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QSPR ANALYSIS OF PHYSICOCHEMICAL PROPERTIES OF ANTI-CANCER DRUGS USING DEGREE BASED GRAPH THEORETICAL DESCRIPTORS

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Abstract. Through topological invariants, chemical graph theory provides a rigorous mathematical framework for describing molecular structure and deciphering chemical behavior. This study builds quantitative structure property relationship (QSPR) models for a group of anticancer medications using ten degree-based descriptors, including the Zagreb indices, atom bond connectivity index, and Randić index. To determine the most predictive descriptors for important physicochemical properties, such as molecular weight, heavy atom count, molar refractivity, boiling point, molar volume, polarizability, and polar surface area, linear, logarithmic, quadratic, and cubic regression models are methodically examined. F-statistics, significance levels, and R^2 , adjusted R^2 standard error are used to evaluate the model's performance. The findings show that a number of degree-based indices have substantial associations with various drug features, with different regression types and descriptors yielding the best accurate

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predictions. Overall, the results show that graph-theoretical invariants are useful and effective techniques for predicting the physicochemical properties of anticancer drugs, providing important information for computational drug design.

Keywords: anti-cancer medications; QSPR modeling; degree dependent topological descriptors; physio-chemical characteristics

2020 AMS Subject Classification: 05C09; 05C92; 92E10

1. INTRODUCTION

Chemical graph theory is an important field with many uses in various branches of chemistry and materials science. Its ability to provide a mathematical framework for understanding the behaviors and structural characteristics of underlying structures is what makes it significant [12]. Chemical informatics, computational chemistry, materials design, and drug discovery are among the domains that benefit from this mathematical framework [34]. In chemical graph theory, topological invariants are mathematical measures that are useful for predicting a chemical compound's strength through QSAR/QSPR analyses [46]. Topological invariants are useful tools for converting a chemical composition into a real number that can be associated with bioactivity and physicochemical characteristics [47]. The degree-based invariants of molecular compounds are the most valuable of the numerous topological invariants that have been studied thus far. The first vertex degree-based topological indices were introduced in the 1970s and are now called Zagreb indices [21]. The development of the topological invariants was made possible by them.

Graph theoretical techniques are used by QSPR models to determine a molecule's structural characteristics, which aid in property prediction. Originally employed in biology and toxicology, these models are now being used more frequently to forecast the characteristics of chemical compounds. To evaluate the relationship between the molecular descriptors and the key characteristics of the chemical structures, they use regression models [2], [24], [25], [35], [38]. Toxicology, pharmacokinetics, pharmacodynamics, chemometrics, and many other fields frequently use QSPR models as a practical and popular research method [6], [9]. They save time and money, enabling us to predict the chemical, physical, pharmaceutical, and biological properties. They also help scientists by providing important information that helps them better

understand how the compound under consideration acts biologically [10], [26]. Applications in material science, organic chemistry, physics, medicine, agriculture, and biology are numerous [28], [33]. According to numerous publications [37], [44], [49], [58], [54], they are effective in predicting characteristics of chemical compounds such as flash point, toxicity, excretion, distribution, absorption, energy, and metabolism.

Kirman et al. [32] discussed degree related topological descriptors of COVID-19 drugs and discovered strong correlations with physicochemical characteristics. Drug discovery was aided by Liu et al. [36], who discussed distance related descriptors for antiviral medications. Havare [23] created QSPR models for cancer medications using M-polynomial. The properties of anti-tuberculosis drugs were correlated with degree-based invariants by Adnan et al. [1]. Shanmukha et al. [53] examined anticancer medications, demonstrating relations among indices and chemical characteristics. Zaman et al. [64] used a linear regression model to create QSPR models for molecular property prediction. Strong predictive power was demonstrated by Ravi and Desikan [50], who created QSPR models for hyaluronic acid-paclitaxel conjugates using reduced reverse degree-based descriptors. Nasir et al. [42] studied blood cancer compounds, Gnanaraj et al. [20] performed QSPR investigation on NSAID medications. Furthermore, medications for cardiovascular disease [15], HIV/AIDS [17], breast cancer [52], colorectal cancer [41], anti-malarial [3], antitumor [40], and infertility treatment drugs [55] have all been studied using QSPR modeling. This paper develops QSPR models for anti-cancer drugs using degree-based descriptors, motivated by these works. The purpose of this research is to analyze various anti-cancer medications in order to forecast their physicochemical characteristics, which could aid in the creation of more potent general medications for cancer patients.

In this regard, graph-theoretical methods are becoming more and more popular as effective methods for simulating intricate pharmaceutical molecules. Essential structural characteristics can be captured by numerical descriptors that rely only on atomic connection when drug molecules are represented as molecular graphs. Degree-based topological indices are particularly useful among the many kinds of descriptors because of their excellent association with physicochemical parameters and ease of calculation. Molecule branching and local connectivity, two important variables affecting molecular size, stability, and intermolecular interactions,

are directly measured by these indices. As a result, adding degree-based descriptors to QSPR modeling provides a strong foundation for forecasting significant physicochemical properties of anticancer medications, promoting logical drug design and lowering the need for lengthy experimental measurements.

The drugs that are used for cancer treatment include an extensive number of therapies that are designed to reduce the growth of cancerous cells, stop tumors from spreading, and increase overall survival. The foundation of many treatment regimens is still traditional chemotherapy, which uses drugs that stop DNA replication or interfere with the cell-division cycle, ultimately killing rapidly proliferating cancer cells [8]. These medications can be quite successful, but they also frequently damage healthy tissues, causing well-known side effects like nausea, exhaustion, and hair loss. By concentrating on particular molecular defects that promote tumor growth, tailored medicines have recently revolutionized the treatment of cancer [56]. These drugs, which include tyrosine kinase inhibitors and monoclonal antibodies, allow for a more specific approach and often generate fewer systemic effects than conventional chemotherapy. By using the body's immune system to recognize and eliminate cancer cells, immunotherapy has introduced yet another level of complexity and given patients with cancers that were previously thought to be incurable new hope [45]. Despite these developments, problems including drug resistance, tumor heterogeneity, and recurrence still make treatment difficult, necessitating continued study to provide more efficient and individualized treatment plans [27]. In order to enhance patient outcomes, current research focuses on creating next-generation precision medications, integrating immunotherapy with targeted drugs, and putting into practice individualized treatment plans powered by genomics and biomarker characterization [60].

Now, we discuss some drugs in Table 1, 2, and Figures 1, 2 and 3, which are commonly used to treat cancer.

2. TOPOLOGICAL INDICES

Using molecular graphs, topological indices are numerical descriptors that depict the structure of chemical compounds. In order to predict physical, chemical, and biological properties without conducting experiments, they are frequently employed in QSAR and QSPR studies. The Randić, Zagreb, and ABC indices are few examples of degree-based topological indices

Drug	Chemical Formula	Mechanism / Target	Clinical Uses
Dactinomycin	$C_{62}H_{86}N_{12}O_{16}$	DNA intercalation; inhibits RNA synthesis; topoisomerase II-mediated DNA breaks	Wilms' tumor, rhabdomyosarcoma, Ewing's sarcoma, testicular cancer, leukemias, lymphomas, lung cancer [4]
Etoposide	$C_{29}H_{32}O_{13}$	Topoisomerase II inhibitor causing DNA double-strand breaks	Small-cell lung cancer, testicular cancer, lymphomas, leukemias [39]
Imatinib	$C_{29}H_{31}N_7O$	Selective inhibitor of BCR-ABL, c-KIT, PDGFRA tyrosine kinases	Chronic myeloid leukemia (CML), gastrointestinal stromal tumors (GIST) [30]
Olaparib	$C_{24}H_{23}FN_4O_3$	PARP inhibition causing synthetic lethality in BRCA1/2-mutated cells	BRCA-mutated ovarian, breast, pancreatic, and prostate cancers [5]
Paclitaxel	$C_{47}H_{51}NO_{14}$	Microtubule stabilization preventing depolymerization; mitotic arrest	Ovarian, breast, lung, pancreatic cancers [59]
Sirolimus	$C_{51}H_{79}NO_{13}$	mTOR inhibition; blocks IL-2-mediated T-cell activation	Immunosuppression; anticancer therapy [57]
Sorafenib	$C_{21}H_{16}ClF_3N_4O_3$	RAF and receptor tyrosine kinase inhibitor; anti-angiogenic	Hepatocellular carcinoma, renal cell carcinoma, thyroid cancer [61]
Temsirolimus	$C_{56}H_{87}NO_{16}$	mTOR inhibitor suppressing cell growth and angiogenesis	Poor-prognosis metastatic renal cell carcinoma [29]
Trabectedin	$C_{39}H_{43}N_3O_{11}S$	Binds DNA minor groove, distorts helix, inhibits transcription-coupled repair	Soft-tissue sarcomas, relapsed ovarian cancer [11]

TABLE 1. Summary of selected anticancer drugs, mechanisms, and clinical applications.

that are based on the degrees of atoms in the molecular graph and represent molecular branching and connectivity. They are useful tools in chemoinformatics and material sciences, with applications ranging from predicting boiling points, stability, bioactivity, toxicity, and drug design. Let $\wp(t)$ be the degree of a vertex t in any given graph.

Drug	Chemical Formula	Mechanism / Target	Clinical Uses
Trametinib	$C_{26}H_{23}FIN_5O_4$	Selective MEK1/2 inhibitor (MAPK/ERK pathway)	BRAF-mutant metastatic melanoma (often with dabrafenib) [16]
Vemurafenib	$C_{23}H_{18}ClF_2N_3O_3S$	Selective inhibitor of BRAF V600E mutation	Metastatic melanoma [7]
Venetoclax	$C_{45}H_{50}ClN_7O_7S$	Selective BCL-2 inhibitor restoring apoptosis	Chronic lymphocytic leukemia (CLL), acute myeloid leukemia (AML) [51]
Vinblastine	$C_{46}H_{58}N_4O_9$	Vinca alkaloid; inhibits microtubule formation; mitotic arrest	Lymphomas, breast cancer, Kaposi's sarcoma, testicular cancer [43]
Vincristine	$C_{46}H_{56}N_4O_{10}$	Vinca alkaloid; blocks microtubule polymerization; metaphase arrest	Acute lymphoblastic leukemia (ALL), lymphomas, neuroblastoma [31]

TABLE 2. Summary of selected anticancer drugs, mechanisms, and clinical applications.

