxifloxacin	285	314.43	305.12	313.26	207.11	330.90	345.40	307.51	338.32	259.26	333.01	310.48
p-Aminosalicylic acid	102.7	111.84	104.79	105.20	150.30	111.00	120.70	101.21	120.26	154.28	120.53	122.89
Pyrazinamide	87.7	91.66	87.56	88.86	102.54	116.50	99.23	86.94	96.48	101.79	94.61	96.28
Rifampin	611.7	577.92	583.43	575.64	571.09	581.96	572.97	577.42	575.75	530.46	586.30	592.51

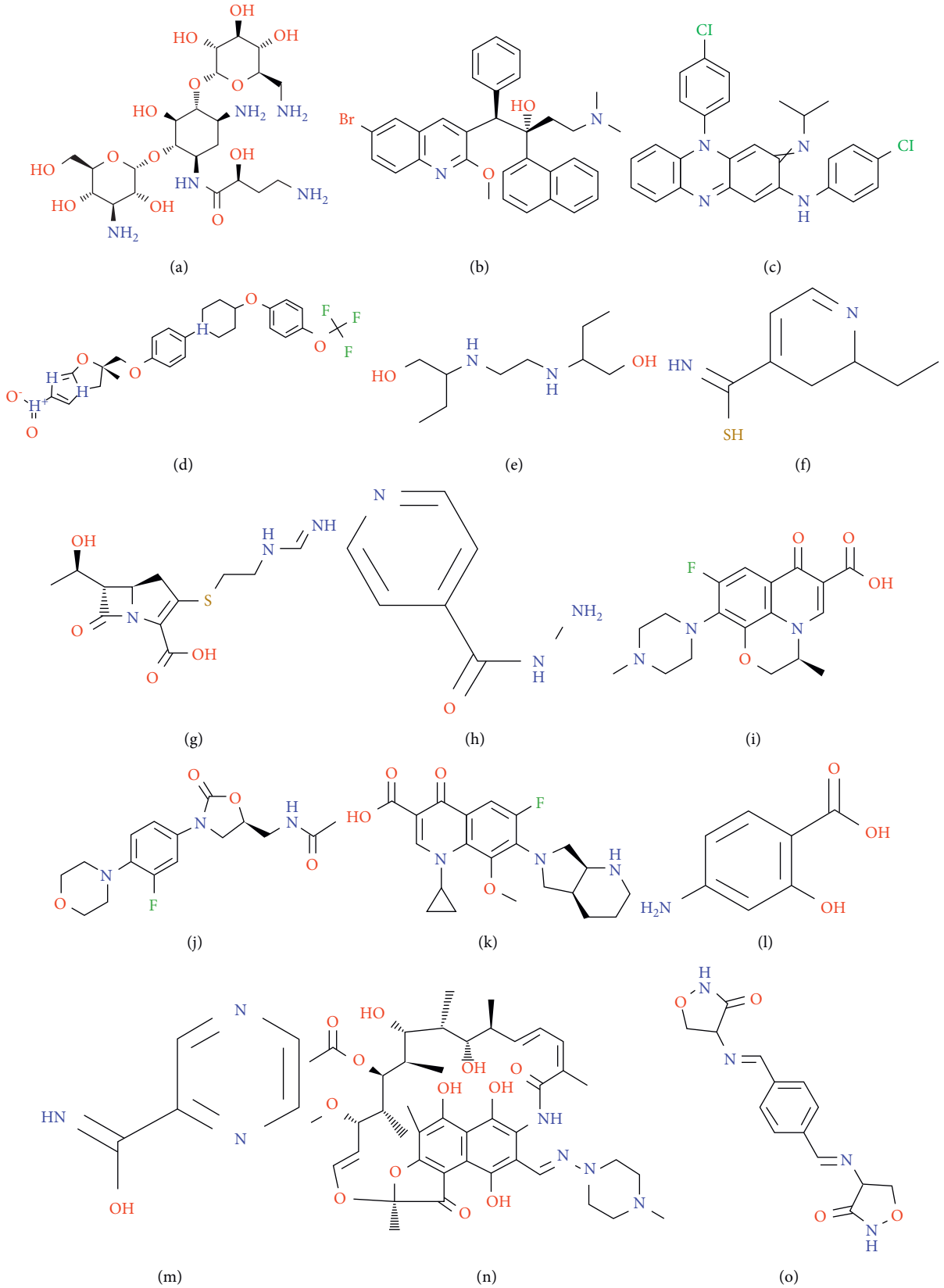

Figure 3: Molecular structure of drugs. (a) Amikacin. (b) Bedaquiline. (c) Clofazimine. (d) Delamanid. (e) Ethambutol. (f) Ethionamide. (g) Imipenem-cilastatin. (h) Isoniazid. (i) Levofloxacin. (j) Linezolid. (k) Moxifloxacin. (l) *p*-aminosalicylic acid. (m) Pyrazinamide. (n) Rifampin. (o) Terizidone.

Table 21: Correlation determination.

