AIMS Mathematics, 7(7): 11829–11850.
DOI: 10.3934/math.2022660
Received: 05 December 2021
Revised: 20 February 2022
Accepted: 02 March 2022
Published: 19 April 2022

http://www.aimspress.com/journal/Math

*Research article*

# Topological indices of novel drugs used in blood cancer treatment and its QSPR modeling

**Sumiya Nasir[1], Nadeem ul Hassan Awan[2], Fozia Bashir Farooq[3,*] and Saima Parveen[2]**

[1] Department of Mathematics and Natural Sciences, College of sciences and Human Studies, Prince Mohammad Bin Fahd University, Khobar 31952, Saudi Arabia
[2] Department of Mathematics, Government College University Faisalabad, Pakistan
[3] Department of Mathematics and statistics, Imam Mohammad Ibn Saud Islamic University, Riyadh 11564, Saudi Arabia

* **Correspondence:** Email: ffarooq@imamu.edu.sa.

**Abstract:** A topological index is a real number obtained from the chemical graph structure. It can predict the physicochemical and biological properties of many anticancer medicines like blood, breast and skin cancer. This can be done through degree-based topological indices. . In this article, the drugs, azacitidine, buslfan, mercaptopurine, tioguanine, nelarabine, etc. which are used in order to cure blood cancer are discussed and the purpose of the QSPR study is to determine the mathematical relation between the properties under investigation (eg, boiling point, flash point etc.) and different descriptors related to molecular structure of the drugs. It is found that topological indices (TIs) applied on said drugs have a good correlation with physicochemical properties in this context.

**Keywords:** Drugs; blood cancer; linear QSPR model; degree-based topological indices
**Mathematics Subject Classification:** 05C09, 05C12, 05C31, 05C07, 05C92, 92E10

## 1. Introduction

Cancer is a dangerous disease and belongs to the family of genetic diseases. It is the uncontrolled magnification of abnormal blood cells in the body that stops normal functions and is prone to infection. The cancer that affects blood cells is known as blood cancer. Leukemia is an example of blood cancer and a mutation in the DNA of blood cells is its main cause, resulting in abnormal behavior of blood

cells. This will not only prone to infection but also in some cases becomes chronic and creates tumors in bones. Throughout the world, nearly 1.24 million people are affected by blood cancer annually. Medicos and scientists are always probing for better ways to care for people fighting cancer. One way to do this is to develop and study incipient drugs. Drug revelation is not an easy task, as it is expensive, time consuming, and challenging in some cases. Numerous ways have been discovered to treat cancer. Drug therapy is one of them. Drug therapy is used to stop the growth of cancer cells and eliminate them from the body, as well as to restore healthy cells. Anticancer drugs are also used to kill and halt this malignant disease and many drugs test are accompanied to fight the fatal disease. This requires timely diagnosis, screening, and medication that benefits patients to control the deadly disease in the future. For further detail see [1–3,14].

Topological Indices (TIs) are termed as numeric descriptors that are obtained from molecular graphs to describe chemical system and are mostly used to investigate the physiochemical properties of several drugs. There are several kinds of polynomials and topological indices which are extensively calculated, represent chemical structure and have vital position in chemical graph theory. Among these classes, degree-based topological indices are of great importance and particularly in chemistry. The use of graph invariants (TIs) in QSPR and QSAR studies has been of key interest in recent years. Topological indices have application in various areas of biology, mathematics, bioinformatics, mathematics, informatics, biology etc., but their utmost significant use to date is in the non-empirical Quantitative Structure- Property Relationships (QSPR) and Quantitative Structure -Activity Relationships (QSAR) [5,18,26]. The ABC index, Wiener index and Randic index are helpful for predicting the bioactivity of drugs. The QSPR models help to determine the optimal relationship between the topological indices and psychochemical characteristic. These psychochemical qualities are being studied because they have a big impact on bioactivity and drug transit in the human body. In this paper, we compute degree-based TIs related to blood cancer drugs. In the same way, anticancer drugs represent chemical compounds on which given topological indices are well defined and discussed in QSPR analysis. The corresponding characteristic calculated in this way is highly correlated with characteristic of blood cancer drugs by the use of linear regression.

## 2. Material and method

In drugs, structure elements denote vertices, and corresponding bonds connecting the atoms are termed edges. Graph G (V, E) is considered as simple, finite, and connected, whereas V and E represented in chemical graph are termed as vertex and edge sets, respectively. Degree of vertex in graph G is number of vertices adjacent to it and is denoted by $d_u$. Valence of a compound in chemistry and the degree of vertex in the graph are closely related concepts, for more details see [4,10,11,13]. Degree-based topological indices used are defined below:

**Def. 2.1 The** ABC index [13] of a molecular graph G is defined as

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

**Def. 2.2** The first-degree-based topological index is Randic index $X(G)$ introduced by Milan Randic in 1975 [15]. Randic index is defined as:

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

**Def. 2.3** The sum connectivity index [16] of a molecular graph G is defined as

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

**Def. 2.4** The GA index [17] of a molecular graph G is defined as:

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

**Def. 2.5** The first and second Zagreb indices [19] of a molecular graph G are defined as follows:

$$M1(G) = \sum_{uv \in E(G)} (d_u + d_v)$$

$$M2(G) = \sum_{uv \in E(G)} (d_u d_v)$$

**Def. 2.6** The harmonic index [20] of a molecular graph G is defined as:

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

**Def. 2.7** The hyper Zagreb index [21] of a molecular graph G is defined as:

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

**Def. 2.8** The forgotten index [23] of a molecular graph G is defined as:

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

The values of physical properties are taken from Chem Spider. It is observed from data Tables 2 and is found these data values are normally distributed. So, linear regression model is most adequate to test and adopt for said analysis. For more information on degree-based topological indices, we refer the reader to visit the following articles [4–9,22,27,28].

The molecular formula for bulasan is $C_8H_{14}N_6S_2$. Busulfan is an antineoplastic alkylating agent and is used for many kinds of cancer. Alkylating agents have the ability to add alkyl groups to several electronegative groups under conditions present in cells. They prohibit tumor development by crosslinking guanine bases in DNA double-helix strands, directly attacking DNA. The strands are unable to separate and uncoil. It is mandatory in DNA replication and cells are no longer divide. The molecular formula of clofarabine is $C_{10}H_{11}ClF\ N_5\ O_5$. Clofarabine interfere in growth of cancer cells. Clofarabine prevents cells from making DNA and RNA by interfering with the synthesis of nucleic acids, thus stopping the growth of cancer cells. The chemical formula of azacitidine is $C_8H_{12}N_4O_5$. Azacytidine has been used as an antineoplastic agent. The molecular formula of meracptopurine is $C_5H_4N_4S$. Mercaptopurine is one of a large series of purine analogues that interfere with nucleic acid

biosynthesis and have been found active against human leukemias. The molecular formula of Tioguanine is $C_5H_5N_5S$. Antineoplastic compound which also has antimetabolite action. The drug is used in the therapy of acute leukemia.

The molecular formula of nelarabine is $C_{11}H1_5N_5$ $S_5$**.** Nelarabine is a purine nucleoside analog and antineoplastic agent used for the treatment of acute T-cell lymphoblastic leukemia and T cell lymphoblastic lymphoma with inadequate clinical response to prior chemotherapeutic treatments. The molecular formula of cytarabine is $C_{11}H1_5N_5$ $S_5$. Cytarabine is an antineoplastic antimetabolite used in the treatment of several forms of leukemia, including acute myelogenous leukemia and meningeal leukemia. The molecular formula of bosutinib is $C_{26}H_{29}Cl_2N_5$ $O_5$. It is used to treat a certain type of chronic myeloid leukemia (a cancer of white blood cells). The molecular formula of dasatinib is $C_{22}H_{26}ClN_7S$.Dasatinib is a tyrosine kinase inhibitor used for the treatment of lymphoblastic or chronic myeloid leukemia. The molecular formula of melphala is $C_{13}H_{18}Cl_2N_2$ $O_2$. Melphalan is an antineoplastic in the class of alkylating agents and is used to treat various forms of cancer. Alkylating agents are so named because of their ability to add alkyl groups to many electronegative groups under conditions present in cells. They stop tumor growth by crosslinking guanine bases in DNA. The molecular formula of dexamethasone is $C_{22}H_{29}FO_5$. Dexamethasone is a glucocorticoid available in various modes of administration that is used for the treatment of various inflammatory conditions, including bronchial asthma, as well as endocrine and rheumatic disorders. The molecular formula of doxorubicine is $C_{27}H_{29}NO_{11}$. Doxorubicin is an antineoplastic in the anthracycline class. Anthracyclines are among the most important antitumor drugs available. Doxorubicin is widely used for the treatment of several solid tumors while daunorubicin and idarubicin are used exclusively for the treatment of leukemia. The molecular formula of carbopalatin is $C_6H_{12}N_2O_4Pt$. Carboplatin is a alkylating agent used to treat advanced ovarian cancer.

