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Topological Descriptors and QSPR Models of Drugs used in Blood Cancer

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Abstract.:In this article, we used M-polynomials to investigate the rela-tionships between topological indices and physicochemical properties of some blood cancer treatment drugs; we used the curvilinear regression method on drugs like azacitidine, buslfan, and mercaptopurine, among others. This article also includes M-polynomial proofs of the closed form of some topological indices of said drugs. The study could be a new at-tempt to improve QSPR model prediction analysis by utilizing the afore-mentioned molecular descriptors, which are used to investigate chemical, medical, and pharmacological properties. Finally, this work demonstrates that topological descriptors can be a cornerstone to designing and synthe-size new blood cancer treatments and other disease drugs.

AMS (MOS) Subject Classification Codes: 68R10 , 92C40 , 92C99 , 90C35 Key Words: Drugs, M-polynomials, regression models, blood cancer.

1. Introduction

Cancer is a dangerous disease that belongs to the genetic disease family. It is the un-controlled magnification of abnormal blood cells in the body that stops normal functions and is prone to infection. Cancer that affects the blood cells is known as blood cancer and Leukemia is an example that belongs to it. This will prone to infection and creates tumors in bones. Annually 1.24 million people are affected by this perilous disease. Sci-entists and Medicos are searching for better treatments to tackle this fatal disease. Drug discovery is not an easy task because it is costly, time-consuming and in some cases dif-ficult. Cancer can be treated in a variety of ways at the early stages of a life-threatening situation. Drug therapy tackles this in an efficient way it will stop the growth of abnor-mal cells. Anticancer drugs kill and halt the menacing disease and many drugs are being tested in order to combat the fatal disease. This necessitates prompt screening, diagnosis

and medication to help patients control the deadly disease in the future. Many medical and pharmaceutical solutions are being developed on a regular basis, which necessitates a significant amount of work to investigate the biological and physiochemical properties of these drugs. Azacitidine, buslfan, nelarabine, and other drugs are all effective treatments for patients with blood cancer. Drug therapy during the early stages of a life-threatening situation has been discovered by scientists [1]. More can be found in [1-3, 14]. Given the rapid technological advancement, many medical and pharmaceutical solutions are being developed consistently, which requires a significant amount of work to examine the biolog-ical and physiochemical properties of these drugs. Using M-polynomials to investigate the relationships between TIs and physical properties of some blood cancer treatment drugs, and, using the curvilinear regression method on drugs like azacitidine, buslfan, and mercap-topurine, among others. This article also includes M-polynomial proofs of the closed form of some topological indices of said drugs and, improving QSPR model prediction analy-sis by utilizing the aforementioned molecular descriptors, which are used to investigate chemical, medical, and pharmacological properties, and, demonstrating topological de-scriptors for a cornerstone to design and synthesize new blood cancer treatments and other disease drugs contributes to Combinatorics, Graph Theory, chemistry topology, Mathemat-ical, Computational, Physical, Electrical and Computer Engineering. The main motivation for the work is to increase the efficiency of the drugs. Previous research on covid-19, anti-cancer, blood cancer, diabetes and QSPR studies of various topological indices for various chemical structures motivated us to work on the current research problem.

2. Material and method

Let G = (V, E) be a simple, finite and connected graph. The degree d(u) of a vertex u is the number of vertices adjacent to u. The edge connecting the vertices u and v will be denoted by uv. We refer to [19] for undefined terms and notation. A molecular graph or a chemical graph is a simple graph related to the structure of a chemical compound in mathematical modelling. This graph's vertex represents an atom of the molecule, and its edges represent atom bonds. A topological index is a numerical parameter derived math-ematically from a graph structure. These topological indices are useful for determining relationships between a molecular compound's structure and its physicochemical proper-ties [18]. The total surface of polychlorophenyles was assessed to calculate with the aid of a symmetric division index in [8]. The heat of the formation of an alkane is best predicted using the augmented Zagreb index in [6]. For more understanding visit the subsequent articles [4, 9, 19, 26-31]. Various regression methods using TIs were implemented for the QSPR and QSAR [5]. Using graph theory, some topological indices of blood cancer drugs were calculated in this study. Later, the best topological indices and curvilinear regression analyses were obtained in order to predict the properties of blood cancer drugs. These TIs were chosen for this QSPR modelling because they are swiftly calculated, information-rich and have a strong predictive power. By using the formulas in Table 1, the topological in-dices via M-polynomials of eleven drugs were computed to design the QSPR. The linear, quadratic, and cubic regression models for the variance of the degree TI were obtained as structure-property models ABC index, sum connectivity index, geometric index, first and second Zagreb index, hyper Zagreb index, harmonic and forgotten index. The Comparison

of linear, quadratic, cubic, logarithmic and exponential QSPR model are given in Table 4-8 respectively. Klavzar and Deutsch defined M-Polynomial [21].

$$M(G_1, x, y) = \sum_{isj} T_{ij} x^i y^j \qquad (2.\ 1)$$

The following operators will be used:
$Q_a(f(\alpha,\beta)) = x^a f(\alpha,\beta), D_\beta(f(\alpha,\beta)) = \beta.\frac{\partial(f(\alpha,\beta)}{\partial\beta}, J(f(\alpha,\beta)) = f(\alpha,\alpha)$
$S_\alpha(f(\alpha,\beta)) = \int_0^\alpha \frac{(f(t,\beta))}{t}dt, S_\beta(f(\alpha,\beta)) = \int_0^\beta \frac{(f(\alpha,t))}{t}dtQ$
$Q_\alpha f(\alpha,\beta) = x\beta^\alpha f(\alpha,\beta)$

See Table 1 for the formulas?