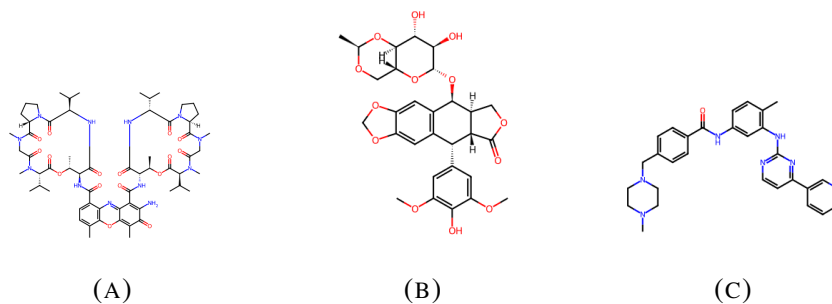


FIGURE 1. (A) Dactinomycin (B) Etoposide (C) Imatinib

Gutman and Trinajestić [21] introduced the first and second Zagreb indices as:

$$M_1(\mathcal{H}) = \sum_{rt \in E_{\mathcal{H}}} (\wp(r) + \wp(t)) \quad M_2(\mathcal{H}) = \sum_{rt \in E_{\mathcal{H}}} \wp(r)\wp(t).$$

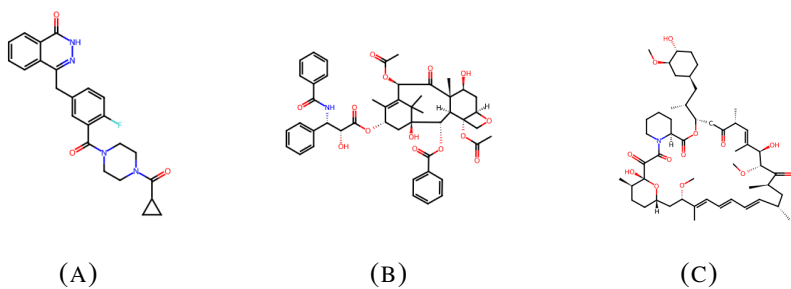
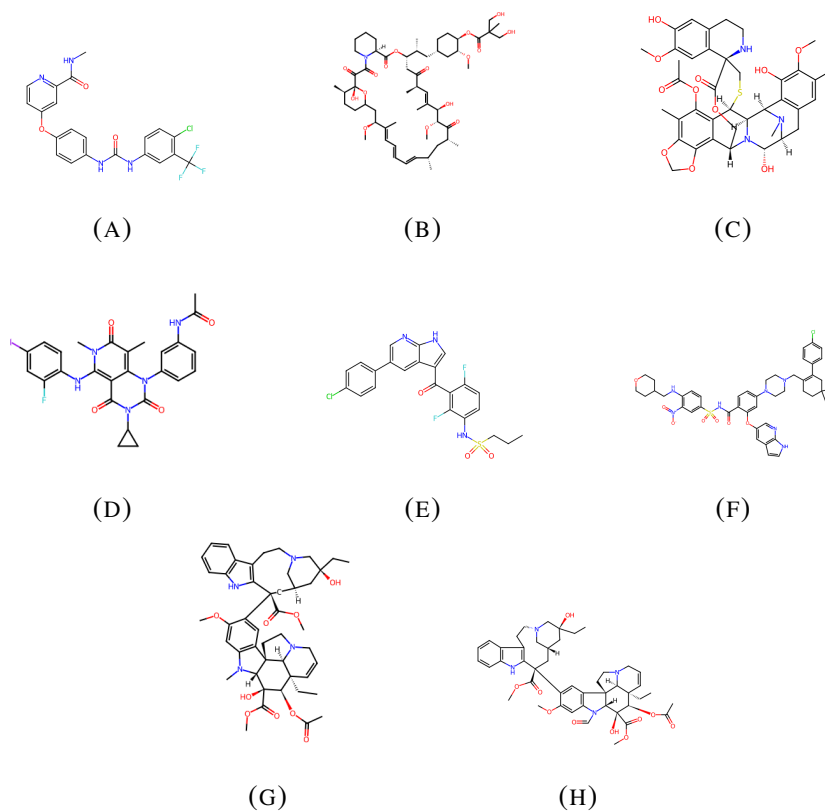


FIGURE 2. (D) Olaparib (E) Paclitaxel (F) Sirolimus

FIGURE 3. (G) Sorafenib (H) Temsirolimus (I) Trabectedin (J) Trametinib
(K) Vemurafenib (L) Venetoclax (M) Vinblastine (N) Vincristine

Estrada et al. [13] gave a topological index called ABC index as:

$$ABC(\mathcal{H}) = \sum_{rt \in E_{\mathcal{H}}} \sqrt{\frac{\wp(r) + \wp(t) - 2}{\wp(r)\wp(t)}}.$$

In [62], Vukičević and Furtula defined the geometric arithmetic index of $\mathcal{H}$ as:

$$GA(\mathcal{H}) = \sum_{rt \in E_{\mathcal{H}}} \frac{2\sqrt{\wp(r)\wp(t)}}{\wp(r) + \wp(t)}.$$

In 1988, Fajtlowicz [14] proposed the Harmonic index as:

$$H(\mathcal{H}) = \sum_{rt \in E_{\mathcal{H}}} \frac{2}{\wp(r) + \wp(t)}.$$

The forgotten index was introduced by Furtula and Gutman [18] as:

$$F(\mathcal{H}) = \sum_{rt \in E_{\mathcal{H}}} (\wp^2(r) + \wp^2(t)).$$

In 1975, the Randić index [48] was defined as follows:

$$RI(\mathcal{H}) = \sum_{rt \in E_{\mathcal{H}}} \frac{1}{\sqrt{\wp(r)\wp(t)}}.$$

[63] provided the sum-connectivity index, which is described as:

$$\chi(\mathcal{H}) = \sum_{rt \in E_{\mathcal{H}}} \frac{1}{\sqrt{\wp(r) + \wp(t)}}.$$

Gutman in [22] introduced the Sombor index as:

$$So(\mathcal{H}) = \sum_{rt \in E_{\mathcal{H}}} \sqrt{\wp^2(r) + \wp^2(t)}.$$

Inspired by the ABC index, Furtula et al. [19] described a new topological index called the augmented Zagreb index, which has the following definition:

$$AZI(\mathcal{H}) = \sum_{rt \in E_{\mathcal{H}}} \left(\frac{\wp(r)\wp(t)}{\wp(r) + \wp(t) - 2} \right)^3.$$

3. MATERIALS AND METHODS

The physicochemical characteristics of fourteen anticancer medications are summarized in Table 3 and are shown as molecular graphs $\mathbb{G}_1 - \mathbb{G}_{14}$. Molecular weight (MW), heavy atom count (HAC), Complexity (CO), boiling point (BP), molar refractivity (MR), polarizability (PO), molecular volume (MV), and polar surface area (PSA) are some of the parameters that highlight the structural and physicochemical diversity of the compounds that were chosen (that are gathered from ChemSpider [65] and PubChem [66]). The information enumerates important molecular traits associated with the physicochemical and biological behavior of the drugs.

For example, Olaparib and Sorafenib have relatively smaller molecular sizes and surface areas than Dactinomycin, which has the highest molecular weight and PSA, suggesting a large and polar structure. While some medications have no recorded data, the boiling point (BP) values are reported where they are available. This study's methodology uses degree-based topolog-

Graphs	Drugs	Properties							
		MW	HAC	CO	BP	MR	PO	MV	PSA
		(g/mol)			°C	(cm ³)	(cm ³)	(cm ³ /mol)	(Å ²)
G ₁	Dactinomycin	1255.4	90	3030	1386	323.7	128.3	880.7	356
G ₂	Etoposide	588.6	42	969	798.1	140.1	55.5	378.5	161
G ₃	Imatinib	493.6	37	706	0	147.1	58.3	393	86.3
G ₄	Olaparib	434.5	32	790	0	116.9	46.3	301.8	82.1
G ₅	Paclitaxel	853.9	62	1790	957.1	219.3	86.5	610.6	221
G ₆	Sirolimus	914.2	65	1760	973	246.7	97.8	773.5	195
G ₇	Sorafenib	464.8	32	646	523.3	113.1	44.8	319.5	92.4
G ₈	Temsirolimus	1030.3	73	2010	1048.4	273.2	108.3	853.1	242
G ₉	Trabectedin	761.8	54	1450	0	195.7	77.6	489.3	194
G ₁₀	Trametinib	615.4	37	1090	0	141.5	56.1	353.1	102
G ₁₁	Vemurafenib	489.9	33	790	711.4	121.6	48.2	332.4	100
G ₁₂	Venetoclax	868.4	61	1640	0	234.4	92.9	647.7	183
G ₁₃	Vinblastine	811	59	1700	0	220.7	87.5	590	154
G ₁₄	Vincristine	825	60	1750	0	221.1	87.6	586.9	171

TABLE 3. Physicochemical properties of anticancer drugs.

ical indices and QSPR modeling to analyze and forecast the physicochemical characteristics

of medications used to treat coronary artery disease. Using degree dependent topological descriptors as the independent variables and the physicochemical characteristics as the dependent variables, we build linear regression model, quadratic regression model, logarithmic regression model, and cubic regression model to correlate the physicochemical characteristics of fourteen cancer disease drug structures. The following lists the mathematical equations for four different regression models included linear, logarithmic, quadratic, and cubic.

$$\begin{aligned}
 (1) \quad & PCP = p[TopInd] + B, \\
 & PCP = p \log[TopInd] + B, \\
 & PCP = q[TopInd]^2 + p[TopInd] + B, \\
 & PCP = s[TopInd]^3 + q[TopInd]^2 + p[TopInd] + B.
 \end{aligned}$$

Here, PCP and $TopInd$ denote the physico-chemical characteristics and index of a given structure, respectively. Also p , q and s used as the regression coefficients and B is a constant.