## 3. Results and discussions

In this section, degree-based TIs are imposed on blood cancer drugs. The relation between QSPR analysis and topological indices depicts that they are highly correlated as regards physicochemical properties use to cure blood cancer. The thirteen medicines azacitidine, buslfan, mercaptopurine, tioguanine, nelarabine, cytarabine, clofarabine, bosutinib, dasatinib, melphala, dexamethasone, doxorubicine, carboplatin are used for this analysis of said disease. The chemical structure for given drugs is shown in Figure 1. In drugs, structure elements denote vertices, and corresponding bonds connecting the atoms are termed edges. Hence, the study used regression analysis for the calculation purpose.

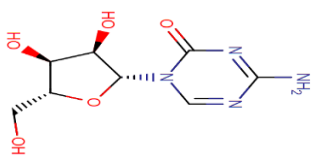
### *3.1. Regression model*

In this article, quantitative structure analysis about nine topological indices is calculated for QSPR modeling purpose. Five physical properties, boiling point (BP), molar volume (MV), molar refractivity (R), complexity and flash point (FP), for 13 medicines arranged in Figure 1, are investigated. We execute the regression analysis for the drugs and tested linear regression model is tested with the help of equation as under:

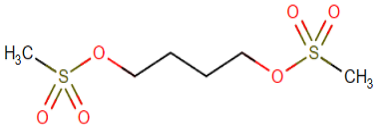
$$P = A + b\,(TI) \tag{1}$$

Here, P is the physicochemical property of the candidate drug. The TI, A, and b represent topological index, constant and regression coefficient, respectively. All data tables are calculated by

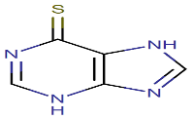
the use of SPSS software version-26 to obtain accurate results. The nine TIs of candidate blood cancer drugs and their physical property are investigated with the help of linear QSPR model. By applying Eq 1, we calculate linear regression model for degree based TIs of candidate drugs given as under.



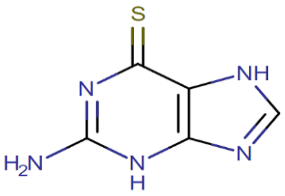
(a) Azacitidine



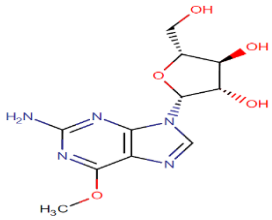
(b) Buslfan



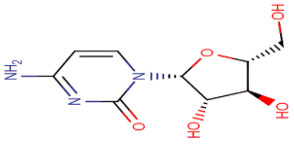
(c) Mercaptopurine



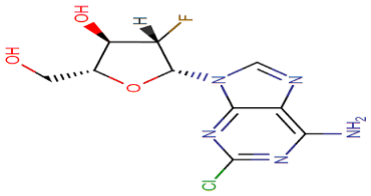
(d) Tioguanine



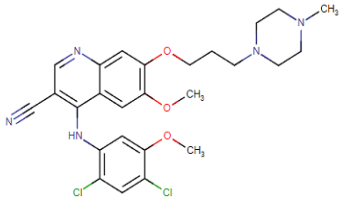
(e) Nelarabine



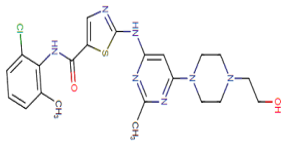
(f) Cytarabine



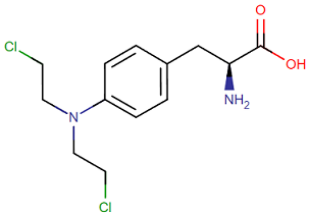
(g) Clofarabine



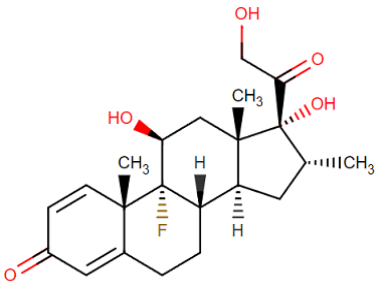
(h) Bosutinib



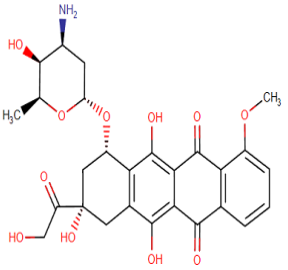
(i) Dasatinib



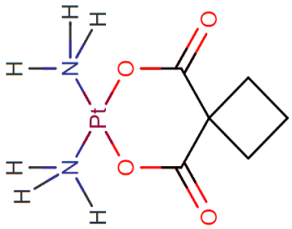
(j) Melphala



(k) Dexamethasone



(l) Doxorubicine



(m) Carboplatin

**Figure 1.** Molecular structure of drugs.

**Theorem 1.** Let $G_1$ be the graph of Azacitidine, the various topological indices of G are given as follows.

i) $ABC(G_1) = 22.04$
ii) $RA(G_1) = 13.12$
iii) $S(G_1) = 13.46$
iv) $GA(G_1) = 27.72$
v) $M1(G_1) = 162$
vi) $M2(G_1) = 209$
vii) $F(G_1) = 516$
viii) $H(G_1) = 11.95$
ix) $HM(G_1) = 934.00$

**Proof.** Let $G_1$ be the graph of Azacitidine with edge set E, Let $E_{m,n}$ represents the class of edges of G joining vertices of degrees $m$ and $n$. With $|E_{1,2}| = 3$, $|E_{1,3}| = 4$, $|E_{1,4}| = 6$, $|E_{2,3}| = 4$, $|E_{2,4}| = 5$, $|E_{3,3}| = 3$, $|E_{3,4}| = 1$, $|E_{4,4}| = 4$.

i) By using definition 2.1 and above given edge partitions $E_{m,n}$we get,

$$(G_1) = = 3\sqrt{\tfrac{1+2-2}{1\times2}} + 4\sqrt{\tfrac{1+3-2}{1\times3}} + 6\sqrt{\tfrac{1+4-2}{1\times4}} + 4\sqrt{\tfrac{2+3-2}{2\times3}} \quad 5\sqrt{\tfrac{2+4-2}{2\times4}} + 3\sqrt{\tfrac{3+3-2}{3\times3}} + 1\sqrt{\tfrac{3+4-2}{3\times4}} = 22.04.$$

ii) By using Definition 2.2 and above given edge partitions $E_{m,n}$we get,

$$RA(GG_1) = = 3\sqrt{\frac{1}{1\times2}} + 4\sqrt{\frac{1}{1\times3}} + 6\sqrt{\frac{1}{1\times4}} + 4\sqrt{\frac{1}{2\times3}} \quad 5\sqrt{\frac{1}{2\times4}} + 3\sqrt{\frac{1}{3\times3}} + 1\sqrt{\frac{1}{3\times4}} + 4\sqrt{\frac{1}{4\times4}} = 13.12.$$

iii) By using Definition 2.3 and above given edge partitions $E_{m,n}$we get,

$$S(G_1) = = 3\sqrt{\tfrac{1}{1+2}} + 4\sqrt{\tfrac{1}{1+3}} + 6\sqrt{\tfrac{1}{1+4}} + 4\sqrt{\tfrac{1}{2+3}} \quad 5\sqrt{\tfrac{1}{2+4}} + 3\sqrt{\tfrac{1}{3+3}} + 1\sqrt{\tfrac{1}{3+4}} + 4\sqrt{\tfrac{1}{4+4}} = 13.46.$$

