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Research Article

Topological Descriptors and QSPR Modelling of HIV/AIDS Disease Treatment Drugs

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A topological index is a real number derived from the structure of a chemical graph. It helps determine the physicochemical and biological properties of a wide range of drugs, and it better reflects the theoretical properties of organic compounds. This is accomplished using degree-based topological indices. We examined some of the physiochemical characteristics of thirteen HIV therapy medications and created a QSPR model utilizing nine of the medication's topological indices. The melting point, boiling point, flash point, complexity, surface tension, etc., of HIV medicines are closely related according to this QSPR model. This work can help to design and synthesize new HIV treatments and other disease drugs.

1. Introduction

About 33 million people have died from HIV infection globally, and numerous mathematical models of the human immune system have developed to represent the full range of infection. Human immunodeficiency virus (HIV) and the immune system have been shown to interact. According to reports, HIV can cause immunodeficiency syndrome (AIDS), which makes it harder for the body to fight off other diseases. About 44,200,000 people have died because of the devastating and incurable HIV virus. According to reports, 1.5 million new HIV infections are reported in 2020, leaving 37.6 million persons worldwide HIV-positive [1]. However, people with HIV are now living longer and healthier lives because of effective treatment, care, assessment, and protection. The HIV virus spreads quickly once it enters the body of a healthy person. The flu, midnight cravings, coughing, weight loss, diarrhea, body pains, joint pain, and dry mouth are some of the early symptoms and indicators of HIV infection. The process is still in its early stages, the virus enters the bloodstream more fully, and the HIV infection spreads across the body more readily than at other times. In addition, HIV-infected viruses can infect the uninfected person through bodily fluids like blood, tears, urine, saliva, and others. It belongs to the genus *Lentivirus* and is responsible for the most serious illness, AIDS (acquired immune deficiency syndrome). HIV directly attacks the immune system [2]. There are numerous recognized targets, and numerous substances have received approval for the treatment of HIV. According to studies, if a single chemical is employed to treat HIV, toxicity and resistance will quickly arise. The major goal of this study project is to examine the system's most important components for the prevention of this viral infection. Without the need for chemical experimentation, the topological index computing technique is being utilized to assess the medicinal characteristics and biochemical data of novel medications, which is particularly welcomed in underdeveloped nations. Numerous investigations have discovered a clear connection between molecular structure and medications and chemical

properties such as boiling and melting points. Gao et al. [3] focused on a family of smart polymers that are frequently employed in the creation of anticancer medications. The results compensate for the lack of chemical and medical experiments and serve as a theoretical foundation topological index utilizing edge division techniques. In recent years, there has been great curiosity in using these invariants (TIs) in QSPR and quantitative structure activity relationship (QSAR) studies. The indices have a lot of uses in countless ranges of chemistry, physics, informatics, and biology QSAR [4]. The ABC index, Wiener index, and Randic index can all be used to predict drug bioactivity. QSPR models sustenance in deciding the best association between TIs and physical properties. Research-based medicinal remedies are being tested as medications by scientists. In this paper, we calculated degree-based TIs for HIV drugs. Similarly, HIV drug on which the specified topological indices are carefully implemented and measured the QSPR technique is performed. With the help of linear regression, the physical characteristic is estimated successfully. It has been discovered that both variables have a good relation.

According to Havare [5], novel medications used in cancer treatment are a costly and complex phenomenon; hence, these are best predicted using this method. QSPR modelling of blood cancer medicines by Nasir et al. [6] demonstrates a significant relationship between TIs and pharmacological characteristics. We are working on the current study issue because of improvements in QSPR investigations for different topological indices for different chemical structures. In order to derive analytically precise equations for particular degree and distance-based topological indices for general networks, Hayat et al. [7] published a computer technique. Experiments are conducted in comparison to the well-known methodologies to show that our method is superior and has a lower level of algorithmic and computing complexity. Antituberculosis drug QSPR modelling is described in [8], and Parveen et al. [9] finished the QSPR analysis of diabetes therapies and identified a best-fit model for it. Vitiligo disease drug modelling is discussed in [10], and the cardiovascular QSPR fitted model is mentioned in [11]. For further investigation, we validate articles [4, 5, 11–15] for more information on degree-based topological indices. Our motivation to work on the current research issue came from studies on COVID-19, anticancer, blood cancer, and QSPR investigations of eigenvalue-based, degree-based entropy, and ve-degree-based topological indices for various chemical structures (see [2, 16–18]). This study's goal is to investigate the usage of TIs in figuring out the physical characteristics and QSPR modelling of the therapeutic management medication regimens for HIV.

2. Materials and Methods

In this study, the drug's structure is represented as a graph, where each vertex $V(G)$ expresses an atom and each edge $E(G)$ represents a chemical connection between these atoms. All graphs are assumed to be simple and linked. The numbers of edges that connect a vertex to other edges determine its degree. Please refer to the book [19] in cases where notations and terminologies are unclear. The degree of a vertex in a graph G is denoted by d_u. For further investigation, we refer [4, 8, 13] and [20] and used the following TIs.

Definition 1. The ABC index is as follows [15]:

$$\mathrm{ABC}(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_{u+} d_v - 2}{d_u d_v}}. \tag{1}$$

Definition 2. The Randic index $RA(G)$ calculated by Milan Randic in 1975 [21] is given under the following expression:

$$RA(G) = \sum_{uv \in E(G)} \sqrt{\frac{1}{d_u d_v}}. \tag{2}$$

Definition 3. The sum connectivity index [22] is given under the following expression:

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

Definition 4. The GA index [23] is given under the following expression:

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

Definition 5. Zagreb indices [24] are given under the following expression:

$$\begin{aligned} M_1(G) &= \sum_{uv \in E(G)} (d_u + d_v), \\ M_2(G) &= \sum_{uv \in E(G)} (d_u d_v). \end{aligned} \tag{5}$$

Definition 6. The harmonic index [25] is given under the following expression:

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

Definition 7. The hyper Zagreb index [26] is defined as follows:

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

Definition 8. The forgotten index [27] is given under the following expression:

$$F(G) = \sum_{uv \in E(G)} \left[(d_u)^2 + (d_v)^2 \right]. \tag{8}$$

Tipranavir is a nonpeptidic protease inhibitor that targets the HIV protease and contains sulfonamides. HIV is treated by the coadministration of ritonavir and tipranavir. A nonpeptidic protease inhibitor of HIV is tipranavir. The protease component of HIV is blocked by protease inhibitors. Lamivudine has the molecular formula C_8H_{11} N_3 O_3S. It is used to treat hepatitis B and type 1 human immunodeficiency virus. It has the molecular formula $C_{31}H_{33}$ F_3N_2 O_5S. It has the molecular formula $C_{32}H_{45}N_3$ O_4S. A powerful inhibitor of the HIV-1 protease is nelfinavir. It is used for the treatment of HIV in adults and children. Maraviroc has the molecular formula $C_{29}H_{41}$ F_2N_5 O_4. It works to combat HIV by obstructing the communication between HIV and CCR5. Emtricitabine is a nucleoside reverse transcriptase inhibitor (NRTI) that is prescribed to treat HIV infection in adults or to prevent HIV infection in high-risk adults and adolescents when taken with tenofovir alafenamide. Emtricitabine is an analogue of cytidine. The medication prevents HIV RNA from being converted to DNA by inhibiting HIV reverse transcriptase. It is identified as a genuine nucleotide analogue in the strictest sense since it has a phosphate group bound to the nitrogenous base. Tenofovir's antiviral properties were initially noted in 1993, and tenofovir disoproxil, the commercial form of this drug, has been accessible since 2008. Tipranavir is a nonpeptidic protease inhibitor that targets the HIV protease and contains sulfonamides. HIV is treated by the coadministration of ritonavir and tipranavir. Etravirine is a type of antiretroviral medication.