Topological indices	Mathematical expression $f(\alpha,\beta)$	Derivation from $M(G,\alpha,\beta)$
ABC(G)	$\sum_{uv\in E(G)}\sqrt{\frac{d_{ut}d_y-2}{d_u d_v}}$	$D_x^{\frac{1}{2}}Q_{x(-2)}JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}[f(x,y)]_{x=y=1}$
S(G)	$\sum_{uv\in E(G)}\sqrt{\frac{1}{d_u+d_v}}$	$S_x^{\frac{1}{2}}J(f(x,y))\|_{x=y=1}$
GA(G)	$\sum_{uv\in E(G)}\frac{2\sqrt{d_u d_v}}{d_u+d_v}$	$2S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}}(f(x,y))\|_{x=y=1}$
$M_1(G_1)$	$\sum_{uv\in E(G)}(d_u+d_v)$	$(D_x+D_y)(f(x,y))\|_{x=y=1}$
$M_2(G)$	$\sum_{uv\in E(G)}(d_u d_v)$	$(D_xD_y)(f(x,y))\|_{x=y=1}$
$F(G)$	$\sum_{uv\in E(G)}[(d_u)^2]+[(d_v)^2]$	$(D_x^2+D_y^2)(f(x,y))\|_{x=y=1}$
$H(G)$	$\sum_{uv\in E(G)}\frac{2}{d_u+d_v}$	$2S_xJ(f(x,y))\|_{x=y=1}$
$HM(G)$	$\sum_{uv\in E(G)}(d_u+d_v)^2$	$D_x^2J(f(x,y))\|_{x=y=1}$

The molecular formula of bulasan is $C_8H_{14}N_6S_2$. Busulfan is an antineoplastic alky-lating agent and is used for many kinds of cancer. They prohibit tumour development by cross-linking guanine bases in DNA. The strands cannot separate and uncoil. It is required for DNA replication, and cells no longer divide. The molecular formula of clofarabine is $C_{10H11}C_lFN_5O_5$. Clofarabine inhibits the growth of cancer cells. The chemical for-mula of azacitidine is $C_8H_{12}N_{4O5}$. Azacytidine has been used in the treatment of cancer. The molecular formula of purixan is $C_5H_4N_4S$. Purixan is found active against human leukemias. The molecular formula of Tioguanine is $C_5H_5N_5S$. The medication is used to treat acute leukaemia. The molecular formula of arranon is $C_{11}H_{15}N_5S_5$. Arranon is 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 vyxeos is $C_{11}H_{15}N_5S_5$. Vyxeos is an antineoplastic anti-metabolite used in the treatment of several forms of leukemia including acute myelogenous leukemia and meningeal leukemia. The molecular formula of bosulif is $C_{26}H_{29}C_{l2}N_5O_5$. It is used to treat a certain type of chronic myeloid leukemia (a cancer of white blood cells). The molecular formula of sprycel is $C_{22}H_{26}ClN_7S$. Sprycel s a tyrosine kinase inhibitor used for the treatment of lymphoblastic or chronic myeloid leukaemia. The molecular formula of evomela is $C_{13}H_{18}C_{l2}N_2O_2$. Evomela is an antineoplastic in the class of alky-lating agents stop tumor growth by cross-linking guanine bases in DNA. The molecular formula of dexadrol is $C_{22}H_{29}FO_5$. Hexadrol is a glucocorticoid that comes in a variety of forms and is used to treat a variety of inflammatory conditions as well as rheumatic disorders and endocrine. The molecular formula of myocet is $C_{27}H_{29}NO_{11}$. Myocet is

an anthracycline-class antineoplastic. Anthracyclines are among the most important anti-tumor drugs on the market. Doxorubicin is widely used to treat a variety of solid tumours, whereas idarubicin and daunorubicin are only used to treat leukaemia. The molecular for-mula of carbopalatin is C6H12N2O4Pt. Carboplatin is an alkylating agent that is used in the treatment of advanced ovarian cancer.The following Table.2 gives the physical proper-ties of said drugs which are taken from ChemSpider.

Table.2 Physical properties of drugs

Name of drug	MV(cm^3)	Boiling Point	Refractive Index (m^3mol^{-1})	Complexity	Flash Point
Azacitidine	117.10	534.21	54.10	384.00	277.00
Buslfan	182.40	464.00	50.90		234.40
Purixan	94.20	491.00	41.00	19.00	250.50
Lanivis	80.20	460.70	46.89	225.00	232.00
Arranon	149.90	721.00	65.80	377.00	389.90
Vyxeos	128.40	547.70	52.60	383.00	283.80
Clofarabine	143.10	550.00	63.60	370.00	286.40
Bosulif	388.30	649.70	142.12	734.00	346.70
Sprycel	366.40		133.08	642.00	
Evomela	231.20	473.00	78.23	265.00	239.00
Hexadrol	296.20	568.20	100.20	805.00	298.00
Myocet	336.60	216.00	134.59	977.00	443.80
Carboplatin		366.40	60.04	177.00	

2.1. **M-polynomials of Blood Cancer Drugs Structures.** In this section, we compute the M-polynomials and the topological indices of the said drugs.

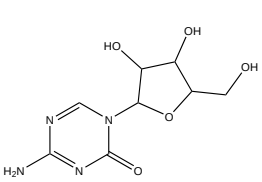
Theorem 2.2. *If G_1 is the chemical graph of Azacitidine, then*

$$M(G_1, x, y) = 3xy^2 + 4xy^2 + 6xy^4 + 4x^2y^3 + 5x^2y^4 + 3x^3y^3 + x^3y^4 + 4x^4y^4$$

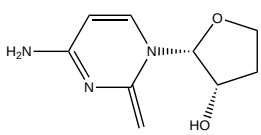
Proof. Let G_1 is the graph of azacitidine with $V = 29$ and $E = 31$. Let $E_{m,n}$ represents vertices of degrees m and n of G_1, then $\mid E_{1,2} \mid= 3, , \mid E_{1,3} \mid= 4, , \mid E_{1,4} \mid= 6, , \mid E_{2,3} \mid= 4, , \mid E_{2,4} \mid= 5, , \mid E_{3,3} \mid= 3, , \mid E_{3,4} \mid= 1, , \mid E_{4,4} \mid= 4$.
From equation 2.1 and edge partition of G_1, we have the desired result $M(G_1, x, y) = 3xy^2 + 4xy^2 + 6xy^4 + 4x^2y^3 + 5x^2y^4 + 3x^3y^3 + x^3y^4 + 4x^4y^4$ □