iv) By using definition 2.4 and above given edge partitions $E_{m,n}$we get,

$$GA(G_1) = = \frac{6\sqrt{1\times2}}{1+2} + \frac{8\sqrt{1\times3}}{1+3} + \frac{12\sqrt{1\times4}}{1+4} + \frac{8\sqrt{2\times3}}{2+3} + \frac{10\sqrt{2\times4}}{2+4} + \frac{6\sqrt{3\times3}}{3+3} + \frac{2\sqrt{3\times4}}{3+4} + \frac{8\sqrt{4\times4}}{4+4} = 27.72$$

v) By using Definition 2.5 and above given edge partitions $E_{m,n}$we get,

$$M1(G_1) = \sum_{uv\in E(G_1)}(s_{u+}s_v) = 3(1+2) + 4(1+3) + 6(1+4) + 4(2+3) + 5(2+4) + 3(3+3) + 1(3+4) + 4(4+4) = 162.$$

vi) By using Definition 2.5 and above given edge partitions $E_{m,n}$we get,

$$M2(G_1) = 3(1\times2) + 4(1\times3) + 6(1\times4) + 4(2\times3) + 5(2\times4) + 3(3\times3) + 1(3\times4) + 4(4\times4) = 209.$$

vii) By using definition 2.6 and above given edge partitions $E_{m,n}$we get,

$$H(G_1) = 6\left(\frac{1}{1+2}\right) + 8\left(\frac{1}{1+3}\right) + 12\left(\frac{1}{1+4}\right) + 8\left(\frac{1}{2+3}\right) + 10\left(\frac{1}{2+4}\right) + 6\left(\frac{1}{3+3}\right) + 2\left(\frac{1}{3+4}\right) + 8\left(\frac{1}{4+4}\right) = 11.95$$

viii) By using definition 2.7 and above given edge partitions $E_{m,n}$we get,

$$HM(G_1) = 3(1+2)^2 + 3(1+3)^2 + 6\,(1+4)^2 + 4(2+3)^2 + 5(2+4)^2 + 3(3+3)^2 + 1(3+4)^2 + 4\,(4+4)^2 = 934$$

ix) By using definition 2.8 and above given edge partitions $E_{m,n}$we get,

$$F(G_1) = 3(1+4) + 4(1+9) + 6(1+16) + 4(4+9) + 5(4+16) + 3(9+9) + 1(9+16) + 4(16+16) = 516.$$

**Theorem2.** Let $G_2$ be the graph of Buslfan, The various Topological indices of $G_2$ are given as follows.

i) $ABC(G_2) = 20.77$
ii) $RA(G_2) = 11.31$
iii) $S(G_2) = 11.04$
iv) $GA(G_2) = 22.23$
v) $M1(G_2) = 148$
vi) $M2(G_2) = 176$
vii) $F(G_2) = 526$
viii) $H(G_2) = 9.45$
ix) $HM(G_2) = 878.00$

**Proof.** Let $G_2$ be the graph of Buslfan with edge set $E'$ , Let $E'_{(m,n)}$ represents the class of edges of $G_2$ joining vertices of degrees $m$ and $n$. With $|E'_{(1,4)}| = 18$, $|E'_{(2,4)}| = 3$, $|E'_{(4,4)}| = 5$.

i) By using definition 2.1 and edge partitions $E'_{(m,n)}$) we get,

$$(G_2) = = 18\sqrt{\tfrac{1+4-2}{1\times4}} + 3\sqrt{\tfrac{2+4-2}{2\times4}} + 5\sqrt{\tfrac{4+4-2}{4\times4}} = 20.77.$$

ii) By using def 2.2 and edge partition $E'_{(m,n)}$) we get,

$$RA(G_2) = 18\sqrt{\frac{1}{1\times4}} + 3\sqrt{\frac{1}{2\times4}} + 5\sqrt{\frac{1}{4\times4}} = 11.31$$

iii) Definition 2.3 and edge partition $E'_{(m,n)}$) gives

$$S(G_2) = 18\sqrt{\tfrac{1}{1+4}} + 3\sqrt{\tfrac{1}{2+4}} + 5\sqrt{\tfrac{1}{4+4}} = 11.04.$$

iv) Using def 2.4 and edge partition $E'_{(m,n)}$) we get,

$$GA(G_2) = \frac{36\sqrt{1\times4}}{1+4} + \frac{6\sqrt{2\times4}}{2+4} + \frac{10\sqrt{4\times4}}{4+4} = 22.23$$

v) Using def 2.5 and edge partition $E^{'}_{(m,n)}$) we get,

$$M1(G_2) = 18(1+4) + 3(2+4) + 5(4+4) = 148$$

vi) Using def 2.5 and edge partition $E^{'}_{(m,n)}$) we get,

$$M2(G_2) = 18(1\times 4) + 3(2\times 4) + 5(4\times 4) = 176$$

vii) Using def 2.6 and edge partition $E^{'}_{(m,n)}$) we get,

$$H(G_2) = 36\left(\frac{1}{1+4}\right) + 6\left(\frac{1}{2+4}\right) + 10\left(\frac{1}{4+4}\right) = 9.45$$

viii) Using def 2.7 and edge partition $E^{'}_{(m,n)}$) we get,

$$HM(G) = 18(1+4)^2 + 3(2+4)^2 + 5\,(4+4)^2 = 878$$

ix) By using def 2.8 and edge partition $E^{'}_{(m,n)}$) we get,

$$F(G_2) = 18(1+16) + 3(4+16) + 5(16+16) = 526$$

One can calculate the topological indices of the remaining drugs by adopting a similar procedure applied in Theorem 1, Theorem 2 and using definitions 2.1 to 2.8. Also, the calculated values of all drugs are listed in Table 2.

Using (1), we have calculated the following diverse linear models for all degree-based topological index, which are given as under:

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

Boiling point = 395.921 + 5.802 [ABC (G)]
Refractive index = 6.034 + 2.468 [ABC (G)]
FP = 197.699 + 3.486 [ABC (G)]
MV = -10.083 + 7.258 [ABC (G)]
Complexity = -107.244 + 18.352 [ABC (G)]

**2. Regression models for the atom-bond connectivity index RA (G)]:**

Boiling point = 385.002+ 10.833[RA (G)]
Refractive index = 4.535 + 4.408 [RA (G)]
FP = 191.561+ 6.451[RA (G)]
MV = -14.889 + 12.947 [RA (G)]
Complexity = -125.985+ 33.119 [RA (G)]

**3. Regression models for atom bond connectivity index S (G):**

Boiling point = 384.612+ 10.664 [S (G)]
Refractive Index = 5.102 + 4.293 [S (G)]
FP = 191.365+ 6.348 [S (G)]
MV = -11.972 + 12.540 [S (G)]
Complexity = -125.538 + 32.402 [S (G)]

**4. Regression models for atom bond connectivity index GA (G):**

Boiling point = 386.718+ 5.013 [GA (G)]
Refractive Index = 6.258 + 2.010 [GA (G)]
FP = 192.642 + 2.985 [GA (G)]
MV = -7.333 + 5.841 [GA (G)]
Complexity = 121.577 + 15.270 [GA (G)]

**5. Regression models for atom bond connectivity index M1 (G):**

Boiling point = 405.004+ .738 [M1 (G)]
Refractive Index = 9.310 + .318[M1 (G)]
FP = 202.599 + 0.448 [M1 (G)]
MV = 1.253 +.932 [M1 (G)]
Complexity = -97.937 + 2.432 [M1 (G)]

**6. Regression models for atom bond connectivity index HM (G):**

Boiling point = 419.068 +.115 [HM (G)]
Refractive index = 13.368 + 0.052 [HM (G)]
FP = 210.170 + 0.071 [HM (G)]
MV = 13.491 + .151 [HM (G)]
Complexity = -78.956 +.404 [HM (G)]

**7. Regression models for atom bond connectivity index M2 (G):**

Boiling point = 414.903+ .535 [M2 (G)]
Refractive index = 13.461 +.233 [M2 (G)]
FP = 208.190 +.327 [M2 (G)]
MV = 15.185 + .677 [M2 (G)]
Complexity = -87.855 + 1.849 [M2 (G)]

**8. Regression models for the atom-bond connectivity index F (G):**

Boiling point = 422.835+ .200 [F (G)]
Refractive Index = 13.494 + .092 [F (G)]
FP = 212.010 +.124 [F (G)]
MV = 13.736 +.273 [F (G)]
Complexity = -71.482 +.717 [F (G)]