3.1. Degree oriented Topological Descriptors Calculation. Using the degree-based edge partitioning of drug molecules for anticancer, which is shown in Table 4, we can determine the degree-based topological invariants.

Next, we acquire the topological indices for the drug Vincristine by using section 2 and Table 4.

- The Zagreb indices

$$\begin{aligned}
 M_1(Vincristine) &= \sum_{rt \in E_{Vincristine}} (\wp(r) + \wp(t)) = 6(1 + 2) + 4(1 + 3) + 2(1 + 4) + 7(2 + 2) \\
 &\quad + 23(2 + 3) + 7(2 + 4) + 7(3 + 3) + 11(3 + 4) = 348
 \end{aligned}$$

$$\begin{aligned}
 M_2(Vincristine) &= \sum_{rt \in E_{Vincristine}} \wp(r)\wp(t) = 6(1 \times 2) + 4(1 \times 3) + 2(1 \times 4) + 7(2 \times 2) \\
 &\quad + 23(2 \times 3) + 7(2 \times 4) + 7(3 \times 3) + 11(3 \times 4) = 449
 \end{aligned}$$

Drug for Anti-cancer	Edge partitions and their respective frequencies								
	(1,2)	(1,3)	(1,4)	(2,2)	(2,3)	(2,4)	(3,3)	(3,4)	(4,4)
Dactinomycin (Actinomycin D)	0	30	0	5	26	0	35	0	0
Etoposide	2	5	0	4	22	0	15	0	0
Imatinib	0	3	0	11	24	0	3	0	0
Olaparib	0	4	0	8	16	0	8	0	0
Paclitaxel (Taxol)	0	11	4	13	19	3	10	7	1
Sirolimus (Rapamycin)	3	14	1	9	26	1	12	2	0
Sorafenib	1	3	3	5	19	0	2	1	0
Temsirolimus	5	14	2	9	26	3	14	3	0
Trabectedin	2	8	0	6	18	2	24	2	0
Trametinib	0	9	0	4	14	0	14	0	0
Vemurafenib	1	4	2	6	13	2	8	0	0
Venetoclax	0	4	4	15	33	3	8	1	0
Vinblastine	5	5	2	7	22	7	8	11	0
Vincristine	6	4	2	7	23	7	7	11	0

TABLE 4. Data on edge partition frequencies for different anticancer medications

- The geometric arithmetic index

$$\begin{aligned}
 GA(Vincristine) &= \sum_{rt \in E_{Vincristine}} \frac{2\sqrt{\wp(r) \times \wp(t)}}{\wp(r) + \wp(t)} \\
 &= \frac{2 \times 6\sqrt{1 \times 2}}{1+2} + \frac{2 \times 4\sqrt{1 \times 3}}{1+3} + \frac{2 \times 2\sqrt{1 \times 4}}{1+4} + \frac{2 \times 7\sqrt{2 \times 2}}{2+2} \\
 &\quad + \frac{2 \times 23\sqrt{2 \times 3}}{2+3} + \frac{2 \times 7\sqrt{2 \times 4}}{2+4} + \frac{2 \times 7\sqrt{3 \times 3}}{3+3} + \frac{2 \times 11\sqrt{3 \times 4}}{3+4} = 64.7431
 \end{aligned}$$

- The atom bond connectivity index

$$\begin{aligned}
 ABC(Vincristine) &= \sum_{rt \in E_{Vincristine}} \sqrt{\frac{\wp(r) + \wp(t) - 2}{\wp(r) \times \wp(t)}} \\
 &= 6\sqrt{\frac{1+2-2}{1 \times 2}} + 4\sqrt{\frac{1+3-2}{1 \times 3}} + 2\sqrt{\frac{1+4-2}{1 \times 4}} + 7\sqrt{\frac{2+2-2}{2 \times 2}}
 \end{aligned}$$

$$\begin{aligned}
& +23\sqrt{\frac{2+3-2}{2 \times 3}} + 7\sqrt{\frac{2+4-2}{2 \times 4}} + 7\sqrt{\frac{3+3-2}{3 \times 3}} + 11\sqrt{\frac{3+4-2}{3 \times 4}} \\
& = 47.1708
\end{aligned}$$

- The Harmonic index

$$\begin{aligned}
H(\text{Vincristine}) &= \sum_{rt \in E_{\text{Vincristine}}} \frac{2}{\wp(r) + \wp(t)} \\
&= 6\left(\frac{2}{1+2}\right) + 4\left(\frac{2}{1+3}\right) + 2\left(\frac{2}{1+4}\right) + 7\left(\frac{2}{2+2}\right) + 23\left(\frac{2}{2+3}\right) \\
&\quad + 7\left(\frac{2}{2+4}\right) + 7\left(\frac{2}{3+3}\right) + 11\left(\frac{2}{3+4}\right) = 27.3095
\end{aligned}$$

- The forgotten index

$$\begin{aligned}
F(\text{Vincristine}) &= \sum_{rt \in E_{\text{Vincristine}}} (\wp^2(r) + \wp^2(t)) = 6[1+4] + 4[1+9] + 2[1+16] + 7[4+4] \\
&\quad + 23[4+4] + 7[4+16] + 7[9+9] + 11[9+16] = 1000
\end{aligned}$$

- The sum-connectivity index

$$\begin{aligned}
\chi(\text{Vincristine}) &= \sum_{rt \in E_{\text{Vincristine}}} \frac{1}{\sqrt{\wp(r) + \wp(t)}} \\
&= \frac{6}{\sqrt{1+2}} + \frac{4}{\sqrt{1+3}} + \frac{2}{\sqrt{1+4}} + \frac{7}{\sqrt{2+2}} + \frac{23}{\sqrt{2+3}} + \frac{7}{\sqrt{2+4}} + \frac{7}{\sqrt{3+3}} \\
&\quad + \frac{11}{\sqrt{3+4}} = 30.0175
\end{aligned}$$

- The Randić index

$$\begin{aligned}
RI(\text{Vincristine}) &= \sum_{rt \in E_{\text{Vincristine}}} \frac{1}{\sqrt{\wp(r)\wp(t)}} \\
&= \frac{6}{\sqrt{1 \times 2}} + \frac{4}{\sqrt{1 \times 3}} + \frac{2}{\sqrt{1 \times 4}} + \frac{7}{\sqrt{2 \times 2}} + \frac{23}{\sqrt{2 \times 3}} + \frac{7}{\sqrt{2 \times 4}} + \frac{7}{\sqrt{3 \times 3}} \\
&\quad + \frac{11}{\sqrt{3 \times 4}} = 28.4254
\end{aligned}$$

- The Sombor index

$$\begin{aligned}
So(\text{Vincristine}) &= \sum_{rt \in E_{\text{Vincristine}}} \sqrt{\wp^2(r) + \wp^2(t)} \\
&= 6\sqrt{1+4} + 4\sqrt{1+9} + 2\sqrt{1+16} + 7\sqrt{4+4} + 23\sqrt{4+9} \\
&\quad + 7\sqrt{4+16} + 7\sqrt{9+9} + 11\sqrt{9+16} = 253.0418
\end{aligned}$$

- The augmented Zagreb

$$\begin{aligned}
 AZI(Vincristine) &= \sum_{rt \in E_{Vincristine}} \left(\frac{\wp(r)\wp(t)}{\wp(r) + \wp(t) - 2} \right)^3 \\
 &= 6 \left(\frac{1 \times 2}{1+2-2} \right)^3 + 4 \left(\frac{1 \times 3}{1+3-2} \right)^3 + 2 \left(\frac{1 \times 4}{1+4-2} \right)^3 + 7 \left(\frac{2 \times 2}{2+2-2} \right)^3 \\
 &\quad + 23 \left(\frac{2 \times 3}{2+3-2} \right)^3 + 7 \left(\frac{2 \times 4}{2+4-2} \right)^3 \\
 &\quad + 7 \left(\frac{3 \times 3}{3+3-2} \right)^3 + 11 \left(\frac{3 \times 4}{3+4-2} \right)^3 \\
 &= 594.0391
 \end{aligned}$$

We calculated the degree-based invariant values for the medications given in Table 5 applying the edge partitioning data from Table 4.

Drug molecules	M_1	M_2	GA	ABC	H	F	χ	RI	So	AZI
Dactinomycin	480	581	91.4555	69.7485	39.5667	1308	43.4162	42.1016	351.2472	747.9219
Etoposide	242	302	46.7713	33.8815	19.6333	648	21.6171	20.2824	174.5590	411.7344
Imatinib	194	224	40.1132	29.1982	17.6000	484	18.9579	18.0300	139.8607	324.2969
Olaparib	176	212	35.1408	25.5699	15.0667	456	16.4214	15.5080	126.9065	296.6250
Paclitaxel	346	429	65.0990	48.9918	27.7833	976	30.5924	29.2723	253.0522	556.2437
Sirolimus	328	384	65.1498	49.1651	29.2048	868	31.3700	30.7496	239.6872	525.9559
Sorafenib	164	187	32.5468	24.7041	14.4190	434	15.6105	15.1512	120.2251	253.8414
Temsirolimus	370	438	72.7108	54.8384	32.5571	996	34.9828	34.3262	270.7120	596.9315
Trabectedin	322	416	60.3153	43.6220	24.7714	894	27.5749	25.6659	232.4085	552.0230
Trametinib	206	253	39.5114	29.4097	16.7667	556	18.4765	17.5783	149.6489	333.8438
Vemurafenib	178	212	34.62299	25.8877	15.0000	480	16.3680	15.6975	129.8595	285.3657
Venetoclax	334	394	65.8155	48.7714	28.2524	886	30.9156	29.2976	242.9087	535.9305
Vinblastine	350	453	64.6865	47.2397	27.0762	1010	29.9012	28.2207	254.6051	592.8047
Vincristine	348	449	64.7431	47.1708	27.3095	1000	30.0175	28.4254	253.0418	594.0391

TABLE 5. Values of the degree-dependent topological invariant that correspond to anticancer drug molecules