Theorem 2.3. *The TIs of the graph azacitidine are*

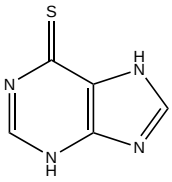
- $ABC(G_1) = 22.04$
- $SCI(G_1) = 13.46$
- $GA(G_1) = 27.72$
- $M_1(G_1) = 162$
- $M_2(G_1) = 209$
- $H(G_1) = 11.95$



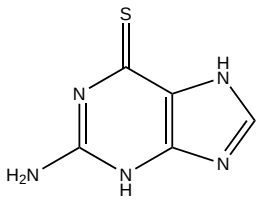
(i) Azacitidine



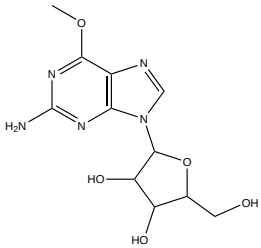
(ii) Vyxeos



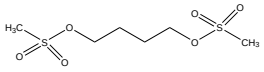
(iii) Purixan



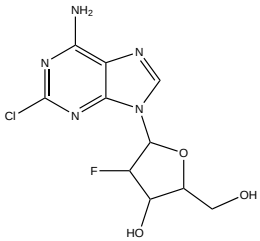
(iv) Lanvis



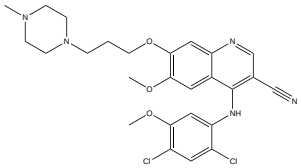
(v) Arranon



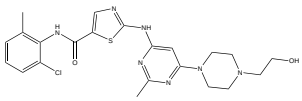
(vi) Buslfan



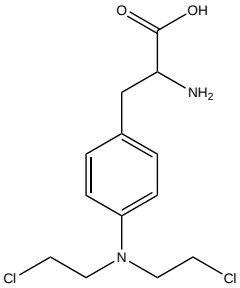
(vii) Clofarabine



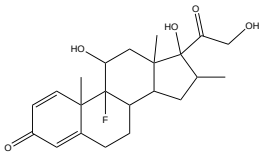
(viii) Busulif



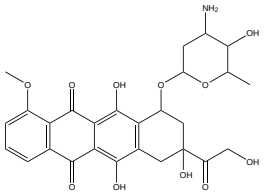
(ix) Sprycel



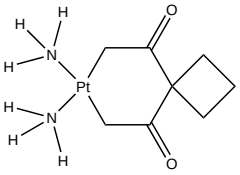
(x) Evomela



(xi) Hexadrol



(xii) Myocet



(xiii) Carboplatin

Figure 1: Molecular structure of drugs

- $HM(G_1) = 934$
- $F(G_1) = 516$

Proof. $S_y{}^{\frac{1}{2}} = \frac{3\sqrt{2}}{2}xy^2 + \frac{4\sqrt{3}}{3}xy^3 + 3xy^4 + \frac{4\sqrt{3}}{3}x^2y^3 + \frac{5}{2}x^2y^4 + \sqrt{3}x^3y^3 + \frac{1}{2}x^3y^4 + 2x^4y^4$

$S_x{}^{\frac{1}{2}}S_y{}^{\frac{1}{2}} = \frac{3\sqrt{2}}{2}xy^2 + \frac{4\sqrt{3}}{3}xy^3 + 3xy^4 + \frac{2\sqrt{6}}{3}x^2y^3 + \frac{5\sqrt{2}}{4}x^2y^4 + x^3y^3 + \frac{\sqrt{3}}{6}x^3y^4 + x^4y^4$

$JS_x{}^{\frac{1}{2}}S_y{}^{\frac{1}{2}} = \frac{3\sqrt{2}}{2}x^3 + \frac{4\sqrt{3}}{3}x^4 + 3x^5 + \frac{2\sqrt{6}}{3}x^5 + \frac{5\sqrt{2}}{4}x^6 + x^6 + \frac{\sqrt{3}}{6}x^7 + x^8$

$Q_{x_{-2}}JS_x{}^{\frac{1}{2}}S_y{}^{\frac{1}{2}} = \frac{3\sqrt{2}}{2}x + \frac{4\sqrt{3}}{3}x^2 + 3x^3 + \frac{2\sqrt{6}}{3}x^3 + \frac{5\sqrt{2}}{4}x^4 + x^4 + \frac{\sqrt{3}}{6}x^5 + x^6$

$D_x{}^{\frac{1}{2}}Q_{x_{(-2)}}JS_x{}^{\frac{1}{2}}S_y{}^{\frac{1}{2}} = \frac{3\sqrt{2}}{2}x + \frac{4\sqrt{6}}{3}x^2 + 3\sqrt{3}x^3 + \frac{2\sqrt{18}}{3}x^3 + \frac{5\sqrt{2}}{2}x^4 + 2x^4 + \frac{\sqrt{15}}{6}x^5 + \sqrt{6}x^6$