**9. Regression models for atom bond connectivity index H (G):**

Boiling point = 377.349 + 12.647 [H (G)]
Refractive Index = 4.240 + 4.943 [H (G)]
FP = 187.144+ 7.500 [H (G)]
MV = -14.817 + 14.434 [H (G)]
Complexity = -136.607 + 37.543 [H (G)]

### *3.2. Quantitative structure analysis and comparison between topological indices and correlation coefficient of physicochemical properties*

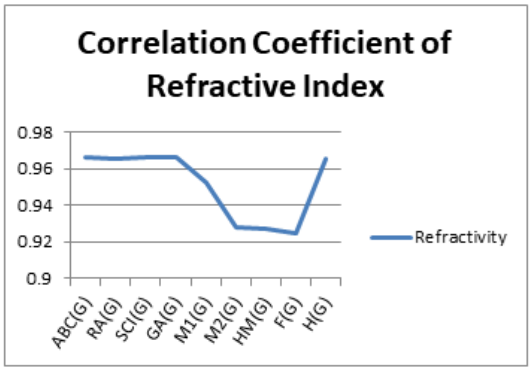
The physicochemical properties of 13 blood cancer drugs are presented in Table 2. Their TI values are listed in Table 1 and computed from their molecular structure. The correlation coefficient between five physicochemical properties and TIs is listed in Table 3. The graph between the correlation coefficient of the physicochemical properties of the drug and the topological index is drawn in Figure 2.

**Table 1.** The TI values of candidate drugs.

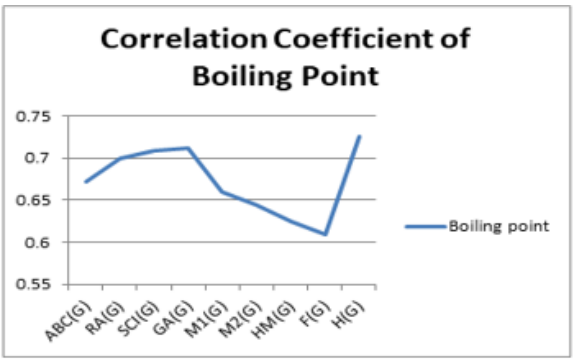
| Name of drug | ABC(G) | RA(G) | S(G) | GA(G) | M1(G) | M2(G) | F(G) | H(G) | HM(G) |
|---|---|---|---|---|---|---|---|---|---|
| Azacitidine | 22.04 | 13.12 | 13.46 | 27.72 | 162 | 209 | 516 | 11.95 | 934.00 |
| Buslfan | 20.77 | 11.31 | 11.04 | 22.23 | 148 | 176 | 526 | 9.45 | 878.00 |
| Mercaptopurine | 10.91 | 6.52 | 6.74 | 14.25 | 76 | 93 | 210 | 6.10 | 396.00 |
| Tioguanine | 12.39 | 7.43 | 7.65 | 16.12 | 86 | 105 | 238 | 6.93 | 448.00 |
| Nelarabine | 27.99 | 16.29 | 16.67 | 35.13 | 206 | 262 | 652 | 14.85 | 1176.00 |
| Cytarabine | 22.77 | 13.55 | 13.68 | 28.62 | 168 | 218 | 536 | 12.32 | 972.00 |
| Clofarabine | 24.24 | 14.04 | 14.43 | 30.59 | 180 | 233 | 570 | 12.82 | 1036.00 |
| Bosutinib | 51.18 | 28.73 | 29.39 | 61.92 | 374 | 467 | 1198 | 25.39 | 2132.00 |
| Dasatinib | 45.50 | 25.95 | 26.60 | 56.11 | 330 | 412 | 1028 | 23.43 | 1852.00 |
| Melphala | 28.12 | 16.18 | 16.15 | 33.33 | 202 | 252 | 656 | 14.28 | 1160.00 |
| Dexamethasone | 44.81 | 24.85 | 25.37 | 54.14 | 354 | 493 | 1242 | 21.86 | 2228.00 |
| Doxorubicine | 52.32 | 30.01 | 30.76 | 65.33 | 396 | 522 | 1288 | 27.11 | 2332.00 |
| Carboplatin | 19.82 | 10.76 | 10.95 | 23.16 | 152 | 202 | 532 | 9.34 | 936.00 |

**Table 2.** Physical properties of drugs.

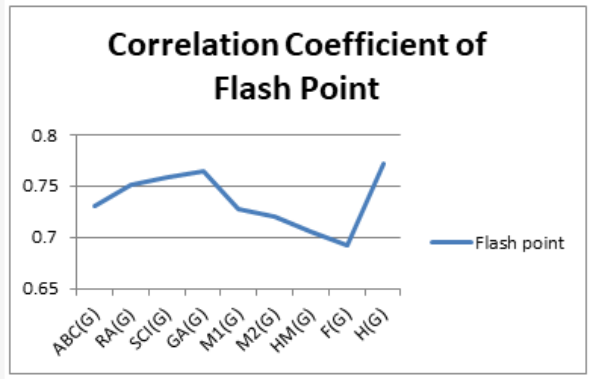
| Name of drug | Molar volume ($cm^3$) | Boiling Point ℃ | Refractive Index ($m^3$ $mol^{-1}$) | Complexity | Flash Point ℃ |
|---|---|---|---|---|---|
| Azacitidine | 117.10 | 534.21 | 54.10 | 384.00 | 277.00 |
| Buslfan | 182.40 | 464.00 | 50.90 | | 234.40 |
| Mercaptopurine | 94.20 | 491.00 | 41.00 | 19.00 | 250.50 |
| Tioguanine | 80.20 | 460.70 | 46.89 | 225.00 | 232.00 |
| Nelarabine | 149.90 | 721.00 | 65.80 | 377.00 | 389.90 |
| Cytarabine | 128.40 | 547.70 | 52.60 | 383.00 | 283.80 |
| Clofarabine | 143.10 | 550.00 | 63.60 | 370.00 | 286.40 |
| Bosutinib | 388.30 | 649.70 | 142.12 | 734.00 | 346.70 |
| Dasatinib | 366.40 | | 133.08 | 642.00 | |
| Melphala | 231.20 | 473.00 | 78.23 | 265.00 | 239.00 |
| Dexamethasone | 296.20 | 568.20 | 100.20 | 805.00 | 298.00 |
| Doxorubicine | 336.60 | 216.00 | 134.59 | 977.00 | 443.80 |
| Carboplatin | | 366.40 | 60.04 | 177.00 | |



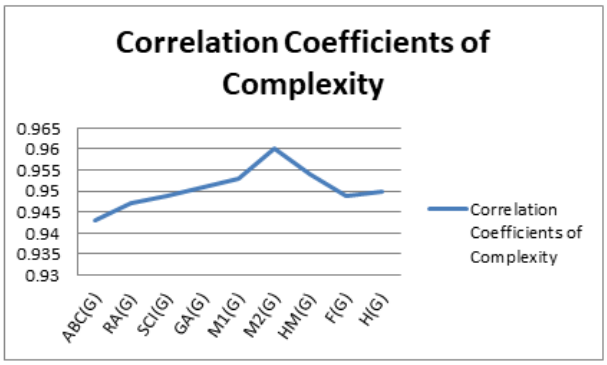

(i) Refractive index on TI



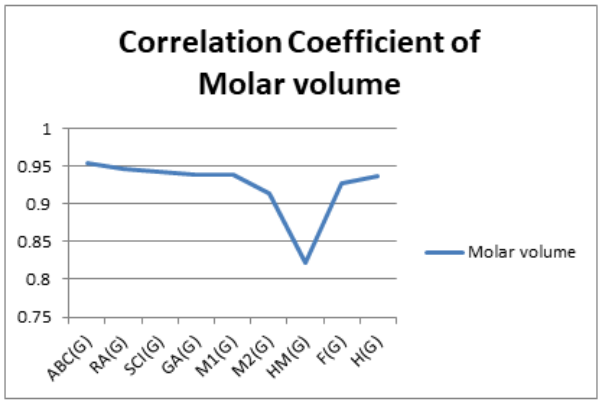

(ii) Boiling Point on TI




(ii) Flash Point in TI




(iv) Complexity on TI




(v) Molar volume on TI

**Figure 2.** Physicochemical properties and Tis.

**Table 3.** Correlation coefficients.

| Topological Index | Correlation coefficient of complexity | Correlation coefficient of refractive index | Correlation coefficient of flash point | Correlation coefficient of boiling point | Correlation coefficient of molar volume |
|---|---|---|---|---|---|
| ABC(G) | 0.943 | 0.966 | 0.731 | 0.672 | 0.953 |
| RA(G) | 0.947 | 0.965 | 0.751 | 0.7 | 0.946 |
| S(G) | 0.949 | 0.966 | 0.759 | 0.708 | 0.942 |
| GA(G) | 0.951 | 0.966 | 0.764 | 0.711 | 0.938 |
| M1(G) | 0.953 | 0.952 | 0.728 | 0.66 | 0.939 |
| M2(G) | 0.96 | 0.928 | 0.72 | 0.645 | 0.913 |
| HM(G) | 0.954 | 0.927 | 0.705 | 0.625 | 0.822 |
| F(G) | 0.949 | 0.925 | 0.692 | 0.609 | 0.927 |
| H(G) | 0.95 | 0.965 | 0.772 | 0.725 | 0.936 |