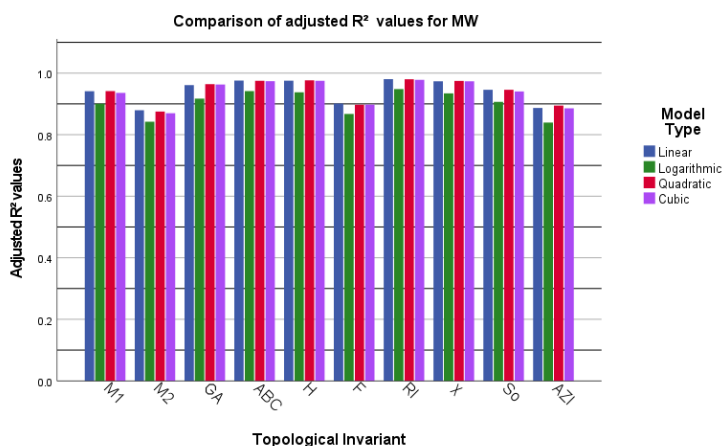
4. RESULTS AND DISCUSSION

SPSS and the R-programming language were used to conduct regression analyses in order to find the worthwhile topological invariant for predicting molecular characteristics. Four regression models (linear, quadratic, logarithmic, and cubic) were evaluated. For each topological index, the best models were chosen based on Quantitative measures including coefficient of determination $\mathbb{R}^2$, adjusted $\mathbb{R}^2$, F-statistic, standard error, and significance ($p < 0.05$). The best model was compared with observed and expected values to provide additional confirmation of predictive stability of the ideal-fitting invariant. The selection methodology relied on balancing reduced standard error, high adjusted $\mathbb{R}^2$, and statistically significant results. This provides a comprehensive, data computed methodology that quantifies the balance among predictive capability and literature interpretation.

4.1. Comparative Evaluation of Regression Models for Molecular Weight Prediction. Table 6 and Figure 4 summarizes the $\mathbb{R}^2$ and adjusted $\mathbb{R}^2$ values for four regression models, where ten degree-based topological indices are treated as independent variables and the molecular weights of fourteen anticancer drugs as the dependent variable.

Topological Invariant	Linear		Logarithmic		Quadratic		Cubic	
	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$
M_1	0.946001	0.941501	0.908057	0.900395	0.950741	0.941784	0.950764	0.935993
M_2	0.888914	0.879657	0.854531	0.842409	0.894365	0.875159	0.900033	0.870043
GA	0.964340	0.961368	0.923791	0.917441	0.969729	0.964225	0.971810	0.963353
ABC	0.977977	0.976142	0.946393	0.941925	0.979026	0.975213	0.979993	0.973990
H	0.977456	0.975578	0.942538	0.937750	0.980445	0.976889	0.980805	0.975046
F	0.908937	0.901348	0.877616	0.867417	0.913401	0.897656	0.921412	0.897835
χ	0.975632	0.973601	0.939615	0.934583	0.978634	0.974749	0.979719	0.973635
RI	0.982296	0.980821	0.952443	0.948480	0.983303	0.980267	0.983350	0.978355
So	0.950343	0.946205	0.913897	0.906722	0.954268	0.945953	0.954268	0.940548
AZI	0.895599	0.886899	0.851721	0.839364	0.911008	0.894828	0.912073	0.885695

TABLE 6. $\mathbb{R}^2$ and adjusted $\mathbb{R}^2$ -values for various regression models are compared.

FIGURE 4. Comparison of adjusted $\mathbb{R}^2$ -values for MW.

The M_1 , GA , H , χ and AZI indices clearly perform best in the quadratic model, while the M_2 , ABC , F , RI , and So indices find their best fits in the cubic model, according to the adjusted $\mathbb{R}^2$ values from Table 6. The Quantitative investigation of the top regression models for every independent variable is displayed in Table 7. The correlation coefficient $\mathbb{R}$, $\mathbb{R}^2$, adjusted $\mathbb{R}^2$, $\mathcal{F}$ -statistic, standard error, p values, and regression equation are all included in this analysis. Using a Linear model, this Quantitative analysis demonstrates that the most predictive index is the Randić index.

Predictor		Goodness of Fit				Sig.		Regression Eq.
Index	Model	$\mathbb{R}$	$\mathbb{R}^2$	adjusted. $\mathbb{R}^2$	Std. Error	$\mathcal{F}$ -statistic	p -quantity	
M_1	Quadratic	0.975059	0.950741	0.941784	58.072140	106.153832	6.44e-08	$MW=0.001804 \times M_1^2 + 1.393368 \times M_1 + 176.317989$
M_2	Linear	0.942822	0.888914	0.879657	83.494576	96.024624	4.46e-07	$MW=1.890177 \times M_2 + 77.19404$
GA	Quadratic	0.984748	0.969729	0.964225	45.523902	176.189712	4.42e-09	$MW=0.055077 \times GA^2 + 7.086753 \times GA + 162.977155$
ABC	Linear	0.988927	0.977977	0.976142	37.176055	532.894823	2.60e-11	$MW=17.711219 \times ABC + 11.871046$
H	Quadratic	0.990174	0.980445	0.976889	36.589507	275.752361	4e-10	$MW=0.220405 \times H^2 + 20.017760 \times H + 126.152914$
F	Linear	0.953382	0.908937	0.901348	75.596197	119.776930	1.34e-07	$MW=0.841506 \times F + 82.400358$
χ	Quadratic	0.989259	0.978634	0.974749	38.246070	251.916072	6.51e-10	$MW=0.181049 \times \chi^2 + 18.489173 \times \chi + 124.040896$
RI	Linear	0.991109	0.982296	0.980821	33.331798	665.831573	7e-12	$MW=29.137534 \times RI + 14.266196$
So	Linear	0.974855	0.950343	0.946205	55.823666	229.658782	3.46e-09	$MW=3.370379 \times So + 35.870889$
AZI	Quadratic	0.954468	0.911008	0.894828	78.054456	56.303617	2e-06	$MW=0.001457 \times AZI^2 + 0.126415 \times AZI + 327.877964$

TABLE 7. Best regression models for MW

Table 8 summarizes the actual and predicted molecular weights of anticancer drugs based on the most accurate forecasting index, and Figure 5 displays the corresponding graphical representation.

Drugs	Actual MW	Predicted MW	Residual	Drugs	Actual MW	Predicted MW	Residual
G_1	1255.4	1241.002997	14.397003	G_8	1030.3	1014.447016	15.852984
G_2	588.6	605.245316	-16.645316	G_9	761.8	762.107230	-0.307230
G_3	493.6	539.615934	-46.015934	G_{10}	615.4	526.454510	88.945490
G_4	434.5	466.131073	-31.631073	G_{11}	489.9	471.652636	18.247364
G_5	853.9	867.188833	-13.288833	G_{12}	868.4	867.926012	0.473988
G_6	914.2	910.233711	3.966289	G_{13}	811	836.547802	-25.547802
G_7	464.8	455.734801	9.065199	G_{14}	825	842.512255	-17.512255

TABLE 8. Predicted vs Actual values for MW using best model

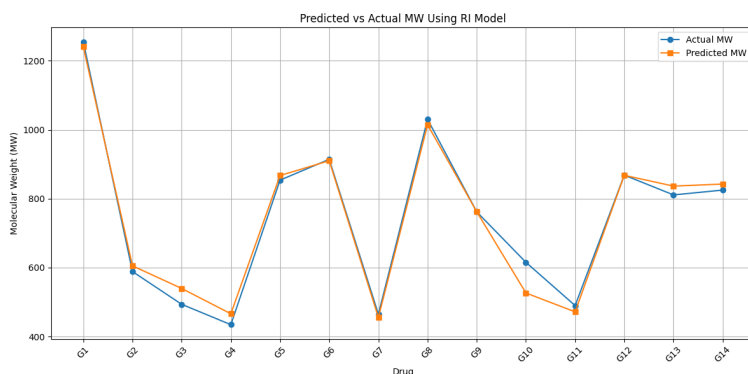


FIGURE 5. Predicted vs Actual values for MW using RI model.

4.2. Comparative Evaluation of Regression Models for HAC Prediction. The $\mathbb{R}^2$ and adjusted $\mathbb{R}^2$ values for the linear regression model, logarithmic regression model, quadratic regression model, and cubic regression model are displayed in Table 9 and Figure 6. In these models, the dependent variable is from the heavy atom counts of fourteen drugs, and the independent variables are from the ten degree-based indices.

Topological Invariant	Linear		Logarithmic		Quadratic		Cubic	
	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$
M_1	0.966883	0.964124	0.928485	0.922525	0.970854	0.965554	0.972013	0.963617
M_2	0.912948	0.905694	0.874988	0.864571	0.918886	0.904137	0.920042	0.896055
GA	0.985908	0.984734	0.948170	0.943851	0.989363	0.987428	0.992117	0.989752
ABC	0.994812	0.994380	0.965827	0.962979	0.995190	0.994316	0.996843	0.995896
H	0.997265	0.997037	0.966977	0.964226	0.998513	0.998243	0.998762	0.998390
F	0.931059	0.925314	0.895393	0.886675	0.936197	0.924597	0.937686	0.918892
χ	0.995189	0.994788	0.962817	0.959718	0.996661	0.996054	0.997909	0.997282
RI	0.999323	0.999266	0.973513	0.971306	0.999541	0.999458	0.999603	0.999484
So	0.970320	0.967847	0.933195	0.927628	0.973615	0.968817	0.974624	0.967011
AZI	0.924690	0.918414	0.880008	0.870009	0.938874	0.927760	0.938986	0.920682

TABLE 9. $\mathbb{R}^2$ and adjusted $\mathbb{R}^2$ -values for various regression models are compared.