$J = 3x^3 + 4x^4 + 10x^5 + 8x^6 + x^7 + 4x^8$
$S_x^{\frac{1}{2}}J = \sqrt{3}x^3 + 2x^4 + 2\sqrt{5}x^5 + \frac{4\sqrt{6}}{3}x^6 + \frac{\sqrt{7}}{7}x^7 + \sqrt{2}x^8$
$D_y{}^{\frac{1}{2}} = 3\sqrt{2}xy^2 + 4\sqrt{3}xy^3 + 12xy^4 + 4\sqrt{3}x^2y^3 + 10x^2y^4 + 3\sqrt{3}x^3y^3 + 2x^3y^4 + 8x^4y^4$
$D_x{}^{\frac{1}{2}}D_y{}^{\frac{1}{2}} = 3\sqrt{2}xy^2 + 4\sqrt{3}xy^3 + 12xy^4 + 4\sqrt{6}x^2y^3 + 10\sqrt{2}x^2y^4 + 9x^3y^3 + 2\sqrt{3}x^3y^4 + 16x^4y^4$
$JD_x{}^{\frac{1}{2}}D_y{}^{\frac{1}{2}} = 3\sqrt{2}x^3 + 4\sqrt{3}x^4 + 12x^5 + 4\sqrt{6}x^5 + 10\sqrt{2}x^6 + 9x^6 + 2\sqrt{3}x^7 + 16x^8$
$S_xJD_x{}^{\frac{1}{2}}D_y{}^{\frac{1}{2}} = \sqrt{2}x^3 + \sqrt{3}x^4 + \frac{12}{5}x^5 + \frac{4\sqrt{6}}{5}x^5 + \frac{5\sqrt{2}}{3}x^6 + \frac{3}{2}x^6 + \frac{2\sqrt{3}}{7}x^7 + 2x^8$
$2S_xJD_x{}^{\frac{1}{2}}D_y{}^{\frac{1}{2}} = 2\sqrt{2}x^3 + 2\sqrt{3}x^4 + \frac{24}{5}x^5 + \frac{8\sqrt{6}}{5}x^5 + \frac{10\sqrt{2}}{3}x^6 + 3x^6 + \frac{4\sqrt{3}}{7}x^7 + 4x^8$
$D_xf(x,y) = 3xy^2 + 4xy^3 + 6xy^4 + 8x^2y^3 + 10x^2y^4 + 9x^3y^3 + 3x^3y^4 + 16x^4y^4$
$D_yf(x,y) = 6xy^2 + 12xy^3 + 24xy^4 + 12x^2y^3 + 20x^2y^4 + 9x^3y^3 + 4x^3y^4 + 16x^4y^4$
$(D_x+D_y)f(x,y) = 32x^4y^4+7x^3y^4+18x^3y^3+30x^2y^4+20x^2y^3+30xy^4+16xy^4+9xy^2$
$D_yf(x,y) = 64x^4y^4 + 12x^3y^4 + 27x^3y^3 + 40x^2y^4 + 24x^2y^3 + 24xy^4 + 12xy^3 + 6xy^2$
$D_x^2 = 3xy^2 + 4xy^3 + 6xy^4 + 16x^2y^3 + 20x^2y^4 + 27x^3y^3 + 9x^3y^4 + 64x^4y^4$
$D_y^2 = 12xy^2 + 36xy^3 + 96xy^4 + 36x^2y^3 + 80x^2y^4 + 27x^3y^3 + 16x^3y^4 + 64x^4y^4$
$(D_x^2 + D_y^2)f(x,y) = 128x^4y^4 + 25x^3y^4 + 54x^3y^3 + 100x^2y^4 + 52x^2y^3 + 102xy^4 + 40xy^4 + 15xy^2$
$S_xJ = x^3 + x^4 + 2x^5 + \frac{4}{3}x^5 + \frac{1}{7}x^7 + \frac{1}{2}x^8$
$2S_xJ = 2x^3 + 2x^4 + 4x^5 + \frac{8}{3}x^6 + \frac{2}{7}x^7 + x^8$
$D_x^2J = 32x^4 + 350x^5 + 72x^6 + 98x^7 + 384x^8$
Hence on simplification with table 1 we get results as:
$ABC(G_1) = (\frac{3\sqrt{22}}{x}{}^1 + \frac{4\sqrt{2}}{\sqrt{3}}3x^2 + 3\sqrt{3}x^3 + \frac{2\sqrt{3}}{\sqrt{6}}3x^3 + \frac{5\sqrt{2}}{2}x^4 + 2x^4 + \frac{\sqrt{5}}{\sqrt{3}}6x^5 + \sqrt{6}x^6)(1,1) = 22.04$
$S(G_1) = (\sqrt{3}x^3 + 2x^4 + 2\sqrt{5}x^5 + \frac{4\sqrt{6}}{3}x^6 + \frac{\sqrt{7}}{7}x^7 + \sqrt{2}x^8)(1,1) = 13.26$
$GA(G_1) = (2\sqrt{2}x^3 + 2\sqrt{3}x^4 + \frac{24}{5}x^5 + \frac{8\sqrt{6}}{5}x^5 + \frac{10\sqrt{2}}{3}x^6 + 3x^6 + \frac{4\sqrt{3}}{7}x^7 + 4x^8)(1,1) = 27.72$
$M_1(G_1) = (32x^4y^4+7x^3y^4+18x^3y^3+30x^2y^4+20x^2y^3+30xy^4+16xy^3+9xy^2)(1,1) = 162$
$M_2(G_1) = (64x^4y^4+12x^3y^4+27x^3y^3+40x^2y^4+24x^2y^3+24xy^4+12xy^3+6xy^2)(1,1) = 209$

$H(G_1) = (2x^3 + 2x^4 + 4x^5 + \frac{8}{3}x^6 + \frac{2}{7}x^7 + x^8)(1,1) = 11.95$
$HM(G_1) = (32x^4 + 350x^5 + 72x^6 + 98x^7 + 384x^8)(1,1) = 934$
$F(G_1) = (128x^4y^4 + 25x^3y^4 + 54x^3y^3 + 100x^2y^4 + 52x^2y^3 + 102xy^4 + 40xy^3 + 15xy^2)(1,1) = 516$

□

By using edge partitioning of drug structures one can easily prove the following theorems