### *3.3. Calculation of statistical parameters*

In this section, QSPR modeling is done to find a relation between physicochemical properties of blood cancer drugs such as medicines azacitidine, buslfan, mercaptopurine, tioguanine, nelarabine, cytarabine, clofarabine, bosutinib, dasatinib, melphala, dexamethasone, doxorubicine, carboplatin and their calculated degree based TIs. whereas TIs, b, r, and N are independent variable, regression model constant, correlation coefficient and sample size respectively. We perceive the correlation coefficient come to be one the experimental and theoretical calculation are close that are marked bold in tables. This type of test can helpful to compare and decide the improvement of model. It is noted the value of r is greater than 0.6 and p value is less than 0.05. Hence, it decides all properties are significant. Tables 4–12 Represent the Statistical parameters used in QSPR models of TIs.

**Table 4.** Statistical parameters used in the QSPR model of ABC (G).

| Physiochemical Property | N | A | b | r | $r^2$ | F | p | Indicator |
|---|---|---|---|---|---|---|---|---|
| Boiling Point | 12 | 395.921 | 5.802 | .672 | .451 | 8.228 | .017 | Significant |
| Refractive index | 13 | 6.034 | 2.468 | .966 | .933 | 154.093 | .000 | Significant |
| Flash point | 11 | 197.699 | 3.486 | .731 | .535 | 10.343 | .011 | Significant |
| Molar volume | 12 | −10.083 | 7.258 | .953 | .909 | 99.904 | .000 | Significant |
| Complexity | 12 | −107.244 | 18.352 | .943 | .889 | 79.955 | .000 | Significant |

**Table 5.** Statistical parameters used in the QSPR model of RA (G).

| Physiochemical Property | N | A | b | r | $r^2$ | F | p | Indicator |
|---|---|---|---|---|---|---|---|---|
| Boiling Point | 12 | 385.002 | 10.833 | .700 | .490 | 9.614 | .011 | Significant |
| Refractive index | 13 | 4.535 | 4.408 | .965 | .932 | 150.523 | .000 | Significant |
| Flash point | 11 | 191.561 | 6.451 | .751 | .564 | 11.648 | .008 | Significant |
| Molar volume | 12 | −14.889 | 12.947 | .946 | .894 | 84.680 | .000 | Significant |
| Complexity | 12 | −125.985 | 33.119 | .947 | .896 | 86.612 | .000 | Significant |

**Table 6.** Statistical parameters used in the QSPR model of S (G).

| Physiochemical Property | N | A | b | r | $r^2$ | F | p | Indicator |
|---|---|---|---|---|---|---|---|---|
| Boiling Point | 12 | 384.612 | 10.664 | .708 | .501 | 10.027 | .010 | Significant |
| Refractive index | 13 | 5.102 | 4.293 | .966 | .934 | 155.042 | .000 | Significant |
| Flash point | 11 | 191.365 | 6.348 | .759 | .576 | 12.232 | .007 | Significant |
| Molar volume | 12 | −11.972 | 12.540 | .942 | .887 | 78.511 | .000 | Significant |
| Complexity | 12 | −125.538 | 32.402 | .949 | .900 | 90.006 | .000 | Significant |

**Table 7.** Statistical parameters used in the QSPR model of GA (G).

| Physiochemical Property | N | A | b | r | $r^2$ | F | p | Indicator |
|---|---|---|---|---|---|---|---|---|
| Boiling Point | 12 | 386.718 | 5.013 | .711 | .505 | 10.202 | .010 | Significant |
| Refractive index | 13 | 6.258 | 2.010 | .966 | .933 | 152.002 | .000 | Significant |
| Flash point | 11 | 192.642 | 2.985 | .764 | .583 | 12.597 | .006 | Significant |
| Molar volume | 12 | −7.333 | 5.841 | .938 | .879 | 72.917 | .000 | Significant |
| Complexity | 12 | −121.577 | 15.270 | .951 | .905 | 95.147 | .000 | Significant |

**Table 8.** Statistical parameters used in the QSPR model of M1 (G).

| Physiochemical Property | N | A | b | r | $r^2$ | F | p | Indicator |
|---|---|---|---|---|---|---|---|---|
| Boiling Point | 12 | 405.004 | .738 | .660 | .436 | 7.721 | .019 | Significant |
| Refractive index | 13 | 9.310 | .318 | .952 | .907 | 106.874 | .000 | Significant |
| Flash point | 11 | 202.599 | .448 | .728 | .530 | 10.153 | .011 | Significant |
| Molar volume | 12 | 1.253 | .932 | .939 | .882 | 74.603 | .000 | Significant |
| Complexity | 12 | −97.937 | 2.432 | .953 | .908 | 98.435 | .000 | Significant |

**Table 9.** Statistical parameters used in the QSPR model of M2 (G).

| Physiochemical Property | N | A | b | r | $r^2$ | F | p | Indicator |
|---|---|---|---|---|---|---|---|---|
| Boiling Point | 12 | 414.903 | .535 | .645 | .416 | 7.127 | .024 | Significant |
| Refractive index | 13 | 13.461 | .233 | .928 | .861 | 67.942 | .000 | Significant |
| Flash point | 11 | 208.190 | .327 | .720 | .518 | 9.666 | .013 | Significant |
| Molar volume | 12 | 15.185 | .677 | .913 | .834 | 50.072 | .000 | Significant |
| Complexity | 12 | −87.855 | 1.849 | .960 | .922 | 118.593 | .000 | Significant |

**Table 10.** Statistical parameters used in the QSPR model of HM (G).

| Physiochemical Property | N | A | b | r | $r^2$ | F | p | Indicator |
|---|---|---|---|---|---|---|---|---|
| Boiling Point | 12 | 419.068 | .115 | .625 | .391 | 6.420 | .030 | Significant |
| Refractive index | 13 | 13.368 | .052 | .927 | .859 | 67.002 | .000 | Significant |
| Flash point | 11 | 210.170 | .071 | .705 | .497 | 8.876 | .015 | Significant |
| Molar volume | 12 | 13.491 | .151 | .822 | .849 | 56.325 | .000 | Significant |
| Complexity | 12 | −78.956 | .404 | .954 | .911 | 102.026 | .000 | Significant |

**Table 11.** Statistical parameters used in the QSPR model of F (G).

| Physiochemical Property | N | A | b | r | $r^2$ | F | p | Indicator |
|---|---|---|---|---|---|---|---|---|
| Boiling Point | 12 | 422.835 | .200 | .609 | .370 | 5.882 | .036 | Significant |
| Refractive index | 13 | 13.494 | .092 | .925 | .855 | 64.869 | .000 | Significant |
| Flash point | 11 | 212.010 | .124 | .692 | .478 | 8.256 | .018 | Significant |
| Molar volume | 12 | 13.736 | .273 | .927 | .859 | 64.032 | .000 | Significant |
| Complexity | 12 | −71.482 | .717 | .949 | .901 | 90.832 | .000 | Significant |

**Table 12.** Statistical parameters used in the QSPR model of H (G).

| Physiochemical Property | N | A | b | r | $r^2$ | F | p | Indicator |
|---|---|---|---|---|---|---|---|---|
| Boiling Point | 12 | 377.349 | 12.647 | .725 | .526 | 11.103 | .008 | Significant |
| Refractive index | 13 | 4.240 | 4.943 | .965 | .930 | 147.100 | .000 | Significant |
| Flash point | 11 | 187.144 | 7.500 | .772 | .596 | 13.299 | .005 | Significant |
| Molar volume | 12 | −14.817 | 14.434 | .936 | .877 | 71.041 | .000 | Significant |
| Complexity | 12 | −136.607 | 37.543 | .950 | .902 | 91.960 | .000 | Significant |

### *3.4. Standard error of estimate (SE) and comparison*

Measure of variation for an observation calculated around the computed regression line is said to be standard error estimate. It measures the amount of accuracy of predictions made around computed regression line and is mentioned in Table 13. We also compare the physicochemical properties of the experimental and theoretical calculated values of the models and are presented in Tables 14–18.