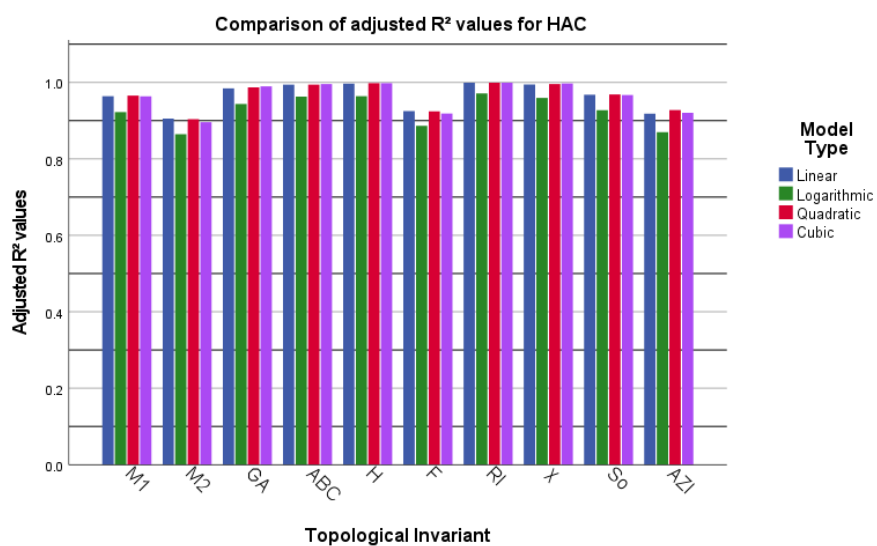


FIGURE 6. Adjusted $\mathbb{R}^2$ -quantities for HAC are compared.

It is evident from Table 9 adjusted R^2 values that the M_1 , So, and AZI indices function best in the quadratic model. The indices GA , ABC , H , χ and RI behaves best in the cubic model. While the other indices M_2 and F reach their peak performance in the linear model. The Quantitative results of the top regression models corresponding to every independent variable is displayed in Table 10. This analysis comprises the regression equation, p quantities, standard error, $\mathcal{F}$ -statistic, adjusted R^2 , and correlation coefficient R . Using a cubic model, the Quantitative investigation emphasize that the Randić index is the best predictor index.

Predictor		Goodness of Fit				Sig.		Regression Eq.
Indep. Variable	Model Type	R	R^2	adjusted. R^2	Std. Error	$\mathcal{F}$ -statistic	p -quantity	
M_1	Quadratic	0.985319	0.970854	0.965554	3.278761	183.202893	3.59e-09	$HAC=0.000121 \times M_1^2 + 0.110945 \times M_1 + 9.549172$
M_2	Linear	0.955483	0.912948	0.905694	5.425158	125.848847	1.02e-07	$HAC=0.140602M_2 + 3.090869$
GA	Cubic	0.996051	0.992117	0.989752	1.788350	419.531530	8.21e-12	$HAC=-0.000239 \times GA^3 + 0.048292 \times GA^2 + (-2.042118) \times GA + 55.755703$
ABC	Cubic	0.998420	0.996843	0.995896	1.131721	1052.580123	8.48e-13	$HAC=(-0.000426) \times ABC^3 + 0.062488 \times ABC^2 + (-1.546583) \times ABC + 38.660388$
H	Cubic	0.999381	0.998762	0.998390	0.708813	2688.469367	7.88e-15	$HAC=(-0.000877) \times H^3 + 0.081834 \times H^2 + (-0.043858) \times H + 17.939095$
F	Linear	0.964914	0.931059	0.925314	4.827954	162.061108	2.50e-08	$HAC=0.062513 \times F + 3.543006$
χ	Cubic	0.998954	0.997909	0.997282	0.920963	1591.157788	1.08e-13	$HAC=(-0.001508) \times \chi^3 + 0.143957 \times \chi^2 + (-2.171424) \times \chi + 36.521679$
RI	Cubic	0.999802	0.999603	0.999484	0.401226	8397.616193	2.66e-17	$HAC=(-0.000360) \times RI^3 + 0.034738 \times RI^2 + 1.123886 \times RI + 8.010198$
So	Quadratic	0.986719	0.973615	0.968817	3.119597	202.949584	2.08e-09	$HAC=0.000204 \times So^2 + 0.161034 \times So + 8.912675$
AZI	Quadratic	0.968955	0.938874	0.927760	4.748226	84.477778	2.11e-07	$HAC=0.000103 \times AZI^2 + 0.015148 \times AZI + 20.437712$

TABLE 10. Best regression models for HAC

Table 11 summarizes the actual and predicted HAC of anticancer medications based on the most accurate forecasting index, and Figure 7 displays the corresponding graphical representation.

Drugs	Actual HAC	Predicted HAC	Residual	Drugs	Actual HAC	Predicted HAC	Residual
G_1	90	90.003547	-0.003547	G_8	73	72.959688	0.040312
G_2	42	42.091947	-0.091947	G_9	54	53.652438	0.3347562
G_3	37	37.456488	-0.456488	G_{10}	37	36.544739	0.455261
G_4	32	32.451172	-0.451172	G_{11}	33	32.819745	0.180255
G_5	62	61.645097	0.354903	G_{12}	61	61.701573	-0.701573
G_6	65	64.948370	0.051630	G_{13}	59	59.301598	-0.301598
G_7	32	31.760722	0.239278	G_{14}	60	59.757113	0.242887

TABLE 11. Predicted vs Actual HAC using RI model.

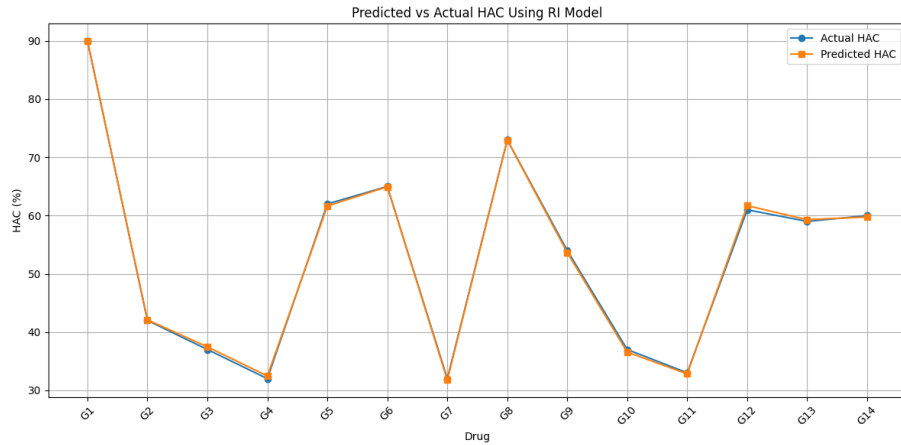


FIGURE 7. Predicted vs Actual HAC using RI model.

4.3. Comparative Evaluation of Regression Models for Complexity Prediction. The $\mathbb{R}^2$ and adjusted $\mathbb{R}^2$ values for the linear regression model, logarithmic regression model, quadratic regression model, and cubic regression model are displayed in Table 12 and Figure 8. In these models, the dependent variable is the set of complexities of fourteen drugs, while the independent variables are the ten degree-based indices.

Table 12 adjusted $\mathbb{R}^2$ values clearly show that the quadratic model is where the M_1 , GA , ABC , H , χ , RI , So and AZI indices perform best. While in the cubic model, the M_2 and F indices

Topological Invariant	Linear		Logarithmic		Quadratic		Cubic	
	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$
M_1	0.949700	0.945509	0.885039	0.875459	0.978442	0.974523	0.978454	0.971990
M_2	0.910414	0.902949	0.847399	0.834683	0.944367	0.934251	0.949916	0.934891
GA	0.950982	0.946897	0.887797	0.878446	0.978226	0.974267	0.978313	0.971807
ABC	0.964247	0.961268	0.907879	0.900202	0.979950	0.976305	0.979987	0.973984
H	0.949917	0.945743	0.894769	0.886000	0.969260	0.963671	0.970247	0.961321
F	0.927018	0.920936	0.865978	0.854809	0.959034	0.951586	0.964636	0.954027
χ	0.955401	0.951685	0.897314	0.888757	0.976010	0.971648	0.976125	0.968962
RI	0.957064	0.953486	0.905255	0.897360	0.971045	0.965780	0.972775	0.964607
So	0.953816	0.949968	0.890163	0.881009	0.980578	0.977047	0.980609	0.974791
AZI	0.900430	0.892132	0.833724	0.819868	0.951881	0.943132	0.954912	0.941386

TABLE 12. $\mathbb{R}^2$ and adjusted $\mathbb{R}^2$ -values for various regression models are compared.

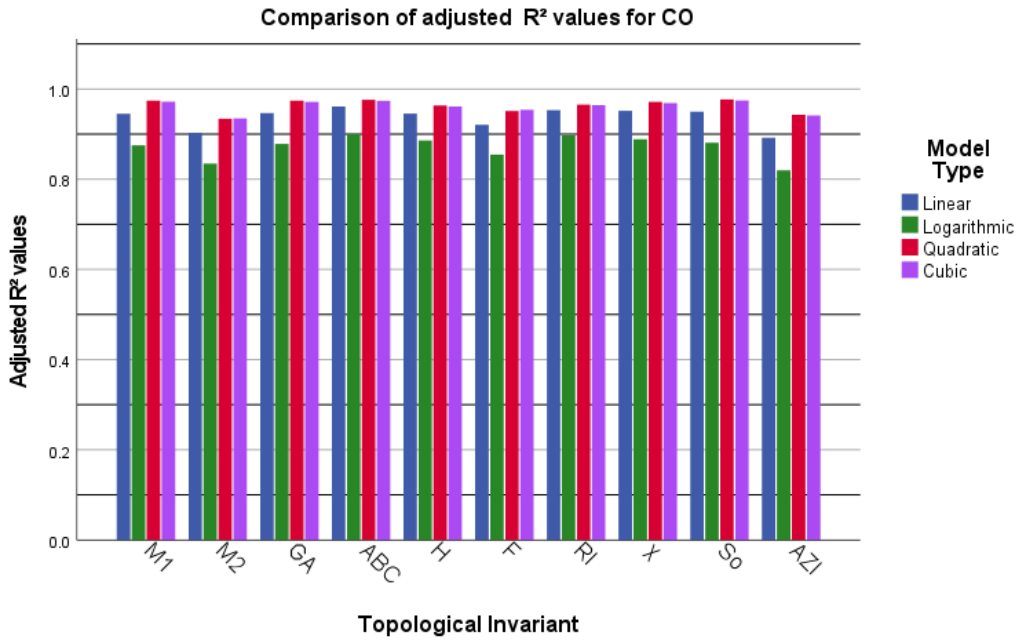


FIGURE 8. Adjusted $\mathbb{R}^2$ -quantities for CO are compared.

reach their peak performance. Table 13 shows the Quantitative investigation of valuable regression models corresponding every independent variable. The regression equation, p quantities, standard error, $\mathcal{F}$ -statistic, adjusted $\mathbb{R}^2$, and correlation coefficient $\mathbb{R}$ are all included in this analysis. The Quantitative investigation emphasize that the Sombor invariant is a best predictor invariant using a quadratic model.