3. Quantitative Structure Analysis and Regression Model

In this section, TIs are performed on HIV drugs. The relationship between QSPR analysis and TIs suggests that the physicochemical characteristics of the disease are highly connected. The thirteen medicines lamivudine, darunavir, Disovey, maraviroc, tenofovir, tipranavir, atazanavir, lopinavir, abacavir, etravirine, nelfinavir, and toreforant are used in the analysis for HIV disease. The drug edifices are exhibited in Figures 1 and 2. We implement regression analysis calculated for this study. Drug computable structure analysis of nine TIs for QSPR modelling tenacity is performed. The nine physical properties, molar refractivity (R), polarity, complexity, molar volume (MV), and enthalpy (E) and boiling point (BP) for nine medicines used in HIV treatment are listed in Table 1. We impose the linear model by using the following equation:

$$P = \alpha + \beta\,(TI). \tag{9}$$

P denotes the physicochemical property of the given drug. The term TI stands for the topological index, α stands for constant, and β stands for the regression coefficient. MATLAB and R-language software are helpful for results. A linear model is used to analyze nine TIs of HIV drugs and their properties.

Let G_1 be graph of lamivudine, and then, TIs are as follows:

(i) $\mathrm{ABC}(G_1) = 11.45$

(ii) $RA(G_1) = 7.20$

(iii) $S(G_1) = 7.42$

(iv) $GA(G_1) = 15.49$

(v) $M1(G_1) = 76$

(vi) $M2(G_1) = 88$

(vii) $F(G_1) = 194$

(viii) $H(G_1) = 6.93$

(ix) $HM(G_1) = 370$

Now, for partition of G_1, $|E_{1,2}| = 1$, $|E_{1,3}| = 2$, $|E_{2,2}| = 2$, $|E_{2,3}| = 9$, and $|E_{3,3}| = 2$.

(i) Applying Definition 1, we obtain $\mathrm{ABC}(G_1) = 1\sqrt{\times 1 + 2 - 2/1 \times 2} + 2\ \sqrt{1 + 3 - 2/1 \times 3} + 2\sqrt{2 + 2 - 2/2 \times 2} + 9\sqrt{2 + 3 - 2/2 \times 3} + 2\sqrt{3 + 3 - 2/3 \times 3} = 11.45$

(ii) Applying Definition 2, we obtain $RA(GG_1) = 1 \times \sqrt{1/1 \times 2} + 2\sqrt{1/1 \times 3} + 2\sqrt{1/2 \times 2} + 9\sqrt{1/2 \times 3} + 2\sqrt{1/3 \times 3} = 7.20$

(iii) Applying Definition 3, we obtain $S(G_1) = 1 \times \sqrt{1/1 + 2} + 2\sqrt{1/1 + 3} + 2\sqrt{1/2 + 2} + 9\sqrt{1/2 + 3} + 2\sqrt{1/3 + 3} = 7.42$

(iv) Applying Definition 4, we obtain $GA(G_1) = 1 \times \sqrt{1 \times 2}/1 + 3 + 2\sqrt{1 \times 3}/1 + 4 + 1 + 4/2 + 3 + 2 + 3/2 + 4 + 2\sqrt{3 \times 3}/3 + 3 = 15.49$

(v) Applying Definition 5, we obtain $M1(G_1) = 1 \times (1 + 2) + 15(1 + 3) + 3(2 + 2) + 1(2 + 3) + 23(3 + 3) = 76$

(vi) Applying Definition 5, we obtain

(vii) $M2(G_1) = 1 \times (1 \times 2) + 2(1 \times 3) + 2(2 \times 2) + 9(2 \times 3) + 2(3 \times 3) = 88$

(viii) Applying Definition 6, we obtain $H(G_1) = 1 \times (1/1 + 2) + 2(1/1 + 3) + 2(1/2 + 2) + 9(1/2 + 3) + 2(1/3 + 3) = 6.93$

(ix) Applying Definition 7, we obtain $HM(G_1) = 1 \times (1 + 2)^2 + 2(1 + 3)^2 + 2(2 + 2)^2 + 9(2 + 3)^2 + 2(3 + 3)^2 = 370$

(x) Applying Definition 8, we obtain $F(G_1) = 1 \times (1 + 4) + 2(1 + 9) + 2(4 + 4) + 9(4 + 9) + 2(9 + 9) = 194$

Also, G_2 be a graph of tipranavir, and then, TIs are as follows:

(i) $\mathrm{ABC}(G_2) = 32.55$

(ii) $RA(G_2) = 19.83$

(iii) $S(G_2) = 20.72$

(iv) $GA(G_2) = 42.93$

(v) $M1(G_2) = 224$

(vi) $M2(G_2) = 265$

(vii) $F(G_2) = 630$

(viii) $H(G_2) = 18.84$

(ix) $HM(G_2) = 1160$

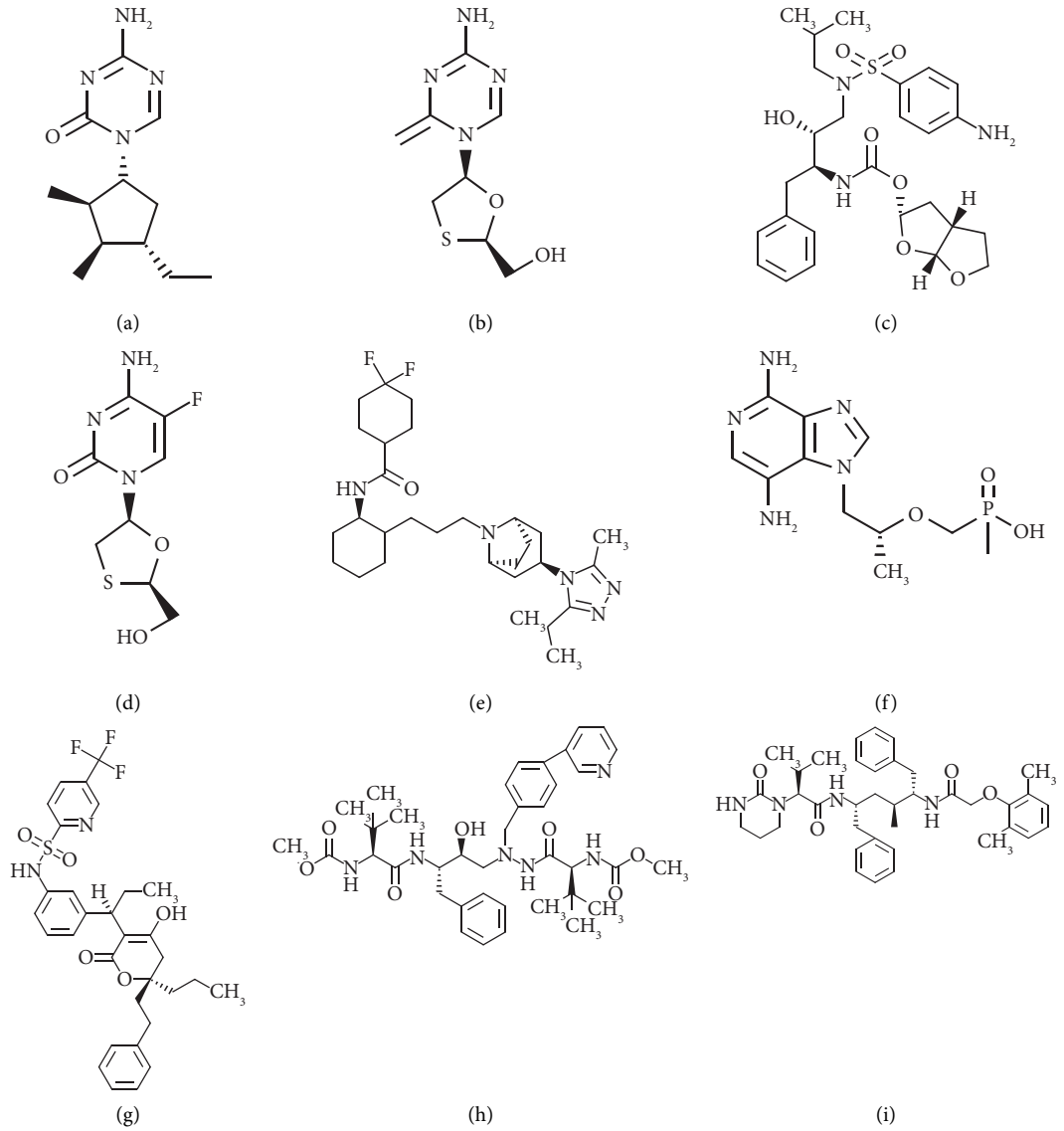


Figure 1: Drug structure. (a) Vidaza. (b) Lamivudine. (c) Darunavir. (d) Disovey. (e) Maraviroc. (f) Tenofovir. (g) Tipranavir. (h) Atazanavir. (i) Lopinavir.

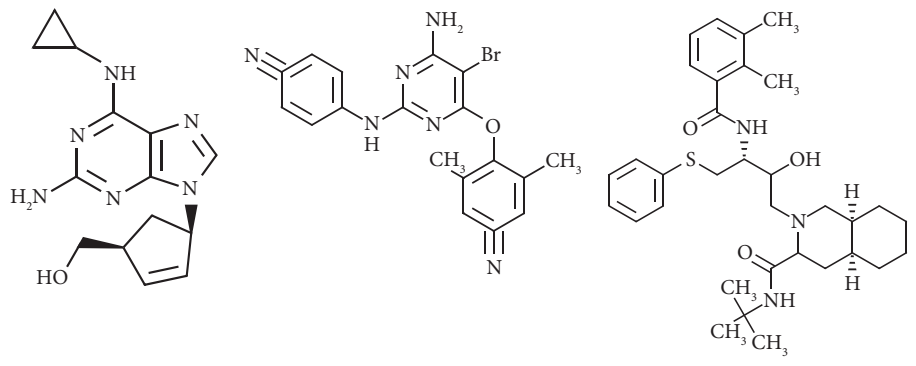
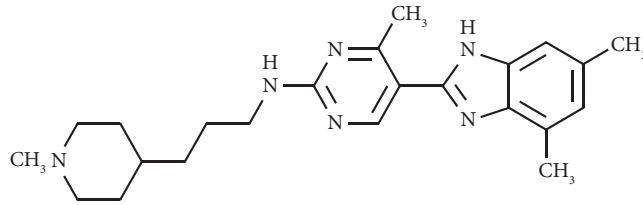


Figure 2: Continued.



(d)

Figure 2: Drug structure. (a) Abacavir. (b) Etravirine. (c) Nelfinavir. (d) Maraviroc.

Table 1: Physical properties of drugs.

Name of drug	Boiling point (°C)	Enthalpy (°C)	Flash point (°C)	Molar refractivity (cm^3)	Polarity (cm^3)	Molar volume (cm^3)	Complexity	Density (g/cm^3)	Polar surface area (A^2)
Vidaza	534.4	93.2	277	51.1	20.3	117.1	384	2.1	141
Lamivudine	475.4	85.2	241.3	54.1	21.5	132.2	331	1.7	113
Darunavir					56.9	408.4	853	1.3	149
Disovey	443.3	80.9	221.9	1.731	21.4	135.2	374	1.8	113
Maraviroc				141.1	55.9	397.8	751	1.3	63
Tenofovir	642.7	94.9	342.5	118.3	46.9	356.1		1.5	195
Tipranavir	712.3	109.3	384.6	152.4	60.4	459		1.3	114
Atazanavir				194	76.9	597.9	1110	1.2	171
Lopinavir	924.2	140.8	512.7	179.2	71	540.5	940	1.2	120
Abacavir	636	98.8	338.4	75.8	30.1	167.7	414	1.7	102
Etravirine	637.4	94.2	339.3	106.9	42.4	275.7	609	1.6	121
Nelfinavir	786.8	120.1	429.7	162.4	64.4	463.1	830	1.2	127
Toreforant	611.2	90.8	323	120.1	47.6	341.7	508	1.1	70

Now, for partition of G_2: $|E_{1,2}| = 2$, $|E_{2,3}| = 12$, $|E_{2,4}| = 6$, $|E_{3,3}| = 2$, $|E_{3,4}| = 4$, $|E_{1,3}| = 1$, $|E_{1,4}| = 6$, and $|E_{2,2}| = 12$.

(i) Applying Definition 1, we obtain $\mathrm{ABC}(G_2) = 2\sqrt{1+2-2/1\times 2}+1\sqrt{1+3-2/1\times 3}+6\sqrt{1+4-2/1\times 4}+12\sqrt{2+2-2/2\times 2}+12\sqrt{2+3-2/2\times 3}+6\sqrt{2+4-2/2\times 4}+2\sqrt{3+3-2/3\times 3}+4\sqrt{3+4-2/3\times 4} = 32.55$

(ii) Applying Definition 2, we obtain $RA(G_2) = 2\sqrt{1/1\times 2}+1\sqrt{1/1\times 3}+6\sqrt{1/1\times 4}+12\sqrt{1/2\times 2}+12\sqrt{1/2\times 3}+6\sqrt{1/2\times 4}+2\sqrt{1/3\times 3}+4\sqrt{1/3\times 4} = 19.83$

(iii) Applying Definition 3, we obtain $S(G_2) = 2\sqrt{1/1+2}+1\sqrt{1/1+3}+6\sqrt{1/1+4}+12\sqrt{1/2+2}+12\sqrt{1/2+3}+6\sqrt{1/2+4}+2\sqrt{1/3+3}+4\sqrt{1/3+4} = 20.72$

(iv) Applying Definition 4, we obtain $GA(G_2) = 2\sqrt{1\times 2}/1+2+1\sqrt{1\times 3}/1+3+1+3/1+4+12\sqrt{2\times 2}/2+2+12\sqrt{2\times 3}/2+3+6\sqrt{2\times 4}/2+4+2\sqrt{3\times 3}/3+3+4\sqrt{3\times 4}/3+4 = 42.93$

(v) Applying Definition 5, we obtain $M1(G_2) = 2(1+2)+1(1+3)+6(1+4)+12(2+2)+12(2+3)+6(2+4)+2(3+3)+4(3+4) = 224$

(vi) Applying Definition 5, we obtain $M2(G_2) = 2(1\times 2)+1(1\times 3)+6(1\times 4)+1(2\times 2)+12(2\times 3)+12(2\times 4)+6(3\times 3)+4(3\times 4) = 265$

(vii) Applying Definition 6, we obtain $H(G_2) = 2(1/1+2)+1(1/1+3)+6(1/1+4)+12(1/2+2)+12(1/2+3)+6(1/2+4)+2(1/3+3)+4(1/3+4) = 18.84$

(viii) Applying Definition 7, we obtain $HM(G_2) = 2(1+2)^2+1(1+3)^2+6(1+4)^2+12(2+2)^2+12(2+3)^2+6(2+4)^2+2(3+3)^2+36 = 1160$

(ix) Applying Definition 8, we obtain $F(G_2) = 2(1+4)+1(1+9)+6(1+16)+12(4+4)+12(4+9)+6(4+16)+2(9+9)+4(9+16) = 630$