**Table 13.** Standard error of estimate.

| Topological Index | Std. Error of the estimate for boiling point | Std. Error of the estimate for refractive index | Std. Error of the estimate for flash point | Std. Error of the estimate for molar volume | Std. Error of the estimate for complexity |
|---|---|---|---|---|---|
| ABC(G) | 125.47771 | 9.78297 | 49.28724 | 34.98955 | 99.29113 |
| RA(G) | 135.48910 | 9.89048 | 47.70434 | 3.69784 | 95.80944 |
| S(G) | 135.49670 | 9.75496 | 47.04354 | 38.98953 | 94.16957 |
| GA(G) | 135.48311 | 9.84552 | 46.64458 | 40.28320 | 91.83836 |
| M1(G) | 135.40209 | 11.57777 | 49.53170 | 39.877986 | 90.43550 |
| M2(G) | 135.28260 | 14.14755 | 50.17335 | 47.32703 | 83.04506 |
| HM(G) | 135.30024 | 14.23249 | 51.27036 | 45.04104 | 88.97405 |
| F(G) | 135.31481 | 14.43119 | 52.18328 | 43.52285 | 93.78305 |
| H(G) | 135.48656 | 9.99697 | 45.90422 | 40.74687 | 93.26266 |

**Table 14.** Comparison of actual and computed values for molar volume from regression models.

| Name of drug | Molar volume of drug | Molar volume from regression model for ABC(G) Index | Molar volume from regression model for RA(G) Index | Molar volume from regression model for SCI(G) Index | Molar volume from regression model for GA(G) Index | Molar volume from regression model for M1(G) Index | Molar volume from regression model for M2(G)Index | Molar volume from regression model for F(G)Index | Molar volume from regression model for H(G) Index | Molar volume from regression model for HM(G)Index |
|---|---|---|---|---|---|---|---|---|---|---|
| Azacitidine | 117.1 $cm^3$ | 149.883 | 139.827 | 156.816 | 154.579 | 152.237 | 156.678 | 154.604 | 157.669 | 154.525 |
| Buslfan | 182.4 $cm^3$ | 140.665 | 107.460 | 126.469 | 122.512 | 139.189 | 134.337 | 157.334 | 121.584 | 146.069 |
| Mercaptopurine | 94.2 $cm^3$ | 69.1017 | 64.0877 | 72.5476 | 75.9012 | 72.085 | 78.146 | 71.066 | 73.2304 | 73.287 |
| Tioguanine | 80.2 $cm^3$ | 79.8436 | 74.8337 | 83.959 | 86.8239 | 81.405 | 86.27 | 78.71 | 85.2106 | 81.139 |
| Nelarabine | 149.9 $cm^3$ | 193.068 | 177.374 | 197.069 | 197.861 | 193.245 | 192.559 | 191.732 | 199.527 | 191.067 |
| Cytarabine | 128.4 $cm^3$ | 155.181 | 144.618 | 159.575 | 159.836 | 157.829 | 162.771 | 160.064 | 163.009 | 160.263 |
| Clofarabine | 143.1 $cm^3$ | 165.850 | 151.091 | 168.980 | 171.343 | 169.013 | 172.926 | 169.346 | 170.226 | 169.927 |
| Bosutinib | 388.3 $cm^3$ | 361.381 | 313.835 | 356.578 | 354.341 | 349.821 | 331.344 | 340.79 | 351.662 | 335.423 |
| Dasatinib | 366.4 $cm^3$ | 320.156 | 288.459 | 321.592 | 320.405 | 308.813 | 294.109 | 294.38 | 323.371 | 293.143 |
| Melphala | 231.2 $cm^3$ | 194.012 | 169.994 | 190.549 | 187.347 | 189.517 | 185.789 | 192.824 | 191.300 | 188.651 |
| Dexamethasone | 296.2 $cm^3$ | 315.148 | 268.132 | 306.167 | 308.898 | 331.181 | 348.946 | 352.802 | 300.710 | 349.919 |
| Doxorubicine | 336.6 $cm^3$ | 369.655 | 336.104 | 373.758 | 374.259 | 370.325 | 368.579 | 365.36 | 376.488 | 365.623 |
| Carboplatin | | 133.770 | 106.036 | 125.341 | 127.944 | 142.917 | 151.939 | 158.972 | 119.996 | 154.827 |

**Table 15.** Comparison of actual and computed values for flash point from regression models.

| Name of drug | Flash point of drug | Flash point computed from regression model for ABC(G) Index | Flash point computed from regression model for RA(G) Index | Flash point computed from regression model for SCI(G) Index | Flash point computed from regression model for GA(G) Index | Flash point computed from regression model for M1(G) Index | Flash point computed from regression model for M2(G)Index | Flash point computed from regression model for F(G)Index | Flash point computed from regression model for H(G) Index | Flash point computed from regression model for HM(G)Index |
|---|---|---|---|---|---|---|---|---|---|---|
| Azacitidine | 277 ℃ | 523.797 | 514.456 | 528.149 | 525.678 | 524.56 | 526.718 | 526.035 | 528.480 | 526.478 |
| Buslfan | 234.4 ℃ | 516.428 | 487.373 | 502.342 | 498.157 | 514.228 | 509.063 | 528.035 | 496.863 | 520.038 |
| Mercaptopurine | 250.5 ℃ | 459.220 | 451.083 | 456.487 | 458.153 | 461.092 | 464.658 | 464.835 | 454.495 | 464.608 |
| Tioguanine | 232 ℃ | 467.807 | 460.074 | 466.191 | 467.527 | 468.472 | 471.078 | 470.435 | 464.992 | 470.588 |
| Nelarabine | 389.9 ℃ | 558.319 | 545.872 | 562.380 | 562.824 | 557.032 | 555.073 | 553.235 | 565.157 | 554.308 |
| Cytarabine | 283.8 ℃ | 528.032 | 518.464 | 530.495 | 530.190 | 528.988 | 531.533 | 530.035 | 533.16 | 530.848 |
| Clofarabine | 286.4 ℃ | 536.561 | 523.881 | 538.493 | 540.065 | 537.844 | 539.558 | 536.835 | 539.483 | 538.208 |
| Bosutinib | 346.7 ℃ | 692.867 | 660.051 | 698.027 | 697.123 | 681.016 | 664.748 | 662.435 | 698.456 | 664.248 |
| Dasatinib | | 659.912 | 638.819 | 668.274 | 667.997 | 648.544 | 635.323 | 628.435 | 673.668 | 632.048 |
| Melphala | 239 ℃ | 559.073 | 539.697 | 556.835 | 553.801 | 554.08 | 549.723 | 554.035 | 557.948 | 552.468 |
| Dexamethasone | 298 ℃ | 655.908 | 621.811 | 655.157 | 658.12 | 666.256 | 678.658 | 671.235 | 653.812 | 675.288 |
| Doxorubicine | 443.8 ℃ | 699.481 | 678.684 | 712.636 | 714.217 | 697.252 | 694.173 | 680.435 | 720.209 | 687.248 |
| Carboplatin | | 5109166 | 486.182 | 501.382 | 502.819 | 517.18 | 522.973 | 529.235 | 495.472 | 526.708 |