Predictor		Goodness of Fit				Sig.		Regression Eq.
Indep. Variable	Model Type	$\mathbb{R}$	$\mathbb{R}^2$	adjusted. $\mathbb{R}^2$	Std. Error	$\mathcal{F}$ -statistic	p -quantity	
M_1	Quadratic	0.989162	0.978442	0.974523	105.135553	249.628793	6.84e-10	$CO=0.012157 \times M_1^2 + (-0.475009) \times M_1 + 461.293033$
M_2	Cubic	0.974636	0.949916	0.934891	168.071016	63.221834	8.35e-07	$CO=0.000039 \times M_2^3 + (-0.037119) \times M_2^2 + 15.779804 \times M_2 + (-1283.796192)$
GA	Quadratic	0.989053	0.978226	0.974267	105.662356	247.091133	7.22e-10	$CO=0.338917 \times GA^2 + (-2.575782) \times GA + 434.704745$
ABC	Quadratic	0.989924	0.979950	0.976305	101.392370	268.814102	4.59e-10	$CO=0.424577 \times ABC^2 + 11.014560 \times ABC + 186.917155$
H	Quadratic	0.984510	0.969260	0.963671	125.545674	173.418472	4.81e-09	$CO=1.534625 \times H^2 + 6.728778 \times H + 314.064335$
F	Cubic	0.982159	0.964636	0.954027	141.229519	90.924286	1.48e-07	$CO=0.000004 \times F^3 + (-0.008067) \times F^2 + 7.683558 \times F + (-1451.089264)$
χ	Quadratic	0.987932	0.976010	0.971648	110.908394	223.760826	1.23e-09	$CO=1.298135 \times \chi^2 + 5.747685 \times \chi + 314.247790$
RI	Quadratic	0.985416	0.971045	0.965780	121.845827	184.449156	3.46e-09	$CO=1.117624 \times RI^2 + 19.304597 \times RI + 184.879216$
So	Quadratic	0.990241	0.980578	0.977047	99.792211	277.681836	3.85e-10	$CO=0.021725 \times So^2 + (-0.210870) \times So + 426.453925$
AZI	Quadratic	0.975644	0.951881	0.943132	157.074645	108.800073	5.66e-8	$CO=0.007288 \times AZI^2 + (-2.754519) \times AZI + 958.020993$

TABLE 13. Best regression models for CO

Table 14 summarizes the actual and predicted complexities of anticancer drugs based on the most accurate forecasting index, and Figure 9 displays the corresponding graphical representation.

Drugs	Actual CO	Predicted CO	Residual	Drugs	Actual CO	Predicted CO	Residual
G_1	3030	3032.699515	-2.699515	G_8	2010	1961.485227	48.514773
G_2	969	1051.623765	-82.623765	G_9	1450	1550.893813	-100.893813
G_3	706	821.924559	-115.924559	G_{10}	1090	881.424345	208.575655
G_4	790	749.579919	40.420081	G_{11}	790	765.429767	24.570233
G_5	1790	1764.262219	25.737781	G_{12}	1640	1657.107496	-17.107496
G_6	1760	1624.011332	135.988668	G_{13}	1700	1781.061467	-81.061467
G_7	646	715.116830	-69.116830	G_{14}	1750	1764.150065	-14.150065

TABLE 14. Predicted vs Actual CO using So model.

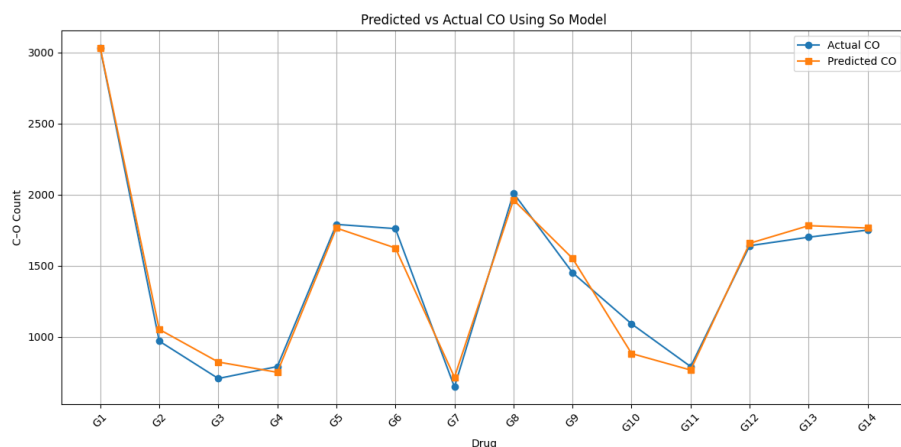


FIGURE 9. Predicted vs Actual CO using So model.

4.4. Comparative Evaluation of Regression Models for Boiling point Prediction. The four regression models' R^2 and adjusted R^2 values are displayed in Table 15 and Figure 10. In these models, the dependent variable is the set of boiling points of fourteen drugs, while the independent variables are from the set of the ten degree-oriented indices.

It is evident from Table 15 adjusted R^2 values that the M_1 , M_2 , F , So , and AZI indices perform best in the cubic model. In the linear model, the GA , ABC , H , χ and RI indices perform at their

Topological Invariant	Linear		Logarithmic		Quadratic		Cubic	
	R^2	adjusted R^2	R^2	adjusted R^2	R^2	adjusted R^2	R^2	adjusted R^2
M_1	0.955821	0.946985	0.915576	0.898692	0.962068	0.943102	0.976400	0.952801
M_2	0.954466	0.945360	0.910762	0.892914	0.960283	0.940424	0.974318	0.948635
GA	0.951228	0.941473	0.909662	0.891595	0.960624	0.940936	0.960624	0.940936
ABC	0.948433	0.938119	0.910287	0.892344	0.955883	0.933824	0.955883	0.933824
H	0.934546	0.921455	0.895805	0.874966	0.946813	0.920219	0.946913	0.920219
F	0.946940	0.936328	0.909694	0.891633	0.952385	0.928577	0.975055	0.950109
χ	0.943789	0.932547	0.904159	0.884991	0.954028	0.931042	0.954028	0.931042
RI	0.934798	0.921758	0.897006	0.876407	0.945710	0.918565	0.945710	0.918565
So	0.954280	0.945136	0.915272	0.898327	0.960292	0.940438	0.976118	0.952236
AZI	0.950542	0.940651	0.899391	0.879269	0.965244	0.947867	0.978965	0.957929

TABLE 15. R^2 and adjusted R^2 -values for various regression models are compared.

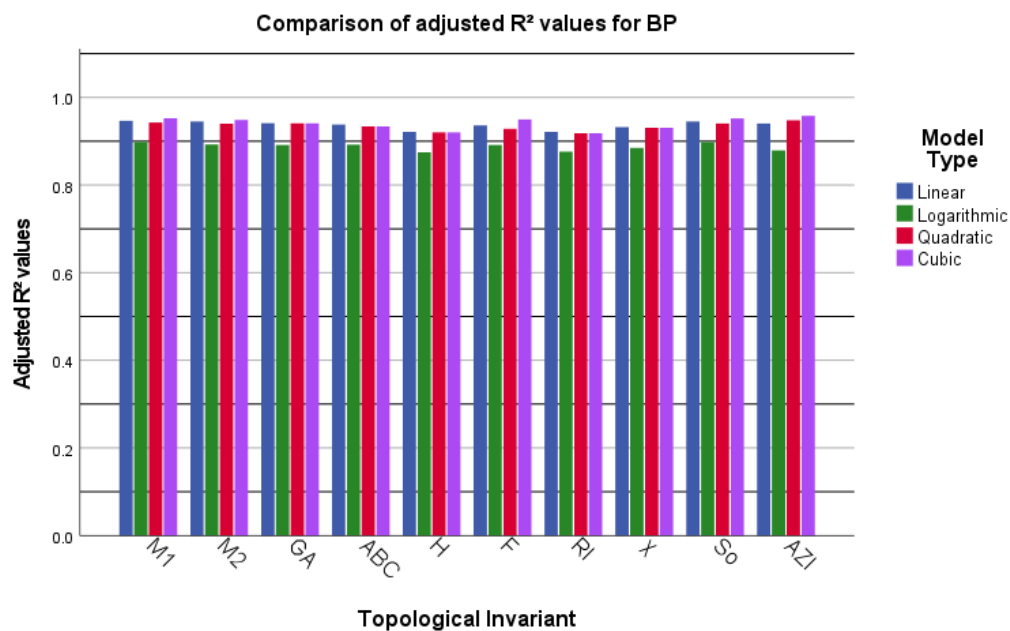


FIGURE 10. Comparison of adjusted R^2 -values for BP.

best. The Quantitative investigation of the valuable regression models corresponding every independent variable is displayed in Table 16. This analysis includes the regression equation, p quantities, standard error, $\mathcal{F}$ -statistic, adjusted $\mathbb{R}^2$, and $\mathbb{R}$ quantities. Using a cubic model, this Quantitative investigation emphasize that the AZI index is the best predictor index.