Topological indices of other drugs can be calculated by means of the identical technique as discussed above and Definitions 1 to 8. Table 2 includes calculated tenets for all drugs' TIs. Figures 3 and 4 depict a graphical representation of calculated TIs for various medicines. Using (1), subsequent diverse linear models to find out other TIs are given as follows:

(1) Regression models of ABC(G) are as follows:

Boiling point = 346.910 + 13.268 [ABC(G)]
Enthalpy = 66.555 + 1.535 [ABC(G)]
Flash point = 163.588 + 8.023 [ABC(G)]
Molar refractivity = −12.048 + 5.276 [ABC(G)]
Polarity = −3.948 + 2.087 [ABC(G)]
Molar volume = −101.097 + 17.791 [ABC(G)]
Complexity = 15.807 + 26.440 [ABC(G)]

(2) Regression models of RA(G) are as follows:

Boiling point = 345.986 + 21.602 [RA(G)]
Enthalpy = 66.296 + 2.509 [RA(G)]
Flash point = 163.035 + 13.062 [RA(G)]

Table 2: TIs of drugs.

Drug	ABC	R	S	GA	$M1$	$M2$	HM	H	F
Vidaza	12.96	8.04	8.25	17.265	88	105	444	7.63	234
Lamivudine	11.45	7.20	7.42	15.49	76	88	370	6.93	194
Darunavir	25.46	15.72	16.13	33.33	171	200	867	14.86	467
Disovey	12.23	7.61	7.83	16.36	82	96	406	7.27	214
Maraviroc	29.42	17.72	18.71	39.63	202	240	1018	17.03	538
Tenofovir	26.37	16.47	16.83	34.29	170	189	822	15.60	444
Tipranavir	32.55	19.83	20.72	42.93	224	265	1160	18.84	630
Atazanavir	38.69	24.01	24.46	50.51	254	287	1250	22.74	676
Lopinavir	34.46	21.71	22.39	46.66	224	255	1068	21.0	558
Abacavir	16.92	10.24	10.92	23.51	118	143	592	10.0	306
Etravirine	20.29	12.33	12.79	26.87	136	158	672	11.73	356
Nelfinavir	32.05	19.30	19.98	41.92	218	255	1114	18.28	604
Toreforant	26.86	16.65	17.11	35.55	176	200	858	15.90	458

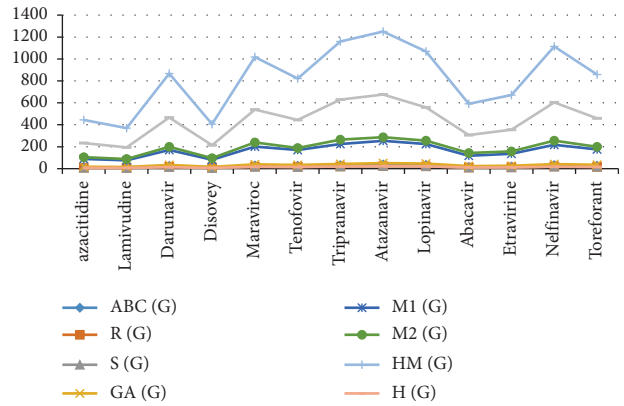


Figure 3: 2D graph of medicines with TIs.

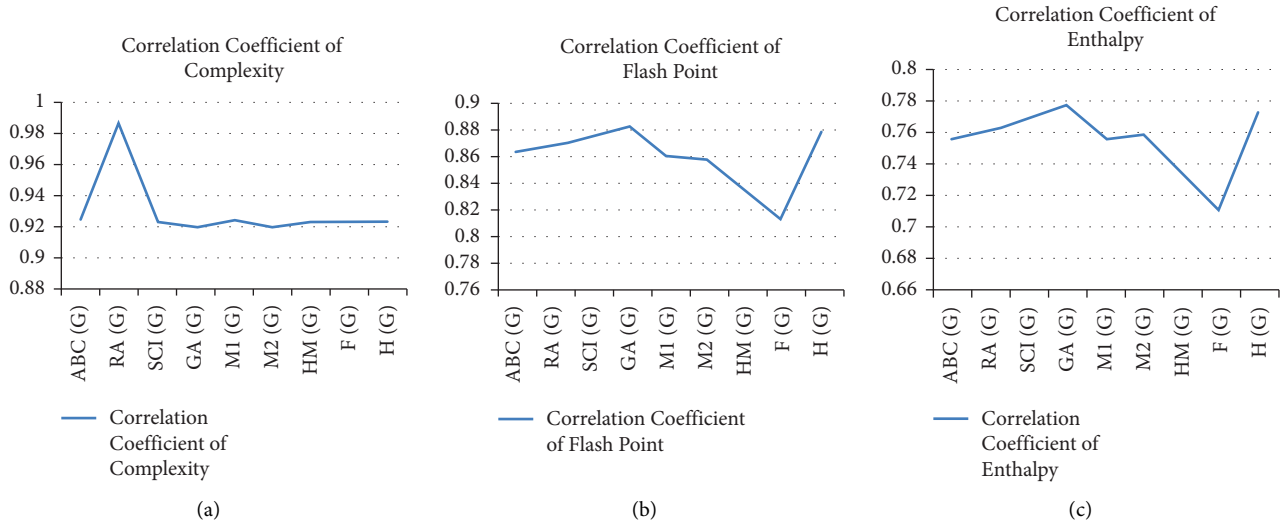


Figure 4: Continued.