**Table 16.** Comparison of actual and computed values for refractive index from regression models.

| Name of drug | Refractive Index of drug | Refractive Index computed from regression model for ABC(G) Index | Refractive Index computed from regression model for RA(G) Index | Refractive Index computed from regression model for SCI(G) Index | Refractive Index computed from regression model for GA(G) Index | Refractive Index computed from regression model for M1(G) Index | Refractive Index computed from regression model for M2(G) Index | Refractive Index computed from regression model for F(G) Index | Refractive Index computed from regression model for H(G) Index | Refractive Index computed from regression model for HM(G) Index |
|---|---|---|---|---|---|---|---|---|---|---|
| Azacitidine | 54.1 ($m^3$ $mol^{-1}$) | 60.4287 | 57.2106 | 62.8857 | 61.9752 | 60.826 | 62.158 | 60.966 | 63.3088 | 61.936 |
| Buslfan | 50.9 ($m^3$ $mol^{-1}$) | 57.2943 | 46.1906 | 52.4967 | 50.9403 | 56.374 | 54.469 | 61.886 | 50.9513 | 59.024 |
| Mercaptopurine | 41 ($m^3$ $mol^{-1}$) | 32.9598 | 31.4238 | 34.0368 | 34.9005 | 33.478 | 35.13 | 32.814 | 34.3923 | 33.96 |
| Tioguanine | 46.89 ($m^3$ $mol^{-1}$) | 36.6125 | 35.0824 | 37.9434 | 38.6592 | 36.658 | 37.926 | 35.39 | 38.4949 | 36.664 |
| Nelarabine | 65.8 ($m^3$ $mol^{-1}$) | 75.1133 | 69.9938 | 76.6663 | 76.8693 | 74.818 | 74.507 | 73.478 | 77.6435 | 74.52 |
| Cytarabine | 52.6 ($m^3$ $mol^{-1}$) | 62.2303 | 58.8415 | 63.8302 | 63.7842 | 62.734 | 64.255 | 62.806 | 65.1377 | 63.912 |
| Clofarabine | 63.6 ($m^3$ $mol^{-1}$) | 65.8583 | 61.0455 | 67.0499 | 67.7439 | 66.55 | 67.75 | 65.934 | 67.6092 | 67.24 |
| Bosutinib | 142.12 ($m^3$ $mol^{-1}$) | 132.346 | 116.454 | 131.273 | 130.717 | 128.242 | 122.272 | 123.71 | 129.742 | 124.232 |
| Dasatinib | 133.08 ($m^3$ $mol^{-1}$) | 118.328 | 107.814 | 119.295 | 119.039 | 114.25 | 109.457 | 108.07 | 120.054 | 109.672 |
| Melphala | 78.23 ($m^3$ $mol^{-1}$) | 75.4341 | 67.4812 | 74.4339 | 73.2513 | 73.546 | 72.177 | 73.846 | 74.8260 | 73.688 |
| Dexamethasone | 100.2 ($m^3$ $mol^{-1}$) | 116.625 | 100.893 | 114.015 | 115.079 | 121.882 | 128.33 | 127.758 | 112.294 | 129.224 |
| Doxorubicine | 134.59 ($m^3$ $mol^{-1}$) | 135.159 | 124.035 | 137.154 | 137.571 | 135.238 | 135.087 | 131.99 | 138.244 | 134.632 |
| Carboplatin | 60.04 ($m^3$ $mol^{-1}$) | 54.9497 | 45.7057 | 52.1103 | 52.8096 | 57.646 | 60.527 | 62.438 | 50.4076 | 62.04 |

**Table 17.** Comparison of actual and computed values for complexity from regression models.

| Name of drug | Complexity of drug | Complexity computed from regression model for ABC(G) Index | Complexity computed from regression model for RA(G) Index | Complexity computed from regression model for SCI(G) Index | Complexity computed from regression model for GA(G) Index | Complexity computed from regression model for M1(G) Index | Complexity computed from regression model for M2(G) Index | Complexity computed from regression model for F(G) Index | Complexity computed from regression model for H(G) Index | Complexity computed from regression model for HM(G)Index |
|---|---|---|---|---|---|---|---|---|---|---|
| Azacitidine | 384 | 297.234 | 269.787 | 310.592 | 301.707 | 296.047 | 298.586 | 298.49 | 312.031 | 298.38 |
| Buslfan | | 273.927 | 186.989 | 232.180 | 217.875 | 261.999 | 237.569 | 305.66 | 218.174 | 275.756 |
| Mercaptopurine | 190 | 92.9763 | 76.0409 | 92.8514 | 96.0205 | 86.895 | 84.102 | 79.088 | 92.4053 | 81.028 |
| Tioguanine | 225 | 120.137 | 103.529 | 122.337 | 124.575 | 111.215 | 106.29 | 99.164 | 123.566 | 102.036 |
| Nelarabine | 377 | 406.428 | 365.832 | 414.603 | 414.858 | 403.055 | 396.583 | 396.002 | 420.906 | 396.148 |
| Cytarabine | 383 | 310.631 | 282.041 | 317.721 | 315.450 | 310.639 | 315.227 | 312.83 | 325.922 | 313.732 |
| Clofarabine | 370 | 337.608 | 298.600 | 342.022 | 345.532 | 339.823 | 342.962 | 337.208 | 344.694 | 339.588 |
| Bosutinib | 734 | 832.011 | 714.906 | 826.756 | 823.941 | 811.631 | 775.628 | 787.484 | 816.609 | 782.372 |
| Dasatinib | 642 | 727.772 | 649.993 | 736.355 | 735.222 | 704.623 | 673.933 | 665.594 | 743.025 | 669.252 |
| Melphala | 265 | 408.814 | 346.954 | 397.754 | 387.372 | 393.327 | 378.093 | 398.87 | 399.507 | 389.684 |
| Dexamethasone | 805 | 715.109 | 597.996 | 696.500 | 705.140 | 762.991 | 823.702 | 819.032 | 684.083 | 821.156 |
| Doxorubicine | 977 | 852.932 | 771.871 | 871.147 | 876.012 | 865.135 | 877.323 | 852.014 | 881.183 | 863.172 |
| Carboplatin | 177 | 256.492 | 183.346 | 229.263 | 232.076 | 271.727 | 285.643 | 309.962 | 214.044 | 299.188 |

**Table 18.** Comparision of actural and computed values for boiling point from regression models.

| Name of drug | Boiling Point of drug | Boiling Point computed from regression model for ABC(G) Index | Boiling Point computed from regression model for RA(G) Index | Boiling Point computed from regression model for SCI(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 for F(G)Index | Boiling Point computed from regression model for H(G) Index | Boiling Point computed from regression model for HM(G)Index |
|---|---|---|---|---|---|---|---|---|---|---|
| Azacitidine | 534.2 ± 60 ℃ at 760 mm Hg | 523.79 | 514.45 | 528.14 | 525.67 | 524.56 | 526.718 | 526.03 | 528.48 | 526.48 |
| Buslfan | 464 ± 28 ℃ at 760 mm Hg | 516.42 | 487.37 | 502.34 | 498.15 | 514.22 | 509.063 | 528.03 | 496.86 | 520.04 |
| Mercaptopurine | 491 ± 25 ℃ at 760 mm Hg | 459.22 | 451.08 | 456.48 | 458.15 | 461.09 | 464.658 | 464.83 | 454.49 | 464.61 |
| Tioguanine | 460.7 ± 37 ℃ at 760 mm Hg | 467.80 | 460.07 | 466.19 | 467.52 | 468.47 | 471.078 | 470.43 | 464.99 | 470.59 |
| Nelarabine | 721 ± 70 ℃ at 760 mm Hg | 558.31 | 545.87 | 562.38 | 562.82 | 557.0 | 555.073 | 553.23 | 565.15 | 554.31 |
| Cytarabine | 547.7 ± 60 ℃ at 760 mm Hg | 528.03 | 518.46 | 530.49 | 530.19 | 528.98 | 531.533 | 530.03 | 533.16 | 530.85 |
| Clofarabine | 550 ± 60 ℃ at 760 mm Hg | 536.56 | 523.88 | 538.49 | 540.06 | 537.84 | 539.558 | 536.83 | 539.48 | 538.21 |
| Bosutinib | 649.7 ± 55 ℃ at 760 mm Hg | 692.86 | 660.05 | 698.02 | 697.12 | 681.01 | 664.748 | 662.43 | 698.45 | 664.25 |
| Dasatinib | | 659.91 | 638.81 | 668.27 | 667.99 | 648.54 | 635.323 | 628.43 | 673.66 | 632.05 |
| Melphala | 473 ± 45 ℃ at 760 mm Hg | 559.07 | 539.69 | 556.83 | 553.80 | 554.08 | 549.723 | 554.03 | 557.94 | 552.47 |
| Dexamethasone | 568.2 ± 5 ℃ at 760 mm Hg | 655.90 | 621.81 | 655.15 | 658.12 | 666.25 | 678.658 | 671.23 | 653.81 | 675.29 |
| Doxorubicine | 216 ± 65 ℃ at 760 mm Hg | 699.48 | 678.68 | 712.63 | 714.21 | 697.25 | 694.173 | 680.43 | 720.20 | 687.25 |
| Carboplatin | 366.4 ± 60 ℃ at 760 mm Hg | 510.91 | 486.18 | 501.38 | 502.81 | 517.18 | 522.973 | 529.23 | 495.47 | 526.71 |

## 4 Conclusions

It is obvious from statistical parameters used in linear QSPR models and topological indices that: ABC (G) index provides high correlated value for molar volume r = 0.953. HM index offers maximum correlated value of complexity i.e. r = 0.954. GA index depicts utmost correlation coefficient of refractive index r=0.966. Harmonic H (G) provides maximum correlated value of flash point r = 0.772.