Topological index	Coefficient of determination of boiling point	Coefficient of determination of enthalpy	Coefficient of determination of flash point	Coefficient of determination of molar refraction	Coefficient of determination of molar volume	Coefficient of determination of polarizability
ABC(G)	0.848	0.750	0.816	0.961	0.947	0.961
R(G)	0.848	0.760	0.804	0.968	0.963	0.969
S(G)	0.845	0.747	0.804	0.967	0.956	0.967
GA(G)	0.799	0.748	0.779	0.826	0.841	0.825
M1(G)	0.808	0.706	0.787	0.949	0.931	0.949
M2(G)	0.848	0.755	0.827	0.909	0.889	0.909
H(G)	0.842	0.748	0.795	0.970	0.964	0.970
HM(G)	0.857	0.761	0.835	0.943	0.919	0.943
ZG3(G)	0.770	0.634	0.721	0.761	0.793	0.761
F(G)	0.841	0.753	0.842	0.940	0.920	0.940
SSD(G)	0.844	0.773	0.831	0.956	0.948	0.956

Table 22: Statistical parameters for the linear QSPR model for $SS\ D(G)$.

Physical property	N	A	b	r	$r2$	F	p	Indicator
Boiling point	14	147.016	5.962	0.925	0.844	71.404	≤0.0001	Significant
Enthalpy	13	38.141	0.795	0.879	0.773	37.471	≤0.0001	Significant
Flash point	14	68.953	3.421	0.912	0.831	58.981	≤0.0001	Significant
Molar refraction	14	4.877	1.371	0.978	0.956	282.000	≤0.0001	Significant
Molar volume	15	16.421	3.803	0.974	0.948	238.815	≤0.0001	Significant
Polarizability	15	1.908	0.544	0.978	0.956	283.014	≤0.0001	Significant

Polarizability = $3.976 + 0.093[F(G)]$

(11) Regression models for symmetric division index: $SS\ D(G)$

Boiling point = $147.016 + 5.962[SS\ D(G)]$

Enthalpy = $38.141 + 0.795[SS\ D(G)]$

Flash point = $68.953 + 3.421[SS\ D(G)]$

Molar refraction = $4.877 + 1.371[SS\ D(G)]$

Molar volume = $16.421 + 3.803[SS\ D(G)]$

Polarizability = $1.908 + 0.544[SS\ D(G)]$

2.2. Computation of Topological Indices and Their Comparison with Correlation Coefficients of Some Physical Properties. Table 1 shows the abovementioned physical properties of 15 drugs used for the treatment of tuberculosis.

In Table 2, the 12 topological indices are computed of the graphs constructed from the molecular structures of the drugs.

In Table 3, the correlation coefficients of the 6 physical properties with respect to each topological index are computed. The graph of the correlation coefficient of all the physical properties such as boiling point, enthalpy, flash point, molar refraction, molar volume, and polarizability on different topological indices are shown in Figure 1. The graphical representation of topological indices of the different medicine is shown in Figure 2.

2.3. Computation of Statistical Parameters. In this section, regression parameters have been computed. N is the sample size, A is constant or Y-intercept, b is slope, r is correlation coefficient, and r^2 is the percentage of the dependent variable variation that a linear model explains. The p value for each term tests the null hypothesis that the coefficient is equal to zero (no effect), whereas a larger (insignificant) p value suggests that changes in the predictor are not associated with changes in the response. Suppose we are doing a test in which the null hypothesis is that all of the regression coefficients are zero. The result of this kind of a test gives us a value called F value. In this case, the model has no predictive capability. With the help of this test, one can compare their model with zero predictor variables and decides whether their added coefficients have improved the model. In Tables 4–13, these statistical parameters are computed for linear QSPR models for different topological indices. All of these analyses show that the p value in each of the model is zero that indicates the significance of the results.

2.4. Standard Error of Estimate. The Standard error of estimate is the measure of variation of an observation made around the computed regression line. Table 14 shows the standard error of estimate for six physical properties corresponding to each topological index.

2.5. Correlation Determination. The correlation determination describes the percentage of relation which gives you more information about the relationship between variables. When you square the correlation coefficient, you end up with the correlation of determination r^2.

2.6. Comparison. In this section, the comparison for known values and computed values from our regression models is

drawn. In Tables 15–20, the comparison of each physical property is shown.

3. Conclusion and Future Study

3.1. Conclusion. Tuberculosis (TB) is a disease and its infection is caused by bacteria "*Mycobacterium tuberculosis*" that usually attacks lungs. It can also spread to other parts of body, like brain and spine and cause death.

A *molecular descriptor* is actually a mathematical formula that can be applied to any graph which models some molecular structure. More precisely, a single number represents a chemical structure. In graph theory, this number is called *topological descriptor*. When a topological descriptor correlates with a molecular property, it is called molecular index or topological index (TI). Thus, a topological graph index is also called a *molecular descriptor*. Mathematically, a *topological index* is a numeric quantity associated with a graph which characterizes the topology of a graph. By computing these topological indices, it is possible to analyze mathematical values and further investigate some physiochemical properties of a molecule. Actually topological indices are designed on the ground of transformation of molecular graph into a number which characterizes the topology of graph.