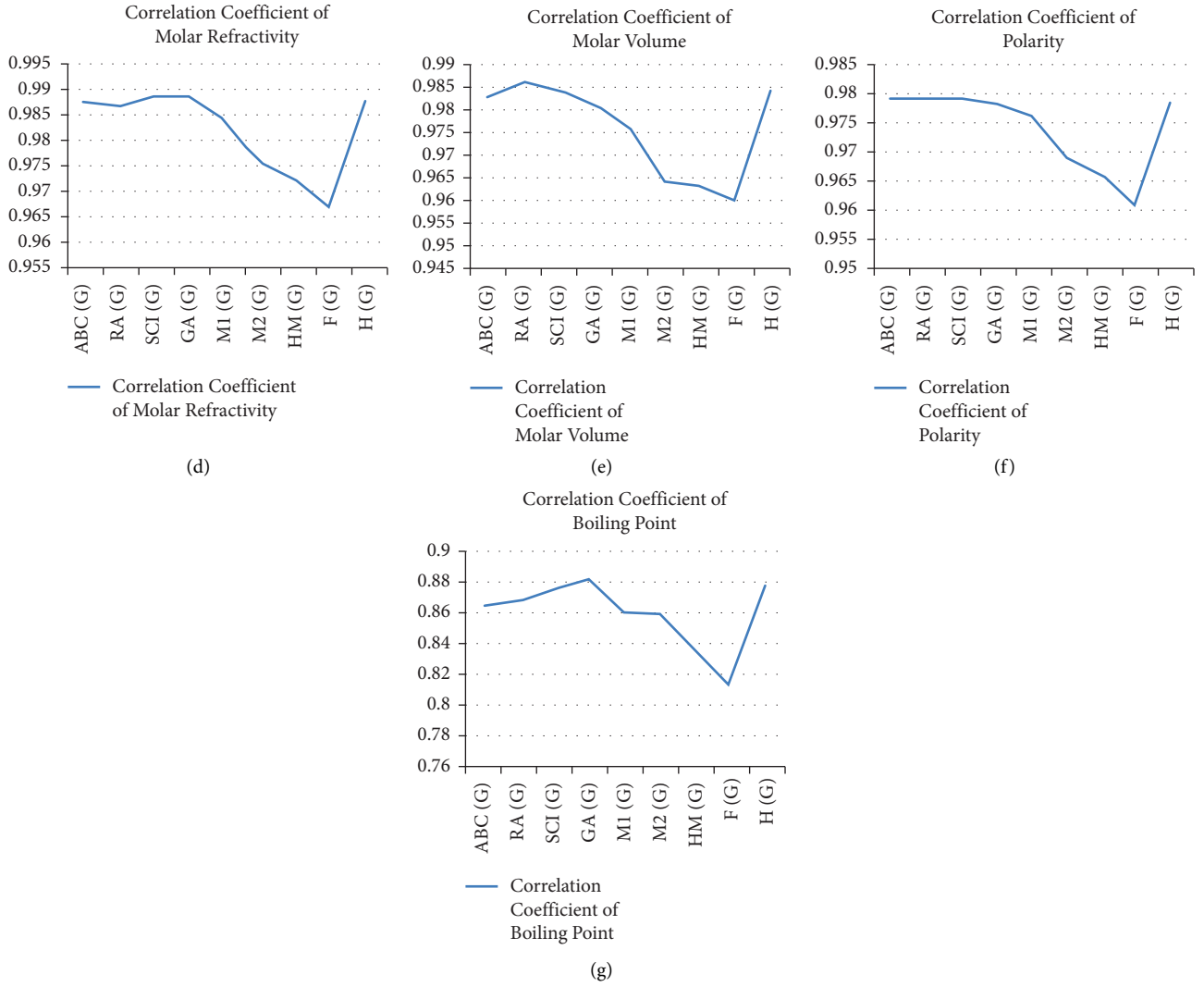


Figure 4: Physicochemical properties and TIs. (a) Complexity on TI. (b) Flash point on TI. (c) Enthalpy on TI. (d) Molar refractivity on TI. (e) Molar volume on TI. (f) Polarity on TI. (g) Boiling point on TI.

Molar refractivity = −11.383 + 8.534 [RA(G)]
Polarity = −3.724 + 3.377 [RA(G)]
Molar volume = −100.628 + 28.88 [RA(G)]
Complexity = 18.898 + 42.774 [RA(G)]

(3) Regression models of $S(G)$ are as follows:

Boiling point = 343.313 + 21.044 [$S(G)$]
Enthalpy = 65.953 + 2.446 [$S(G)$]
Flash point = 161.415 + 12.725 [$S(G)$]
Molar refractivity = −12.807 + 8.332 [$S(G)$]
Polarity = −4.191 + 3.294 [$S(G)$]
Molar volume = −103.688 + 28.110 [$S(G)$]
Complexity = 13.333 + 41.709 [$S(G)$]

(4) Regression models of GA(G) are as follows:

Boiling point = 335.740 + 10.330 [GA(G)]
Enthalpy = 64.945 + 1.205 [GA(G)]
Flash point = 156.835 + 6.246 [GA(G)]
Molar refractivity = −14.735 + 4.051 [GA(G)]
Polarity = −4.838 + 1.599 [GA(G)]
Molar volume = −107.878 + 13.609 [GA(G)]
Complexity = 8.000 + 20.107 [GA(G)]

(5) Regression models of $M1(G)$ are as follows:

Boiling point = 345.584 + 1.993 [$M1(G)$]
Enthalpy = 66.272 + 0.231 [$M1(G)$]
Flash point = 162.775 + 1.205 [$M1(G)$]
Molar refractivity = −13.422 + 0.797 [$M1(G)$]
Polarity = −4.538 + 0.315 [$M1(G)$]
Molar volume = −104.247 + 2.678 [$M1(G)$]
Complexity = 0.879 + 4.042 [$M1(G)$]

(6) Regression models of HM(G) are as follows:

Boiling point = 359.791 + 0.383 [HM(G)]
Enthalpy = 67.889 + 0.045 [HM(G)]
Flash point = 171.354 + 0.232 [HM(G)]
Molar refractivity = −10.462 + 0.157 [HM(G)]
Polarity = −3.571 + 0.062 [HM(G)]
Molar volume = −94.808 + 0.527 [HM(G)]
Complexity = −2.288 + 0.818 [HM(G)]

Table 3: Parameters for ABC(G).

Physiochemical property	N	A	b	r	r^2	F
Boiling point	10	346.910	13.268	0.8646	0.747	20.745
Enthalpy	10	66.555	1.535	0.756	0.572	9.3870
Flash point	10	163.588	8.023	0.864	0.747	20.674
Molar refractivity	11	−12.048	5.276	0.988	0.976	372.71
Polarity	13	−3.948	2.087	0.979	0.959	235.30
Molar volume	13	−101.097	17.791	0.983	0.967	294.56
Complexity	12	15.807	26.440	0.925	0.857	48.093

Table 4: Parameters for RA(G).

Physiochemical property	N	A	b	r	r^2	F
Boiling point	10	345.986	21.602	0.867	0.753	21.415
Enthalpy	10	66.296	2.509	0.762	0.581	9.7550
Flash point	10	163.035	13.062	0.867	0.752	21.335
Molar refractivity	11	−11.383	8.534	0.987	0.974	343.27
Polarity	13	−3.724	3.377	0.978	0.957	228.49
Molar volume	13	−100.628	28.88	0.985	0.972	349.02
Complexity	12	18.898	42.774	0.927	0.860	49.278

Table 5: Parameters for $S(G)$.

Physiochemical property	N	A	b	r	r^2	F
Boiling point	10	343.313	21.044	0.876	0.767	22.257
Enthalpy	10	65.953	2.446	0.771	0.595	10.020
Flash point	10	161.415	12.725	0.875	0.766	22.174
Molar refractivity	11	−12.807	8.332	0.988	0.977	354.92
Polarity	13	−4.191	3.294	0.978	0.958	222.09
Molar volume	13	−103.688	28.110	0.983	0.967	293.43
Complexity	12	13.333	41.709	0.923	0.852	46.611

Table 6: Parameters for GA(G).

Physiochemical property	N	A	b	r	r^2	F
Boiling point	10	335.740	10.330	0.882	0.778	24.605
Enthalpy	10	64.945	1.205	0.778	0.606	10.790
Flash point	10	156.835	6.246	0.881	0.777	24.507
Molar refractivity	11	−14.735	4.051	0.988	0.977	394.91
Polarity	13	−4.838	1.599	0.9783	0.957	222.73
Molar volume	13	−107.878	13.609	0.980	0.961	250.47
Complexity	12	8.000	20.107	0.919	0.845	43.674

Table 7: Parameters for $M1(G)$.

Physiochemical property	N	A	b	r	r^2	F
Boiling point	10	345.584	1.993	0.860	0.739	19.905
Enthalpy	10	66.272	0.231	0.755	0.570	9.3100
Flash point	10	162.775	1.205	0.859	0.739	19.847
Molar refractivity	11	−13.422	0.797	0.984	0.968	276.75
Polarity	13	−4.538	0.315	0.975	0.952	200.05
Molar volume	13	−104.247	2.678	0.975	0.952	200.30
Complexity	12	0.879	4.042	0.923	0.853	46.618

Table 8: Parameters for $M2(G)$.

Physiochemical property	N	A	b	r	r^2	F
Boiling point	10	342.262	1.737	0.858	0.737	19.632
Enthalpy	10	65.611	0.203	0.759	0.577	9.5570
Flash point	10	160.757	1.050	0.858	0.736	19.583
Molar refractivity	11	−14.752	0.695	0.975	0.951	178.21
Polarity	13	−5.166	0.275	0.968	0.938	151.55
Molar volume	13	−107.540	2.326	0.964	0.929	132.77
Complexity	12	−17.017	3.573	0.919	0.845	43.699

Table 9: Parameters for HM(G).