Theorem 2.4. *The G_2 is the chemical graph of buslfan*

$$M(G_2, x, y) = 18xy^4 + 3x^2y^4 + 5x^4y^4$$

Theorem 2.5. *The G_3 is the chemical graph of purixan*

$$M(G_3, x, y) = 5xy^3 + 4x^2y^4 + 6x^3y^3$$

Theorem 2.6. *The G_4 is the chemical graph of lanvis*

$$M(G_4, x, y) = 6xy^3 + 4x^2y^4 + 7x^3y^3$$

Theorem 2.7. *The G_5 is the chemical graph of nelarabine*
$M(G_5, x, y) = 3xy^2 + 3xy^3 + 9xy^4 + 7x^2y^3 + 6x^2y^4 + 5x^3y^3 + x^3y^4 + 4x^4y^4$

Theorem 2.8. *The G_6 is the chemical graph of Cytarabine* $M(G_6, x, y) = 3xy^2 + 5xy^3 + 6xy^4 + 2x^2y^3 + 5x^2y^4 + 5x^3y^3 + x^3y^4 + 4x^4y^4$

Theorem 2.9. *The G_7 is the chemical graph of Clofarabine* $M(G_7, x, y) = 2xy^2 + 4xy^3 + 7xy^4 + 6x^2y^3 + 4x^2y^4 + 5x^3y^3 + x^3y^4 + 4x^4y^4$

Theorem 2.10. *The G_8 is the chemical graph of Bosutinib* $M(G_8, x, y) = xy^2 + 8xy^3 + 23xy^4 + 6x^2y^3 + 3x^2y^4 + 17x^3y^3 + 6x^3y^4 + 4x^4y^4$

Theorem 2.11. *The G_9 is the chemical graph of Dasatinib* $M(G_9, x, y) = xy^2 + 10xy^3 + 8xy^4 + x^2y^3 + 16x^2y^4 + 7x^3y^3 + 2x^3y^4 + 16x^4y^4$

Theorem 2.12. *The G_{10} is the chemical graph of Melphalan* $M(G_{10}, x, y) = xy^2 + 7xy^3 + 13xy^4 + x^2y^3 + 7x^3y^3 + 5x^3y^4 + 3x^4y^4$

Theorem 2.13. *The G_{11} is the chemical graph of Dexamethasone* $M(G_1 1, x, y) = 3xy^2 + 5xy^3 + 3xy^4 + 4x^2y^4 + 5x^3y^3 + 16x^3y^4 + 24x^4y^4$

Theorem 2.14. *The G_{12} is the chemical graph of Doxorubicine* $M(G_{12}, x, y) = 5xy^2 + 8xy^3 + 19xy^4 + 2x^2y^3 + 7x^2y^4 + 16x^3y^3 + 6x^3y^4 + 8x^4y^4$

Theorem 2.15. *The $G_1 3$ is the chemical graph of Carboplatin* $M(G_{13}, x, y) = 2xy^3 + 12xy^4 + 2x^2y^3 + 2x^2y^4 + 2x^3y^4 + 6x^4y^4$

Using table 1 and theorems 2.4 to 2.16, one can calculate the TIs of the remaining drugs, which is summarised in the following table

Table.3 The TIs values of candidate drugs

Name of drug	ABC(G)	RA(G)	S(G)	GA(G)	$M_1(G)$	$M_2(G)$	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
Meracaptopurine	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
Melaphala	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

3. Quantitative Structure Analysis and Regression Models

In order to find the usefulness of a topological index, we have to predict regression models between calculated topological indices and physicochemical properties. In Tables 1 and 3, we have tabulated calculations of the above TIs and physicochemical properties of molecular structures, respectively. These values are useful for creating regression models. The data set of the above-mentioned molecular structures consists of the following physic-ochemical properties as given in Table 2.

Regression models are used to fit the curves. Accordingly, we studied linear, quadratic, cubic, logarithmic, and exponential regression models. We constructed regression models of the above-mentioned topological indices with the physicochemical properties of mole-cular structures as shown in Table 5. In the regression model table, we considered the square of the coefficient of the correlation (R^2), the F-ratio test, and significance (sig). The model with the maximum R^2 is preeminent forecaster or goodness of fit of the regression model. For the model to be efficient, if the F-ratio test is greater than one and the sig value is less than 0.05, then the topological indices reliably predict the dependent variable for the particular physicochemical property. Here, we have shown a few best predictors of the topological index regression models for the particular physicochemical property. As a result, the regression model is the best to test and use for this analysis. We used some regression models to fit curves rather than straight lines. Curvilinear regression analysis is the name given to this method. In this study, we tested the following equations;

$Y = a + b_1X_1$ (Linear Equation)

$Y = a + b_1X_1 + b_2X_1^2$ (Quadratic Equation)

$Y = a + b_1X_1 + b_2X_1^2 + b_3X_1^3$ (Cubic Equation)

where Y is dependent variable, a is the regression model constant, , $X_i(i = 1, 2, 3)$ are independent variables, $b_i(i = 1, 2, 3)$ are the coefficients for the individual descriptor is the number of samples used for building the regression equation. It obviously clear that the best predictive model has minimum error and The parameters will be considered for the model's goodness of fit. Todeschini [10] selected the best goodness of fit in models by using any of the parameters $max(R^2), max(F)$. The curvilinear regression analyses and other results were obtained by using the Statistic, MATLAB, Sage math, SPSS statistical

software. The curvilinear regression models' independent variables are the Randic index, first and second Zagreb indices, GA index, ABC index, Forgotten index and Harmonic Index of eleven blood cancer drugs.