Predictor		Goodness of Fit				Sig.		Regression Eq.
Indep. Variable	Model Type	$\mathbb{R}$	$\mathbb{R}^2$	adjusted. $\mathbb{R}^2$	Std. Error	$\mathcal{F}$ -statistic	p -quantity	
M_1	Cubic	0.988130	0.976400	0.952801	59.715986	41.373536	6e-3	BP=0.000046 $\times M_1^3$ + (-0.043322) $\times M_2^2$ + 14.940018 $\times M_1$ + (-910.472205)
M_2	Cubic	0.987075	0.974318	0.948635	62.295460	37.937058	7e-3	BP=0.000023 $\times M_2^3$ + (-0.026028) $\times M_2^2$ + 10.862406 $\times M_2$ + (-708.780992)
GA	Linear	0.975309	0.951228	0.941473	66.496812	97.516914	1.82e-4	BP=12.506491 $\times GA$ + 184.313846
ABC	Linear	0.973875	0.948433	0.938119	68.375418	91.961023	2.09e-4	BP=16.217282 $\times ABC$ + 202.153395
H	Linear	0.966719	0.934546	0.921455	77.034136	71.388987	3.81e-4	BP=28.164763 $\times H$ + 197.049646
F	Cubic	0.987449	0.975055	0.950109	61.394866	39.087762	7e-3	BP=0.000002 $\times F^3$ + (-0.006774) $\times f^2$ + 6.218985 $\times F$ + (-1072.020699)
χ	Linear	0.971488	0.943789	0.932547	71.387874	83.950478	2.6e-4	BP=25.988533 $\times \chi$ + 193.806010
RI	Linear	0.966850	0.934798	0.921758	76.885154	71.685313	3.77e-4	BP=26.272232 $\times RI$ + 209.876248
So	Cubic	0.987987	0.976118	0.952236	60.072090	40.872650	6e-3	BP=0.00125 $\times So^3$ + (-0.085785) $\times So^2$ + 21.523845 $\times So$ + (-984.826540)
AZI	Cubic	0.989426	0.978965	0.957929	56.378412	46.539023	5e-3	BP=0.000011 $\times AZI^3$ + (-0.016125) $\times AZI^2$ + 8.578143 $\times AZI$ + (-755.220665)

TABLE 16. Best regression models for BP

Table 17 summarizes the actual and predicted complexities of anticancer medications based on the most forecasting index, and Figure 11 displays the corresponding graphical representation.

Drugs	Actual BP	Predicted BP	Residual	Drugs	Actual BP	Predicted BP	Residual
G_1	1386	1242.599307	143.400693	G_8	1048	959.299083	89.100917
G_2	798.1	810.894781	-12.794781	G_9	-	916.744082	-
G_3	-	705.966718	-	G_{10}	-	720.662792	-
G_4	-	657.579048	-	G_{11}	711.4	635.192460	76.207540
G_5	957.1	920.291563	36.808437	G_{12}	-	903.859489	-
G_6	973	896.296539	76.703461	G_{13}	-	954.877879	-
G_7	523.3	563.165681	-39.865681	G_{14}	-	956.187857	-

TABLE 17. Predicted vs Actual BP using AZI model

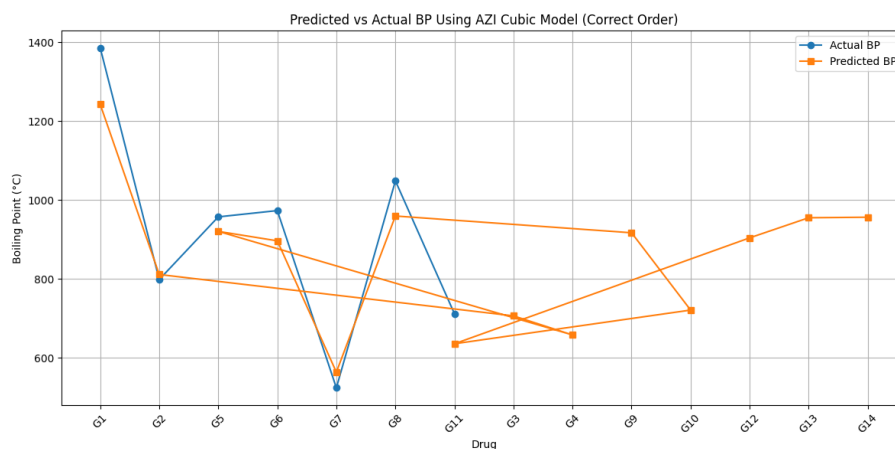


FIGURE 11. Actual and predicted BP using AZI model.

4.5. Comparative Evaluation of Regression Models for molar refractivity prediction.

The R^2 and adjusted R^2 values for the linear regression model, logarithmic regression model, quadratic regression model, and cubic regression model are displayed in Table 18 and Figure 12. In these models, the dependent variable is the set of boiling points of fourteen medications, and the independent variables are from the set of the ten degree-oriented indices.

Topological Invariant	Linear		Logarithmic		Quadratic		Cubic	
	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$
M_1	0.942426	0.937628	0.911742	0.904388	0.943641	0.933393	0.946604	0.930585
M_2	0.881148	0.871244	0.851274	0.838880	0.883496	0.862314	0.884042	0.849255
GA	0.970026	0.967529	0.939514	0.934473	0.970990	0.965715	0.977062	0.970181
ABC	0.978094	0.976269	0.956704	0.953096	0.978175	0.974207	0.983098	0.978027
H	0.988359	0.987388	0.964555	0.961601	0.988432	0.986328	0.990835	0.988086
F	0.900870	0.892609	0.872343	0.861705	0.902816	0.885146	0.903152	0.874098
χ	0.982387	0.980919	0.956990	0.953406	0.982505	0.979325	0.986827	0.982875
RI	0.988493	0.987534	0.969531	0.966992	0.988651	0.986587	0.990397	0.987516
So	0.945843	0.941330	0.916338	0.909366	0.946707	0.937017	0.949649	0.934544
AZI	0.900971	0.892718	0.863575	0.852206	0.909269	0.892773	0.909270	0.882051

TABLE 18. $\mathbb{R}^2$ and adjusted $\mathbb{R}^2$ -values for various regression models are compared.

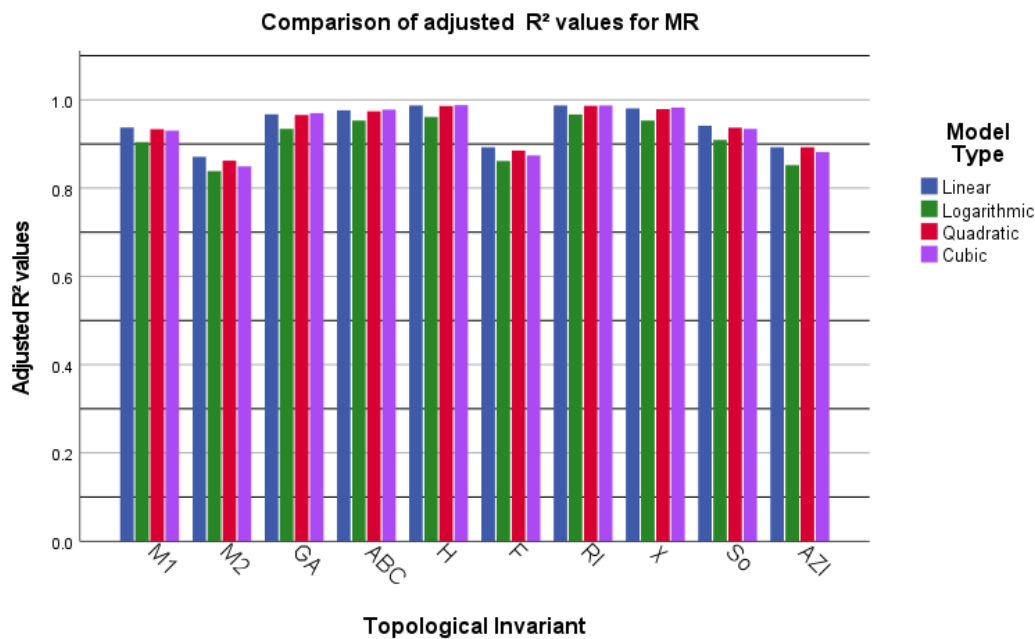


FIGURE 12. Comparison of adjusted $\mathbb{R}^2$ -values for MR.

It is evident from Table 18 adjusted $\mathbb{R}^2$ values that the M_1 , M_2 , F , χ , RI and So indices perform best in the Linear model, while the GA , ABC , H and χ indices find their best fits in the cubic model. At the same time, AZI perform at their best in the quadratic model. The Quantitative investigation of the top regression models for every independent variable is displayed in Table 19. This analysis includes the regression equation, p quantities, standard error, $\mathcal{F}$ -statistic, adjusted $\mathbb{R}^2$, and $\mathbb{R}$ quantities. Using a cubic model, this Quantitative investigation emphasize that H index is the strongest predictor index.

Predictor		Goodness of Fit				Sig.		Regression Eq.
Indep. Variable	Model Type	$\mathbb{R}$	$\mathbb{R}^2$	adjusted. $\mathbb{R}^2$	Std. Error	$\mathcal{F}$ -statistic	p -quantity	
M_1	Linear	0.970786	0.942426	0.937628	16.271972	196.426089	8.43e-09	$MR=666835 \times M_1 + 1.601420$
M_2	Linear	0.938695	0.881148	0.871244	23.379165	88.965845	6.71e-07	$MR=0.509441 \times M_2 + 14.394272$
GA	Cubic	0.988464	0.977062	0.970181	11.251069	141.986090	1.70e-08	$MR=(-0.001307) \times GA^3 + 0.253009 \times GA^2 + (-11.677148) \times GA + 277.137025$
ABC	Cubic	0.991513	0.983098	0.978027	9.658064	193.877638	3.71e-09	$MR=(-0.002711) \times ABC^3 + 0.383460 \times ABC^2 + (-12.148148) \times ABC + 226.819076$
H	Cubic	0.995407	0.990835	0.988086	7.111722	360.382016	1.74e-10	$MR=(-0.010055) \times H^3 + 0.827744 \times H^2 + (-12.915843) \times H + 162.371149$
F	Linear	0.949142	0.900870	0.892609	21.351525	109.052759	2.24e-07	$MR=0.226787 \times H + 15.810927$
χ	Cubic	0.993392	0.986827	0.982875	8.526199	249.713117	1.07e-09	$MR=(-0.010349) \times \chi^3 + 0.933718 \times \chi^2 + (-18.668730) \times \chi + 222.434880$
RI	Linear	0.994230	0.988493	0.987534	7.274699	1030.803282	5.26e-13	$MR=7.912519 \times RI + (-4.050611)$
So	Linear	0.972545	0.945843	0.941330	15.781646	209.578641	5.83e-09	$MR=0.910216 \times So + 2.873347$
AZI	Quadratic	0.953556	0.909269	0.892773	21.335211	55.118977	1.85e-06	$MR=0.000290 \times AZI^2 + 0.134456 \times AZI + 59.7936824$

TABLE 19. Best regression models for MR

Table 20 summarizes the actual and predicted molar refractivities of anticancer drugs based on the most accurate forecasting index, and Figure 13 displays the corresponding graphical representation.