Physiochemical property	N	A	b	r	r^2	F
Boiling point	10	359.791	0.383	0.834	0.696	16.095
Enthalpy	10	67.889	0.045	0.733	0.538	8.1740
Flash point	10	171.354	0.232	0.834	0.696	16.062
Molar refractivity	11	−10.462	0.157	0.971	0.944	152.23
Polarity	13	−3.571	0.062	0.965	0.932	138.44
Molar volume	13	−94.808	0.527	0.963	0.927	128.19
Complexity	12	−2.288	0.818	0.922	0.850	45.563

Table 10: Parameters for $H(G)$.

Physiochemical property	N	A	b	r	r^2	F
Boiling point	10	341.898	22.900	0.877	0.769	23.360
Enthalpy	10	65.670	2.671	0.774	0.599	10.467
Flash point	10	160.565	13.847	0.876	0.768	23.265
Molar refractivity	11	−12.255	8.994	0.987	0.975	353.68
Polarity	13	−3.957	3.555	0.977	0.956	219.94
Molar volume	13	−102.314	30.381	0.984	0.969	315.39
Complexity	12	18.702	44.784	0.922	0.851	46.094

Table 11: Parameters for $F(G)$.

Physiochemical property	N	A	b	r	r^2	F
Boiling point	10	375.225	0.683	0.813	0.661	13.676
Enthalpy	10	69.871	0.079	0.710	0.505	7.1550
Flash point	10	180.685	0.413	0.813	0.661	13.652
Molar refractivity	11	−6.426	0.285	0.966	0.934	127.81
Polarity	13	−2.049	0.113	0.961	0.924	122.38
Molar volume	13	−82.530	0.960	0.960	0.922	118.34
Complexity	12	12.530	1.504	0.923	0.852	46.103

Table 12: Correlation coefficients.

Topological index	Correlation coefficient						
	Boiling point	Enthalpy	Flash point	Refractivity	Polarity	Molar volume	Complexity
ABC(G)	0.865	0.757	0.864	0.988	0.979	0.983	0.926
RA(G)	0.868	0.763	0.868	0.987	0.979	0.986	0.986
$S(G)$	0.876	0.771	0.876	0.989	0.979	0.984	0.923
GA(G)	0.882	0.779	0.882	0.989	0.978	0.981	0.919
$M1(G)$	0.860	0.756	0.860	0.984	0.976	0.976	0.924
$M2(G)$	0.859	0.760	0.858	0.976	0.969	0.964	0.919
HM(G)	0.835	0.734	0.835	0.972	0.966	0.963	0.922
$F(G)$	0.813	0.711	0.813	0.967	0.961	0.960	0.923
$H(G)$	0.877	0.774	0.877	0.988	0.978	0.984	0.923

Table 13: Coefficient of determination.

Topological index	Coefficient of determination						
	Boiling point	Enthalpy	Flash point	Refractivity	Polarity	Molar volume	Complexity
ABC	0.748	0.573	0.747	0.976	0.959	0.967	0.857
RA	0.753	0.582	0.753	0.974	0.958	0.972	0.860
S	0.767	0.595	0.767	0.977	0.958	0.968	0.852
GA	0.779	0.606	0.778	0.978	0.957	0.962	0.845
$M1$	0.740	0.571	0.739	0.969	0.952	0.952	0.854
$M2$	0.737	0.577	0.737	0.952	0.938	0.930	0.845
HM	0.697	0.539	0.696	0.944	0.933	0.928	0.851
F	0.661	0.505	0.661	0.934	0.924	0.922	0.852
H	0.769	0.599	0.769	0.975	0.956	0.969	0.852

Table 14: Standard error estimate.

Topological index	Standard error estimate (SEE)						
	Boiling point	Enthalpy	Flash point	Refractivity	Polarity	Molar volume	Complexity
ABC	71.58823	12.310425	43.3625	7.82587	3.89592	29.68461	105.49552
RA	70.73892	12.174462	42.85357	8.14629	3.95113	27.34072	104.39851
S	69.71392	12.079252	42.23289	8.01478	4.00531	29.74006	106.91801
GA	67.07459	11.814988	40.63925	7.60775	3.9998	32.10131	109.91429
$M1$	72.69719	12.33944	44.02479	9.04492	4.21016	35.7233	106.91065
$M2$	73.06861	12.247025	44.24284	11.17462	4.80072	43.35636	109.88778
HM	78.46519	12.792877	47.50065	12.04107	5.00822	44.06804	107.95832
F	82.92827	13.245201	50.19557	13.07199	5.30333	45.72923	107.41857
H	68.43589	11.923726	41.46483	8.02852	4.02395	28.71903	107.42736

Table 15: Comparison of polarity.

Name of drug	Polarity of drug	Polarity computed from regression model								
		ABC	R	S	GA	$M1$	$M2$	F	H	HM
Vidaza	$20.3 \pm 5.0\,cm^3$	23.09952	23.42708	22.9845	22.76874	23.182	23.709	24.393	23.16765	23.96
Lamivudine	$21.5 \pm 5.0\,cm^3$	19.94815	20.5904	20.25048	19.93051	19.402	19.034	19.873	20.67915	19.37
Darunavir	56.9	49.18702	49.36244	48.94122	48.45667	49.327	49.834	50.722	48.8703	50.18
Disovey		21.57601	21.97497	21.60102	21.32164	21.292	21.234	22.133	21.88785	21.6
Maraviroc	$55.9 \pm 5.0\,cm^3$	57.45154	56.11644	57.43974	58.53037	59.092	60.834	58.745	56.58465	59.55
Tenofovir	$46.9 \pm 5.0\,cm^3$	51.08619	51.89519	51.24702	49.99171	49.012	46.809	48.123	51.501	47.39
Tipranavir	$60.4 \pm 5.0\,cm^3$	63.98385	63.24191	64.06068	63.80707	66.022	67.709	69.141	63.0192	68.35
Atazanavir	$76.9 \pm 5.0\,cm^3$	76.79803	77.35777	76.38024	75.92749	75.472	73.759	74.339	76.8837	73.93
Lopinavir	$71.00 \pm 0.0\,cm^3$	67.97002	69.59067	69.56166	69.77134	66.022	64.959	61.005	70.698	62.65
Abacavir	$30.10 \pm 0.0\,cm^3$	31.36404	30.85648	31.77948	32.75449	32.632	34.159	32.529	31.593	33.13
Etravirine	$42.4 \pm 0.0\,cm^3$	38.39723	37.91441	37.93926	38.12713	38.302	38.284	38.179	37.74315	38.09
Nelfinavir	$64.4 \pm 0.0\,cm^3$	62.94035	61.4521	61.62312	62.19208	64.132	64.959	66.203	61.0284	65.5
Toreforant	$47.6 \pm 0.0\,cm^3$	52.10882	52.50305	52.16934	52.00645	50.902	49.834	49.705	52.5675	49.63

Table 16: Comparison of Molar Volume.