Regression model 2-57-10	**Refractivity**				**Regression model**	**Refractivity Point**			
	Molecular descriptor	**R Square**	**F**	**Sig**		**Molecular descriptor**	**R Square**	**F**	**Sig**
Linear Model	ABC(G)	0.933	154.093	000	**Logarithmic Model**	ABC(G)	0.827	52.416	000
	S(G)	0.934	155.042	000		S(G)	0.837	56.567	000
	GA(G)	0.933	152.002	000		GA(G)	0.843	58.946	000
	M1(G)	0.907	106.874	000		M1(G)	0.802	44.586	000
	M2(G)	0.861	67.942	000		M2(G)	0.773	37.449	000
	HM(G)	0.859	67.002	000		HM(G)	0.752	33.324	000
	F(G)	0.855	64.869	000		F(G)	0.732	29.976	000
	H(G)	0.930	147.1	000		H(G)	0.836	56.036	000
Quadratic Model	ABC(G)	0.952	99.878	000	**Exponential Model**	ABC(G)	0.955	232.739	000
	S(G)	0.952	99.647	000		S(G)	0.951	214.865	000
	GA(G)	0.948	90.695	000		GA(G)	0.950	207.857	000
	M1(G)	0.917	55.502	000		M1(G)	0.936	160.612	000
	M2(G)	0.861	31.027	000		M2(G)	0.899	98.077	000
	HM(G)	0.861	31.003	000		HM(G)	0.900	98.646	000
	F(G)	0.859	30.586	000		F(G)	0.897	96.144	000
	H(G)	0.950	95.124	000		H(G)	0.947	197.267	000
Cubic Model	ABC(G)	0.953	60.898	000					
	S(G)	0.954	61.977	000					
	GA(G)	0.949	56.22	000					
	M1(G)	0.924	36.586	000					
	M2(G)	0.911	30.799	000					
	HM(G)	0.919	33.942	000					
	F(G)	0.923	35.742	000					
	H(G)	0.953	61.434	000					

Table 4. Regression models between topological indices and physicochemical boiling point of molecular structures

Boiling Point					**Boiling Point**				
Regression model	**Molecular descriptor**	R^2	**F**	**Sig**	**Regression model**	**Molecular descriptor**	R^2	**F**	**Sig**
	ABC(G)	0.002	0.017	0.898		ABC(G)	0.001	0.009	0.926
	S(G)	0.001	0.014	0.907		S(G)	0.002	0.021	0.888
	GA(G)	0.002	0.016	0.901		GA(G)	0.002	0.02	0.89
Linear Model	M1(G)	0.003	0.028	0.87	**Logaritmic Model**	M1(G)	0.001	0.005	0.944
	M2(G)	0.005	0.046	0.834		M2(G)	0.000	0.002	0.964
	HM(G)	0.004	0.043	0.839		HM(G)	0.000	0.001	0.975
	F(G)	0.004	0.041	0.843		F(G)	0.000	0.001	0.981
	H(G)	0.002	0.016	0.902		H(G)	0.003	0.027	0.873
	ABC(G)	0.150	0.796	0.48		ABC(G)	0.034	0.351	0.567
	S(G)	0.232	1.361	0.305		S(G)	0.035	0.359	0.562
	GA(G)	0.252	1.516	0.271		GA(G)	0.036	0.372	0.556
Quadratic Model	M1(G)	0.171	0.928	0.43	**Exopnential Model**	M1(G)	0.038	0.391	0.546
	M2(G)	0.191	1.066	0.384		M2(G)	0.042	0.438	0.523
	HM(G)	0.141	0.736	0.506		HM(G)	0.040	0.418	0.533
	F(G)	0.108	0.543	0.599		F(G)	0.038	0.4	0.541
	H(G)	0.289	1.828	0.216		H(G)	0.036	0.378	0.553
Cubic Model	ABC(G)	0.323	1.275	0.347					
	S(G)	0.465	2.321	0.152					
	GA(G)	0.515	2.834	0.106					
	M1(G)	0.599	3.99	0.052					
	M2(G)	0.751	8.032	0.008					
	HM(G)	0.693	6.034	0.019					
	F(G)	0.611	4.192	0.047					
	H(G)	0.552	3.29	0.079					

Table 5. Regression models between topological indices and physicochemical properties of melting point of molecular structures

Melting Point					**Melting Point**				
Regression model	**Molecular descriptor**	R^2	**F**	**Sig**	**Regression model**	**Molecular descriptor**	R^2	**F**	**Sig**
	ABC(G)	0.909	99.904	0.000		ABC(G)	0.831	49.795	0.000
	S(G)	0.887	78.511	0.000		S(G)	0.814	43.636	0.000
	GA(G)	0.879	72.917	0.000		GA(G)	0.810	42.719	0.000
Linear Model	M1(G)	0.882	74.603	0.000	**Logarithmic Model**	M1(G)	0.807	41.739	0.000
	M2(G)	0.834	50.072	0.000		M2(G)	0.773	34.008	0.000
	HM(G)	0.849	56.325	0.000		HM(G)	0.776	34.56	0.000
	F(G)	0.859	61.032	0.000		F(G)	0.773	33.994	0.000
	H(G)	0.877	71.041	0.000		H(G)	0.804	40.916	0.000
	ABC(G)	0.912	46.795	0.000		ABC(G)	0.894	84.043	0.000
	S(G)	0.891	36.926	0.000		S(G)	0.864	63.499	0.000
	GA(G)	0.883	34.015	0.000		GA(G)	0.853	58.169	0.000
Quadratic Model	M1(G)	0.883	33.923	0.000	**Exponential Model**	M1(G)	0.873	68.918	0.000
	M2(G)	0.834	22.643	0.000		M2(G)	0.832	49.595	0.000
	HM(G)	0.850	25.413	0.000		HM(G)	0.855	59.177	0.000
	F(G)	0.859	27.475	0.000		F(G)	0.872	67.831	0.000
	H(G)	0.882	33.494	0.000		H(G)	0.853	57.982	0.000
Cubic Model	ABC(G)	0.921	30.971	0.000					
	S(G)	0.903	24.863	0.000					
	GA(G)	0.895	22.726	0.000					
	M1(G)	0.901	24.303	0.000					
	M2(G)	0.89	21.555	0.000					
	HM(G)	0.912	27.795	0.000					
	F(G)	0.930	35.608	0.000					
	H(G)	0.899	23.6817	0.000					

Table 6. Regression models between topological indices and physicochemical property complexity of molecular structures