Molecular topological indices play a significant role in mathematical chemistry, especially in quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) investigations. (11) is used to correlate the various physical properties of various drugs used for the treatment of tuberculosis with some topological indices. Therefore, it is an efficient way to avoid expensive and time-consuming laboratory experiments. The purpose of computing these 11 topological indices is that no single topological index is found yet that can be efficient (given in various tables) for all physical properties of these drugs.

Tables 1 and 2 gives the values of physical properties and topological indices of medicines (Figure 3), respectively. Table 3 and graphs (Figure 1) shows how degree-based topological indices and physical properties of medicine correlate. Upon examining correlation coefficients horizontally for physical properties under consideration, we see that $H(G)$ index gives highest correlation coefficient for molar refraction ($r = 0.985$), molar volume ($r = 0.982$), and polarizability ($r = 0.985$). $HM(G)$ index gives highest correlation coefficient for boiling point ($r = 0.925$). $F(G)$ has highest correlation coefficient for flash point ($r = 0.925$). $SS\ D$ gives highest correlation coefficient for boiling point and enthalpy. When we look vertically, boiling point has also good correlation with $ABC(G)$ and $R(G)$, i.e., ($r = .921$) for both. Enthalpy has also good correlation with $R(G)$ and $HM(G)$, i.e., ($r = 0.872$). Flash point has also good correlation with $SS\ D(G)$, i.e., ($r = 0.812$). Molar refraction has also good correlation with $R(G)$, i.e., ($r = 0.984$). Molar volume has also good correlation with $R(G)$, i.e., ($r = 0.981$). Polarizability has also good correlation with $R(G)$ and $S(G)$, i.e., $r = .984$.

While examining correlation determination (Table 21) horizontally for physical properties under consideration, we see that $H(G)$ index gives highest correlation determination for molar refraction ($r^2 = 0.970$), molar volume ($r^2 = 0.964$), and polarizability ($r^2 = 0.970$). $HM(G)$ index gives highest correlation determination for boiling point ($r^2 = 0.857$). $F(G)$ has highest correlation determination for flash point ($r^2 = 0.842$). $SS\ D$ gives highest correlation determination for boiling point and enthalpy ($r^2 = 0.773$). When we look vertically, boiling point has also good correlation with $ABC(G)$ and $R(G)$, i.e., ($r^2 = 0.848$) for both. Enthalpy has also good correlation with $R(G)$ and $HM(G)$, i.e., ($r \geq 0.760$). Flash point has also good correlation with $SS\ D(G)$ and $HM(G)$, i.e., ($r^2 = .0.831$). Molar refraction has also good correlation with $R(G)$, i.e., ($r^2 = 0.968$). Molar volume has also good correlation with $R(G)$, i.e., ($r^2 = 0.963$). Polarizability has also good correlation with $R(G)$ and $S(G)$, i.e., $r^2 = 0.969$. One can easily gather from the table of statistical parameters for the linear QSPR models for different degree-based topological indices that are as follows:

Harmonic index $H(G)$ has positive and highly significant correlation coefficient for molar refraction ($r = 0.985$), molar volume ($r = 0.982$), and polarizability ($r = 0.985$).

Sum-connectivity $S(G)$ index and hyper-Zagreb index $HM(G)$ has highly significant correlation coefficient for boiling point, i.e., ($r = 0.925$).

Sum-connectivity $S(G)$ index also has highly significant correlation coefficient for enthalpy.

Forgotten topological index $F(G)$ has highly significant correlation coefficient for flash point ($r = 0.917$).

From Table 21, we can also see high percentage correlation between degree-based topological index and physical properties of medicines.

Harmonic index $H(G)$ has positive and high percentage of correlation for molar refraction ($r^2 = 0.970$), molar volume ($r^2 = 0.964$), and polarizability ($r^2 = 0.970$).

Hyper-Zagreb index $HM(G)$ has high percentage of correlation correlation for boiling point, i.e., ($r^2 = 0.857$).

Sum-connectivity $S(G)$ index also has high percentage of correlation for enthalpy ($r^2 = 0.773$).

Forgotten topological index $F(G)$ has high percentage of correlation for flash point ($r^2 = 0.842$).

Tables 4–13 and 22 show different statistical parameters of correlation between values of eleven degree based topological indices and six physical properties of medicine. We could not find any correlation between degree-based topological index and melting point of antituberculosis drugs.

This work indicated that this theocratical analysis may help the chemist and people working in pharmaceutical industry to predict properties of antituberculosis drugs

without experimenting. It is also possible that different composition of these drugs may be used for different diseases; of course it depends on the range of the topological indices which are computed in this work. In this work, we have found the correlation coefficient for different topological indices; this will help the chemist to design new drugs based on the combination of positively high correlated drugs.

3.2. Future Study. In a similar pattern, relation between physical properties for different drugs/medicine for the treatment/preventive measures of a particular disease and Topological indices can be established to estimate physical properties of newly discovered medicine or candidate drug(s) of particular disease.

It will be very important to find a topological index that can correlate with all the physical properties.

Data Availability

The physical property data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors have no conflicts of interest.

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