Name of drug	Molar volume of drug	Molar volume computed from regression model								
		ABC	*R*	*S*	GA	*M*1	*M*2	*F*	*H*	HM
Vidaza	$117.1 \pm 7.0\ cm^3$	129.4744	131.5672	128.2195	127.0814	131.417	136.69	142.11	129.493	139.18
Lamivudine	$132.2 \pm 5.0\ cm^3$	102.61	107.308	104.8882	102.9254	99.281	97.148	103.71	108.2263	100.182
Darunavir	$408.4 \pm 7.0\ cm^3$	351.8619	353.3656	349.7263	345.71	353.691	357.66	365.79	349.1477	362.101
Disovey		116.4869	119.1488	116.4133	114.7652	115.349	115.756	122.91	118.5559	119.154
Maraviroc	$397.8 \pm 3.0\ cm^3$	422.3142	411.1256	422.2501	431.4467	436.709	450.7	433.95	415.0744	441.678
Tenofovir	$356.1 \pm 3.0\ cm^3$	368.0517	375.0256	369.4033	358.7746	351.013	332.074	343.71	371.6296	338.386
Tipranavir	$459 \pm 3.0\ cm^3$	478.0001	472.0624	478.7512	476.3564	495.625	508.85	522.27	470.064	516.512
Atazanavir	$597.9 \pm 3.0\ cm^3$	587.2368	592.7808	583.8826	579.5126	575.965	560.022	566.43	588.5499	563.942
Lopinavir	$540.5 \pm 3.0\ cm^3$	511.9809	526.3568	525.6949	527.1179	495.625	485.59	453.15	535.687	468.028
Abacavir	$167.7 \pm 3.0\ cm^3$	199.9267	195.1032	203.2732	212.0696	211.757	225.078	211.23	201.496	217.176
Etravirine	$275.7 \pm 3.0\ cm^3$	259.8824	255.4624	255.8389	257.7958	259.961	259.968	259.23	254.0551	259.336
Nelfinavir	$463.1 \pm 3.0\ cm^3$	469.1046	456.756	457.9498	462.6113	479.557	485.59	497.31	453.0507	492.27
Toreforant	$341.7 \pm 3.0\ cm^3$	376.7693	380.224	377.2741	375.922	367.081	357.66	357.15	380.7439	357.358

Table 17: Comparison of Enthalpy.

Name of drug	Enthalpy of drug	Enthalpy computed from regression model								
		ABC	*R*	*S*	GA	*M*1	*M*2	*F*	*H*	HM
Vidaza	$93.2 \pm 3.0^{\circ}C$	86.4486	86.46836	86.1325	85.74933	86.6	86.926	88.357	86.04973	87.869
Lamivudine	$85.2 \pm 3.0^{\circ}C$	84.13075	84.3608	84.1023	83.61045	83.828	83.475	85.197	84.18003	84.539
Darunavir		105.6361	105.7375	105.407	105.1077	105.773	106.211	106.764	105.3611	106.9
Disovey		85.32805	85.38949	85.1052	84.6588	85.214	85.099	86.777	85.08817	86.159
Maraviroc		111.7147	110.7555	111.718	112.6992	112.934	114.331	112.373	111.1571	113.7
Tenofovir	$94.9 \pm 3.0^{\circ}C$	107.033	107.6192	107.119	106.2645	105.542	103.978	104.947	107.3376	104.88
Tipranavir	$109.3 \pm 3.0^{\circ}C$	116.5193	116.0495	116.634	116.6757	118.016	119.406	119.641	115.9916	120.09
Atazanavir		125.9442	126.5371	125.782	125.8096	124.946	123.872	123.275	126.4085	124.14
Lopinavir	$140.8 \pm 3.0^{\circ}C$	119.4511	120.7664	120.719	121.1703	118.016	117.376	113.953	121.761	115.95
Abacavir	$98.8 \pm 3.0^{\circ}C$	92.5272	91.98816	92.6633	93.27455	93.53	94.64	94.045	92.38	94.529
Etravirine	$94.2 \pm 3.0^{\circ}C$	97.70015	97.23197	97.2373	97.32335	97.688	97.685	97.995	97.00083	98.129
Nelfinavir	$120.1 \pm 3.0^{\circ}C$	115.7518	114.7197	114.824	115.4586	116.63	117.376	117.587	114.4959	118.02
Toreforant	$90.8 \pm 3.0^{\circ}C$	107.7851	108.0709	107.804	107.7828	106.928	106.211	106.053	108.1389	106.5

Table 18: Comparison of Molar refractivity.

Name of drug	Molar refractivity of drug	Molar refractivity computed from regression model								
		ABC	*R*	*S*	GA	*M*1	*M*2	*F*	*H*	HM
Vidaza	$51.1 \pm 5.0\ cm^3$	129.4744	131.5672	128.2195	127.0814	131.417	136.69	142.11	129.493	139.18
Lamivudine		102.61	107.308	104.8882	102.9254	99.281	97.148	103.71	108.2263	100.182
Darunavir		351.8619	353.3656	349.7263	345.71	353.691	357.66	365.79	349.1477	362.101
Disovey		116.4869	119.1488	116.4133	114.7652	115.349	115.756	122.91	118.5559	119.154
Maraviroc		422.3142	411.1256	422.2501	431.4467	436.709	450.7	433.95	415.0744	441.678
Tenofovir	$342.5 \pm 3.0\ cm^3$	368.0517	375.0256	369.4033	358.7746	351.013	332.074	343.71	371.6296	338.386
Tipranavir	$384.6 \pm 3.0\ cm^3$	478.0001	472.0624	478.7512	476.3564	495.625	508.85	522.27	470.064	516.512
Atazanavir		587.2368	592.7808	583.8826	579.5126	575.965	560.022	566.43	588.5499	563.942
Lopinavir	$512.7 \pm 3.0\ cm^3$	511.9809	526.3568	525.6949	527.1179	495.625	485.59	453.15	535.687	468.028
Abacavir	$338.4 \pm 3.0\ cm^3$	199.9267	195.1032	203.2732	212.0696	211.757	225.078	211.23	201.496	217.176
Etravirine	$339.3 \pm 3.0\ cm^3$	259.8824	255.4624	255.8389	257.7958	259.961	259.968	259.23	254.0551	259.336
Nelfinavir	$429.7 \pm 3.0\ cm^3$	469.1046	456.756	457.9498	462.6113	479.557	485.59	497.31	453.0507	492.27
Toreforant	$323 \pm 3.0\ cm^3$	376.7693	380.224	377.2741	375.922	367.081	357.66	357.15	380.7439	357.358

Table 19: Comparison of Complexity.

Name of drug	Complexity of drug	Complexity computed from regression model								
		ABC	R	S	GA	$M1$	$M2$	F	H	HM
Vidaza	384	358.4694	362.801	357.4323	355.1474	356.575	358.148	364.466	360.4039	360.904
Lamivudine	331	318.545	326.8708	322.8138	319.4574	308.071	297.407	304.306	329.0551	300.372
Darunavir	853	688.9694	691.3053	686.0992	678.1663	692.061	697.583	714.898	684.1922	706.918
Disovey		339.1682	344.4081	339.9145	336.9505	332.323	325.991	334.386	344.2817	329.82
Maraviroc	751	793.6718	776.8533	793.7084	804.8404	817.363	840.503	821.682	781.3735	830.436
Tenofovir		713.0298	723.3858	715.2955	697.469	688.019	658.28	680.306	717.3324	670.108
Tipranavir		876.429	867.1064	877.5435	871.1935	906.287	929.828	960.05	862.4326	946.592
Atazanavir	1110	1038.771	1045.902	1033.535	1023.605	1027.547	1008.434	1029.234	1037.09	1020.212
Lopinavir	940	926.9294	947.5215	947.1975	946.1926	906.287	894.098	851.762	959.166	871.336
Abacavir	414	463.1718	456.9038	468.7953	480.7156	477.835	493.922	472.754	466.542	481.968
Etravirine	609	552.2746	546.3014	546.7911	548.2751	550.591	547.517	547.954	544.0183	547.408
Nelfinavir	830	863.209	844.4362	846.6788	850.8854	882.035	894.098	920.946	837.3535	908.964
Toreforant	508	725.9854	731.0851	726.974	722.8039	712.271	697.583	701.362	730.7676	699.556

Table 20: Comparison of Boiling point.