Complexity					**Complexity**				
Regression model	**Molecular descriptor**	R^2	**F**	**Sig**	Regression model	**Molecular descriptor**	R^2	**F**	**Sig**
	ABC(G)	0.889	79.955	0.000		ABC(G)	0.889	79.955	0.000
	S(G)	0.900	90.006	0.000		S(G)	0.851	57.091	0.000
	GA(G)	0.905	95.147	0.000		GA(G)	0.857	60.113	0.000
Linear Model	M1(G)	0.908	98.435	0.000	**Logaritmic Model**	M1(G)	0.833	49.841	0.000
	M2(G)	0.922	118.59	0.000		M2(G)	0.835	50.599	0.000
	HM(G)	0.911	102.03	0.000		HM(G)	0.813	43.338	0.000
	F(G)	0.901	90.832	0.000		F(G)	0.795	38.665	0.000
	H(G)	0.902	91.96	0.000		H(G)	0.855	58.959	0.000
	ABC(G)	0.891	36.851	0.000		ABC(G)	0.604	15.241	0.003
	S(G)	0.901	41.054	0.000		S(G)	0.611	15.683	0.003
	GA(G)	0.906	43.403	0.000		GA(G)	0.607	15.446	0.003
Quadratic Model	M1(G)	0.914	47.833	0.000	**Exponential Model**	M1(G)	0.611	15.69	0.003
	M2(G)	0.929	58.779	0.000		M2(G)	0.613	15.815	0.003
	HM(G)	0.92	51.495	0.000		HM(G)	0.612	15.799	0.003
	F(G)	0.912	46.362	0.000		F(G)	0.612	15.744	0.003
	H(G)	0.903	41.964	0.000		H(G)	0.614	15.887	0.003
Cubic Model	ABC(G)	0.896	22.971	0.000					
	S(G)	0.905	25.482	0.000					
	GA(G)	0.911	27.42	0.000					
	M1(G)	0.927	34.112	0.000					
	M2(G)	0.939	41.106	0.000					
	HM(G)	0.931	36.226	0.000					
	F(G)	0.924	32.59	0.000					
	H(G)	0.908	26.202	0.000					

Table 7. Regression models between topological indices and physicochemical propertiey flash point of molecular structures

Flash Point					**Flash Point**				
Regression model	**Molecular descriptor**	R^2	**F**	**Sig**	**Regression model**	**Molecular descriptor**	R^2	**F**	**Sig**
	ABC(G)	0.535	10.343	0.011		ABC(G)	0.491	8.699	0.016
	S(G)	0.576	12.232	0.007		S(G)	0.533	10.282	0.011
	GA(G)	0.583	12.597	0.006		GA(G)	0.546	10.819	0.009
Linear Model	M1(G)	0.530	10.153	0.011	**Logarithmic Model**	M1(G)	0.490	8.64	0.017
	M2(G)	0.518	9.666	0.013		M2(G)	0.490	8.637	0.017
	HM(G)	0.497	8.876	0.015		HM(G)	0.460	7.652	0.022
	F(G)	0.478	8.256	0.018		F(G)	0.435	6.941	0.027
	H(G)	0.596	13.299	0.005		H(G)	0.550	10.994	0.009
	ABC(G)	0.538	4.661	0.045		ABC(G)	0.550	11.005	0.009
	S(G)	0.580	5.524	0.031		S(G)	0.593	13.09	0.006
	GA(G)	0.586	5.657	0.029		GA(G)	0.600	13.519	0.005
Quadratic Model	M1(G)	0.532	4.542	0.048	**Exponential Model**	M1(G)	0.547	10.879	0.009
	M2(G)	0.518	4.3	0.054		M2(G)	0.537	10.442	0.010
	HM(G)	0.497	3.945	0.064		HM(G)	0.515	9.548	0.013
	F(G)	0.497	3.672	0.074		F(G)	0.496	8.852	0.016
	H(G)	0.602	6.059	0.025		H(G)	0.612	14.205	0.004
Cubic Model	ABC(G)	0.584	3.281	0.089					
	S(G)	0.630	3.968	0.061					
	GA(G)	0.642	4.193	0.054					
	M1(G)	0.598	3.473	0.079					
	M2(G)	0.543	2.772	0.120					
	HM(G)	0.516	2.486	0.145					
	F(G)	0.497	2.302	0.164					
	H(G)	0.655	4.428	0.048					

4. CONCLUSION

The QSPR study has shown that molecular descriptors (TIs) are best tools to predict physicochemical properties of drugs used for chemical, medical, and pharmaceutical char-acteristics. In the linear regression model, all molecular descriptors are best predicted with the mentioned physicochemical properties. In a quadratic regression model, molecular descriptor S (G) is best predicted with refractivity, melting point and complexity. In a loga-rithmic regression model, molecular descriptor ABC (G) is best predicted with refractivity. In an exponential regression model, molecular descriptors M1 (G) and HM (G) are best predicted with molar refractivity. The results of the above study may be used in the fur-ther development of drugs used for chemical, medical, and pharmaceutical characteristics. Also the obtained theoretical results have promising aspects and provide a cornerstone in designing new drugs.

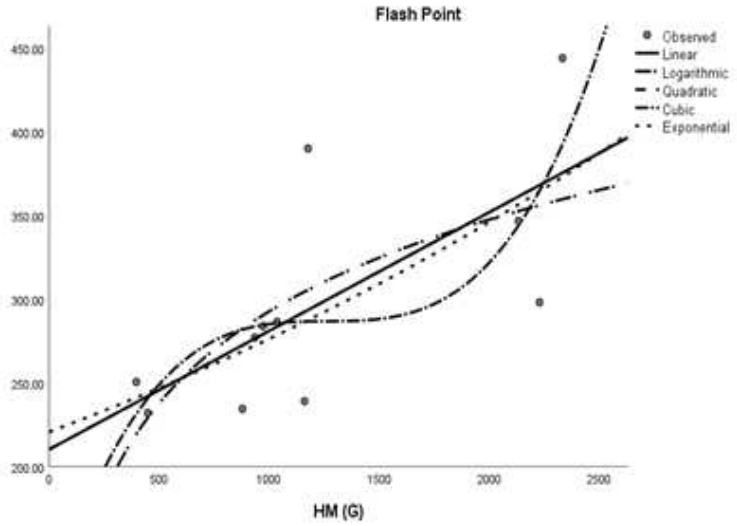


Figure 2: Logarithmic regression model of GA (G) with refractivity.