In this paper, we have computed topological indices and relate it with linear QSPR model for the drugs used to cure blood cancer. The results obtained in this way will helpful for designing some new drugs to obtain preventive measure for the said disease in pharmaceutical industry. The correlation coefficient has significant contribution to the range of topological indices for these drugs. The results are an eye-opener for the researcher working on drugs science in pharmaceutical industry and provide a way to estimate physicochemical properties for novice discoveries of anticancer medicines to cure other specific cancer disease.

## Conflict of interest

We declare no conflict of interest.

## References


1. B. Figuerola, C. Avila, The phylum bryozoa as a promising source of anticancer drugs, *Mar. Drugs*, **17** (2019), 477. https://doi.org/10.3390/md17080477
2. G. Genovese, A. K. Kähler, R. E. Handsaker, J. Lindberg, S. A. Rose, S. F. Bakhoum, et al., Clonal hematopoiesis and blood-cancer risk inferred from blood DNA sequence, *New Eng. J. Med.*, **371** (2014), 2477–2487. https://doi.org/10.1056/NEJMoa1409405
3. T. Terwilliger, M. J. B. C. J. Abdul-Hay, Acute lymphoblastic leukemia: A comprehensive review and 2017 update, *Blood Cancer J.*, **7** (2017), e577–e577. https://doi.org/10.1038/bcj.2017.53
4. A. Aslam, Y. Bashir, S. Ahmad, W. Gao, On topological indices of certain dendrimer structures, *Z. Naturforsch.*, 72 (2017), 559–566. https://doi.org/10.1515/zna-2017-0081
5. S. M. Hosamani, D. Perigidad, S. Jamagoud, Y. Maled, S. Gavade, QSPR anlysis of certain degree based topological indices, *J. Statis. Appl. Prob.*, **6** (2017), 1–11. https://doi.org/10.18576/jsap/060211
6. M. Randic, Comparative structure-property studies: regressions using a single descriptor, *Croat. Chem. Acta*, **66** (1993), 289–312.
7. M. Randic, Quantitative structure-propert relationship: boiling points and planar benzenoids, *New J. Chem.*, **20** (1996) 1001–1009.
8. M. C. Shanmukha, N. S. Basavarajappa, K. N. Anilkumar, Predicting physico-chemical properties of octane isomers using QSPR approach, *Malaya J. Math.*, **8** (2020) 104–116. https://doi.org/10.26637/MJM0801/0018
9. S. Hayat, M. Imran, J. Liu, Correlation between the Estrada index and Q-electronic energies for benzenoid hydrocarbons with applica-tions to boron nanotubes, *Int. J. Quant. Chem.,* 2019. https://doi.org/10.1002/qua.26016
10. A. Aslam, S. Ahmad, W. Gao, On topological indices of boron triangular nanotubes, *Z. Naturforsch.*, **72** (2017), 711–716. https://doi.org/10.1515/zna-2017-0135
11. S. Hayat, S. Wang, J. Liu, Valency-based topological descrip-tors of chemical networks and their applications, *Appl. Math. Model.*, 2018. https://doi.org/10.1016/j.apm.2018.03.016
12. S. Hayat, M. Imran, J. Liu, An efficient computational technique for degree and distance based topological descriptors with applications, 2019. https://doi.org/10.1109/ACCESS.2019.2900500

13. E. Estrada, L. Torres, L. Rodriguez, I. Gutman, An atom-bond connectivity index: Modeling the enthalpy of formation of alkanes, *Indian J. Chem.,* **37A** (1998), 849–855.
14. T. Barbui, J. Thiele, H. Gisslinger, H. M. Kvasnicka, A. M. Vannucchi, P. Guglielmelli, et al., The 2016 WHO classification and diagnostic criteria for myeloproliferative neoplasms: document summary and in-depth discussion, *Blood Cancer J.,* **8** (2018), 1–11. https://doi.org/10.1038/s41408-018-0054-y
15. M. Randic, On Characterization of molecular branching, *J. Am. Chem. Soc.*, **97** (1975), 6609–6615. https://doi.org/10.1021/ja00856a001
16. B. Zhou, N. Trinajstic, On general sum-connectivity index, *J. Math. Chem.*, **47** (2010), 210–218. https://doi.org/10.1007/s10910-009-9542-4
17. D. Vukicevic, B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem.*, **46** (2009), 1369–1376. https://doi.org/10.1007/s10910-009-9520-x
18. M., Adnan, S. A. U. H. Bokhary, G. Abbas, T. Iqbal, Degree-based topological indices and QSPR analysis of antituberculosis drugs, *J. Chem.,* 2022, Article ID 5748626. https://doi.org/10.1155/2022/5748626
19. I. Gutman, Degree based topological indices, *Croat. Chem. Acta*, **86** (2013), 351–361. https://doi.org/10.5562/cca2294
20. S. Fajtlowicz, On conjectures of grafitti II, *Congr. Numerantium*, **60** (1987), 189–197.
21. G. H. Shirdel, H. RezaPour, A. M. Sayadi, The hyper-zagreb index of graph operations, *Iran. J. Math. Chem.*, **4** (2013), 213–220.
22. M. Imran, M. K. Siddiqui, A. Q. Baig, W. Khalid, H. Shaker, Topological properties of cellular neural networks, *J. Intell. Fuzzy Syst.,* **37** (2019), 3605–3614. https://doi.org/10.3233/JIFS-181813
23. B. Furtula, I. Gutman, A forgotton topological index, *J. Math. Chem.,* **53** (2015), 213–220. https://doi.org/10.1007/s10910-015-0480-z
24. W. Gao, W. Wang, M. K. Jamil, M. R. FArhani, Electron energy studing of moleculer structurevia forgotten topological index computation, *J. Chem.,* 2016. https://doi.org/10.1155/2016/1053183
25. I. B. M. Corp, Released. IBM SPSS Statistics for Windows, Version 24.0 (Armonk, NY: IBM Corp., 2016).
26. J. Liu, M. Arockiaraj, M. Arulperumjothi, S. Prabhu, Distance based and Bond additive topological indices of certain repurposed antiviral drug compounds tested for treating COVID-19, *Int. J. Quantum Chem.*, **121** (2021), e26617. https://doi.org/10.1002/qua.26617
27. S. Prabhu, G. Murugan, M. Arockiaraj, M. Arulperumjothi, V. Manimozhi, Molecular topological characterization of three classes of polycyclic aromatic hydrocarbons, *J. Mol. Struct.*, **1229** (2021), 129501. https://doi.org/10.1016/j.molstruc.2020.129501
28. S. Prabhu, Y. S. Nisha, M. Arulperumjothi, D. Sagaya Rani Jeba, V. Manimozhi, On detour index of Cycloparaphenylene and polyphenylene molecular structures, *Sci. Rep-UK,* 2021. https://doi.org/10.1038/s41598-021-94765-6
29. Y. Chu, K. Julietraja, P. Venugopal, M. K. Siddiqui, S. Prabhu, Degree- and irregularity-based molecular descriptors for benzenoid systems, *Eur. Phys. J. Plus,* **136** (2021), 78. https://doi.org/10.1140/epjp/s13360-020-01033-z