Name of drug	Boiling point of drug	Boiling point computed from regression model								
		ABC	R	S	GA	$M1$	$M2$	F	H	HM
Vidaza	534.4 ± 6.0°C	518.8633	519.6661	516.926	514.0875	520.968	524.647	535.047	516.625	529.8
Lamivudine	475.4 ± 5.0°C	498.8286	501.5204	499.4595	495.7517	497.052	495.118	507.727	500.595	501.5
Darunavir		684.7133	685.5694	682.7527	680.0389	686.387	689.662	694.186	682.192	691.9
Disovey		509.1776	510.3772	508.0875	504.7388	509.01	509.014	521.387	508.381	515.3
Maraviroc		737.2546	728.7734	737.0462	745.1179	748.17	759.142	742.679	731.885	749.7
Tenofovir	642.7.5 ± 55°C	696.7872	701.7709	697.4835	689.9557	684.394	670.555	678.477	699.138	674.6
Tipranavir	712.3 ± 37°C	778.7834	774.3537	779.3447	779.2069	792.016	802.567	805.515	773.334	804.1
Atazanavir		860.2489	864.65	858.0492	857.5083	851.806	840.781	836.933	862.644	838.5
Lopinavir	924.2 ± 55°C	804.1253	814.9654	814.4882	817.7378	792.016	785.197	756.339	822.798	768.8
Abacavir	636 ± 55°C	571.4046	567.1905	573.1135	578.5983	580.758	590.653	584.223	570.898	586.5
Etravirine	637.4 ± 55°C	616.1177	612.3387	612.4658	613.3071	616.632	616.708	618.373	610.515	617.2
Nelfinavir	786.8 ± 37°C	772.1494	762.9046	763.7721	768.7736	780.058	785.197	787.757	760.51	786.5
Toreforant	611.2 ± 55°C	703.2885	705.6593	703.3758	702.9715	696.352	689.662	688.039	706.008	688.4

Table 21: Comparison of flash point.

Name of drug	Flash point of drug	Flash point computed from regression model								
		ABC	R	S	GA	$M1$	$M2$	F	H	HM
Vidaza	277 ± 32°C	267.5661	268.0535	266.3963	264.6722	268.815	271.007	277.327	266.2176	274.362
Lamivudine	241.3 ± 30°C	255.4514	257.0814	255.8345	253.5855	254.355	253.157	260.807	256.5247	257.194
Darunavir		367.8536	368.3696	366.6693	365.0142	368.83	370.757	373.556	366.3314	372.498
Disovey		261.7093	262.4368	261.0518	259.0196	261.585	261.557	269.067	261.2327	265.546
Maraviroc		399.6247	394.4936	399.4998	404.364	406.185	412.757	402.879	396.3794	407.53
Tenofovir	342.5 ± 31.5°C	375.1545	378.1661	375.5768	371.0103	367.625	359.207	364.057	376.5782	362.058
Tipranavir	384.6 ± 26.5°C	424.7367	422.0545	425.077	424.9758	432.695	439.007	440.875	421.4425	440.474
Atazanavir		473.9979	476.6536	472.6685	472.3205	468.845	462.107	459.873	475.4458	461.354
Lopinavir	512.7 ± 34.3°C	440.0606	446.611	446.3278	448.2734	432.695	428.507	411.139	451.352	419.13
Abacavir	338.4 ± 31.5°C	299.3372	296.7899	300.372	303.6785	304.965	310.907	307.063	299.035	308.698
Etravirine	339.3 ± 26.5°C	326.3747	324.0895	324.1678	324.665	326.655	326.657	327.713	322.9903	327.258
Nelfinavir	429.7 ± 31.5°C	420.7252	415.1316	415.6605	418.6673	425.465	428.507	430.137	413.6882	429.802
Toreforant	90.8 ± 34.3°C	379.0858	380.5173	379.1398	378.8803	374.855	370.757	369.839	380.7323	370.41

(7) Regression models of $M2(G)$ are as follows:

Boiling point = 342.262 + 1.737 $[M2(G)]$
Enthalpy = 65.611 + 0.203 $[M2(G)]$
Flash point = 160.757 + 1.050 $[M2(G)]$
Molar refractivity = −4.752 + 0.695 $[M2(G)]$
Polarity = −5.166 + 0.275 $[M2(G)]$
Molar volume = −107.540 + 2.326 $[M2(G)]$
Complexity = −17.017 + 3.573 $[M2(G)]$

(8) Regression models of $F(G)$ are as follows:

Boiling point = 375.225 + 0.683 $[F(G)]$
Enthalpy = 69.871 + 0.079 $[F(G)]$

Flash point = 180.685 + 0.413 [$F(G)$]
Molar refractivity = −6.426 + 0.285 [$F(G)$]
Polarity = −2.049 + 0.113 [$F(G)$]
Molar volume = −82.830 + 0.960 [$F(G)$]
Complexity = 12.530 + 1.504 [$F(G)$]

(9) Regression models of $H(G)$ are as follows:

Boiling point = 341.898 + 22.900 [$H(G)$]
Enthalpy = 65.670 + 2.671 [$H(G)$]
Flash point = 160.565 + 13.847 [$H(G)$]
Molar refractivity = −12.255 + 8.994 [$H(G)$]
Polarity = −3.957 + 3.555 [$H(G)$]
Molar volume = −102.314 + 30.381 [$H(G)$]
Complexity = 18.702 + 44.784 [$H(G)$]

Tables [4–7, 11–14, 16] represent the statistical parameters used in QSPR models of TIs.

3.1. Statistical Parameters Comparison between TIs and Correlation Coefficient of Properties. The correlation between Therapeutic Indices (TIs) and the physical properties of drugs used for HIV disease treatment, including medications like lamivudine, darunavir, disovey, maraviroc, tenofovir, tripranavir, atazanavir, lopinavir, abacavir, etravirine, nelfinavir, toreforant, is effectively established through the implementation of Quantitative Structure-Property Relationship (QSPR) modeling. This sort of analysis can be useful for the model. It is eminent that the value of p is less than 0.05 and r is greater than 0.6. Hence, it concluded entirely properties given in Tables 3–11 which are significant. Table 12 lists the correlation coefficients. Figure 3 depicts the graph.

3.2. Standard Error of Estimate (SEE), Correlation Determination, and Comparison. Measure of variation for an observation calculated around the computed regression line is said to be the standard error estimate. It examines the extent of accuracy of predictions made about the calculated regression line in Table 13. Table 14 shows correlation. Tables 15–21 compare the physicochemical properties of the experimental and theoretical calculated tenets of the models.

4. Conclusions

It is noted harmonic $H(G)$ provides the maximum correlated value of molar polarity $r = 0.979$. The ABC(G) index provides a high correlated value for molar volume $r = 0.984$. The $H(G)$ index offers the maximum correlated value of the flash point, i.e., $r = 0.882$. GA(G) and $H(G)$ indices depict the utmost correlation coefficient of BP $r = 0.877$. Harmonic $H(G)$ provides the maximum correlated value of molar refractivity $r = 0.989$. No correlation is present between TIs and density, polar surface area, and surface tension. In this work, the TIs for drugs used to treat HIV disease were computed, and they were contrasted with a linear QSPR model. Using the data gathered in this manner, the pharmaceutical industry will be able to create new medications to discover preventative treatments for the aforementioned illness. The variety of topological indicators for these medications is strongly affected by the correlation coefficient. The results offer a technique to evaluate physicochemical features for new discoveries of other disorders and are eye-opening for researchers working on drug science in the pharmaceutical sector [28].

Data Availability

The data used to support the findings of this study are available upon reasonable request to the corresponding author.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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