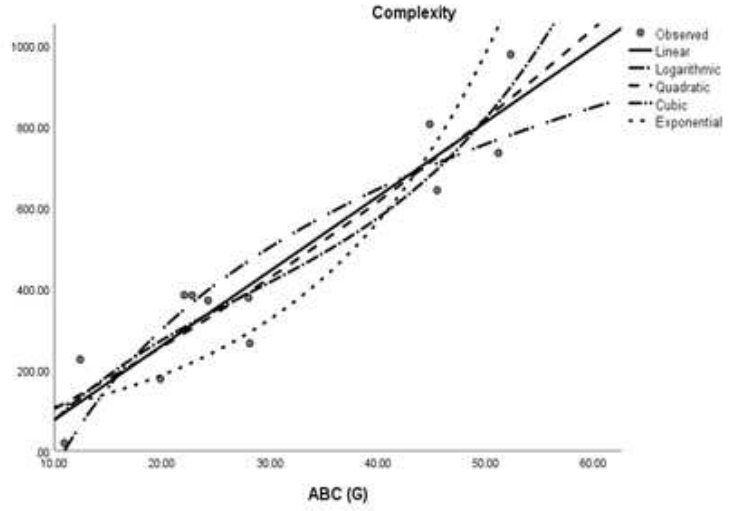


Figure 3: Exponential regression model of ABC (G) with refractivity.

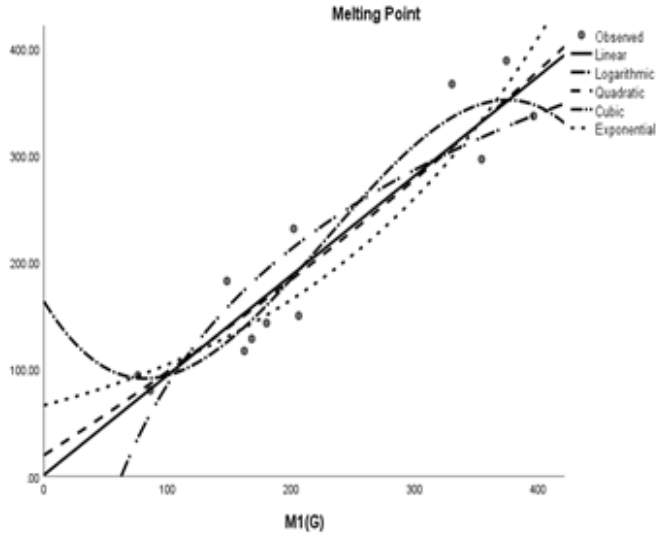


Figure 4: Linear regression model of M1 (G) with melting point.

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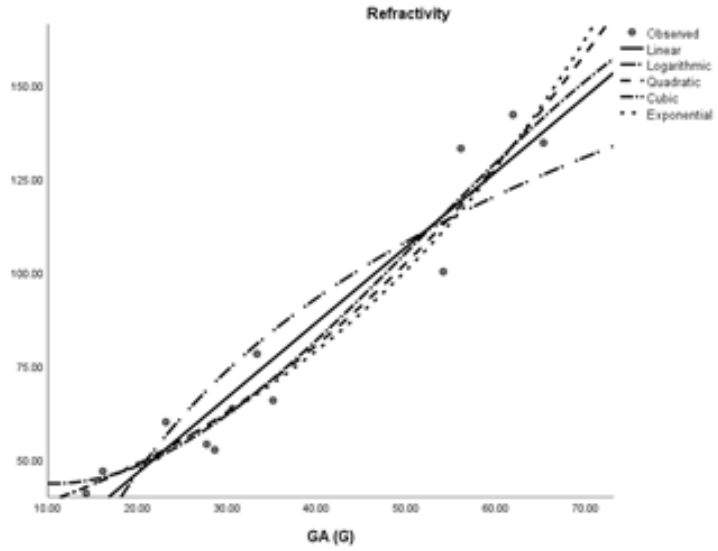

Figure 5: Quadratic regression model of GA(G) with refractivity.

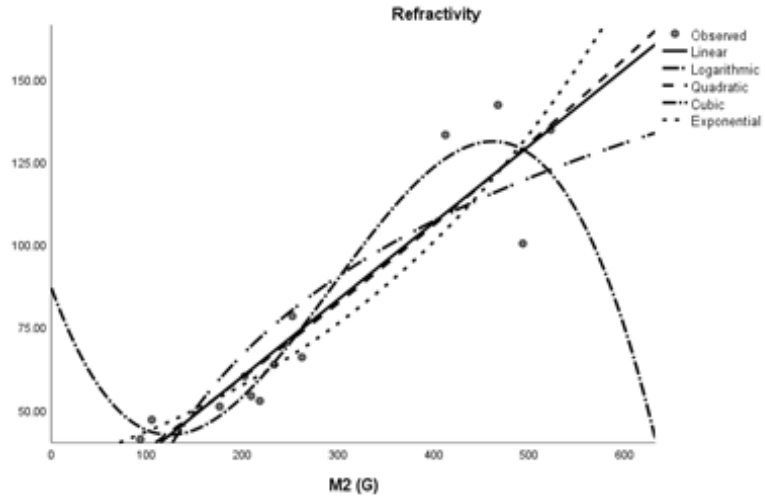

Figure 6: Cubic regression model of ABC (G) with refractivity.

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