Drugs	Actual MR	Predicted MR	Residual	Drugs	Actual MR	Predicted MR	Residual
G_1	323.7	324.353825	-0.653825	G_8	273.2	272.256425	0.943575
G_2	140.1	151.762058	-11.662058	G_9	195.7	197.510938	-1.810938
G_3	147.1	136.636686	10.463314	G_{10}	141.5	131.118160	10.381840
G_4	116.9	121.284073	-4.384073	G_{11}	121.6	120.940279	0.659721
G_5	219.3	226.829631	-7.529631	G_{12}	234.4	231.420852	2.979148
G_6	246.7	240.702538	5.997462	G_{13}	220.7	219.902426	0.797574
G_7	113.1	118.088774	-4.988774	G_{14}	221.1	222.187813	-1.087813

TABLE 20. Predicted vs Actual MR using H model

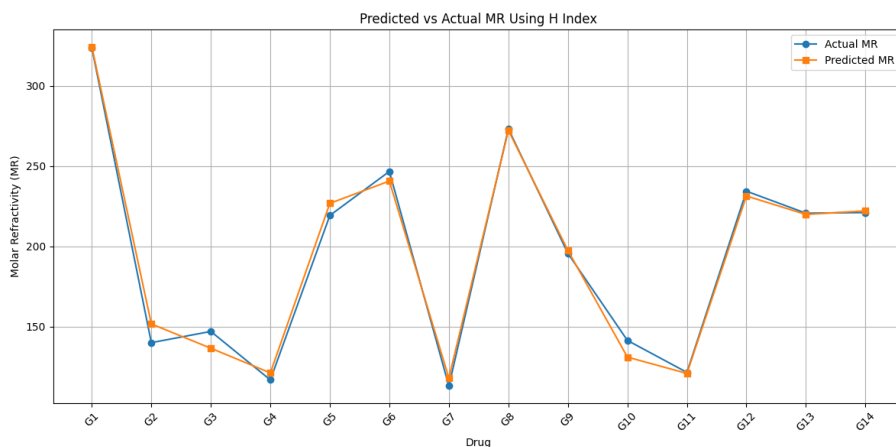
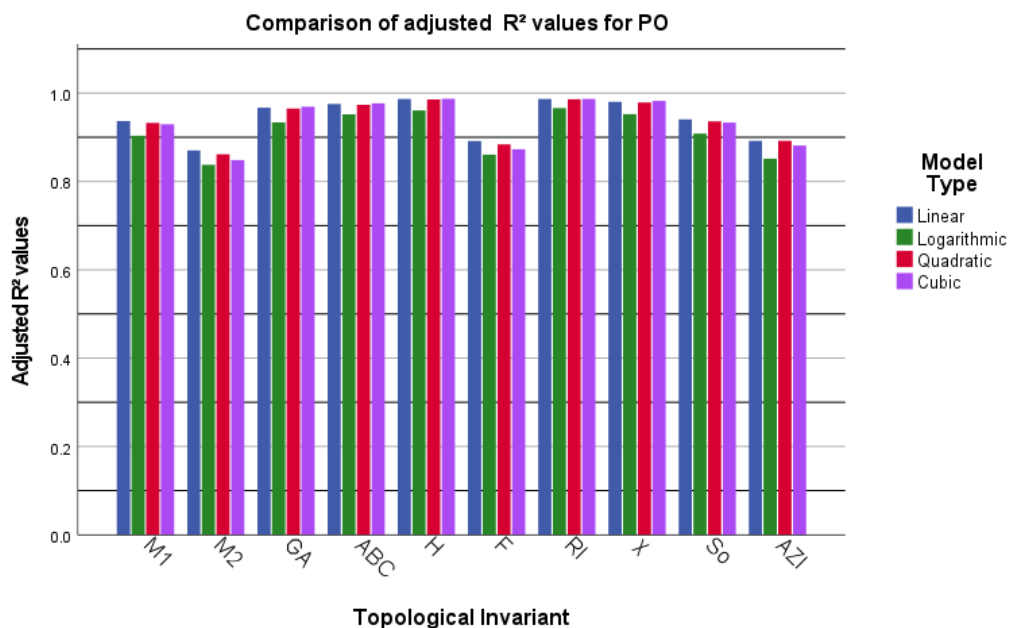


FIGURE 13. Actual and predicted MR using H model.

4.6. Comparative Evaluation of Regression Models for PO prediction. Table 21 and Figure 14 show the R^2 and adjusted R^2 values for the linear regression model, logarithmic regression model, quadratic regression model, and cubic regression model. The sets of values for the ten degree-based indices are the independent variables in these models, while the dependent variable is the collection of polarizabilities of fourteen medications. The M_1 , M_2 , F , χ , RI , and So indices perform best in the linear model, as shown by Table 21 adjusted R^2 values, while the

Topological Invariant	Linear		Logarithmic		Quadratic		Cubic	
	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$
M_1	0.941807	0.936957	0.911001	0.903585	0.943065	0.932714	0.945958	0.929745
M_2	0.880469	0.870508	0.850506	0.838049	0.882871	0.861575	0.883453	0.848488
GA	0.969568	0.967032	0.938891	0.933799	0.970577	0.965227	0.976588	0.969564
ABC	0.977550	0.975679	0.955993	0.952325	0.977618	0.973548	0.982462	0.977200
H	0.987982	0.986981	0.963978	0.960976	0.988070	0.985901	0.990445	0.987578
F	0.900034	0.891704	0.871446	0.860733	0.902023	0.884209	0.902395	0.873114
χ	0.981947	0.980443	0.956368	0.952732	0.982083	0.978825	0.986356	0.982262
RI	0.988079	0.987085	0.968914	0.966323	0.988217	0.986074	0.989933	0.986913
So	0.945191	0.940624	0.915567	0.908531	0.946091	0.936289	0.948956	0.933643
AZI	0.900487	0.892194	0.862965	0.851546	0.908912	0.892351	0.908912	0.881586

TABLE 21. Comparison of $\mathbb{R}^2$ and adjusted $\mathbb{R}^2$ -values for 4 models.FIGURE 14. Comparison of adjusted $\mathbb{R}^2$ -quantities for PO.

GA, ABC, H and χ indices find their best matches in the cubic model. At the same time, AZI perform best in the quadratic model analysis. Table 22 shows the Quantitative analysis of the

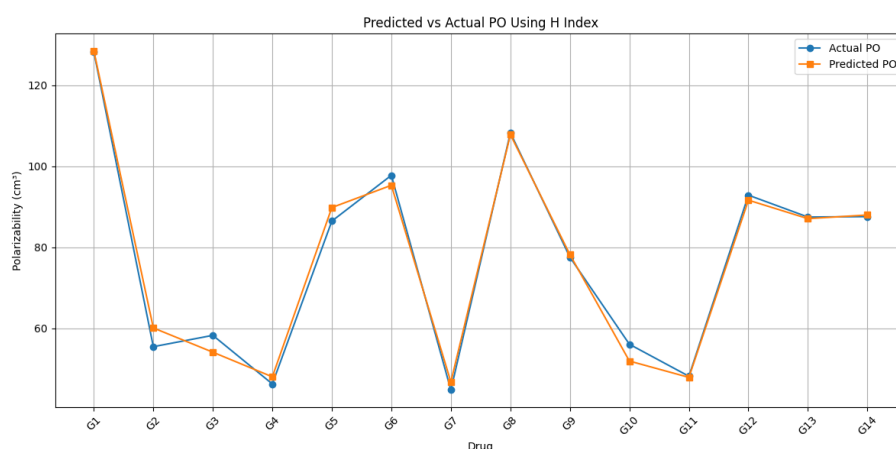
valuable regression models for every independent variable. The regression equation, p quantities, standard error, $\mathcal{F}$ -statistic, adjusted $\mathbb{R}^2$, and $\mathbb{R}$ quantities are all included in this analysis. This Quantitative analysis demonstrates that the H index is the dominant predictor index using a cubic model.

Predictor		Goodness of Fit				Sig.		Regression Eq.
Indep. Variable	Model Type	$\mathbb{R}$	$\mathbb{R}^2$	adjusted. $\mathbb{R}^2$	Std. Error	$\mathcal{F}$ -statistic	p -quantity	
M_1	Linear	0.970467	0.941807	0.936957	6.483140	194.209003	8.99e-09	$PO=0.264179 \times M_1 + 0.638863$
M_2	Linear	0.938333	0.880469	0.870508	9.291569	88.392272	6.95e-07	$PO=0.201813 \times M_2 + 5.711042$
GA	Cubic	0.988225	0.976588	0.969564	4.504632	139.043252	1.89e-08	$PO=(-0.000515) \times GA^3 + 0.099835 \times GA^2 + (-4.605701) \times GA + 109.473731$
ABC	Cubic	0.991192	0.982462	0.977200	3.898798	186.728866	4.46e-09	$PO=(-0.001066) \times ABC^3 + 0.150829 \times ABC^2 + (-4.768349) \times ABC + 89.302464$
H	Cubic	0.995211	0.990445	0.987578	2.877766	345.522673	2.15e-10	$PO=(-0.003961) \times H^3 + 0.326440 \times H^2 + (-5.087311) \times H + 64.153438$
F	Linear	0.948701	0.900034	0.891704	8.497177	108.040868	2.35e-07	$PO=0.089834 \times F + 6.277786$
χ	Cubic	0.993154	0.986356	0.982262	3.438882	240.966127	1.27e-09	$PO=(-0.004078) \times \chi^3 + 0.368211^2 + (-7.355468) \times \chi + 87.827846$
RI	Linear	0.994021	0.988079	0.987085	2.934358	994.589328	6.51e-13	$PO=3.135067 \times RI + (-1.609636)$
So	Linear	0.972209	0.945191	0.940624	6.291782	206.943010	6.26e-9	$PO=0.360593 \times So + 1.143989$
AZI	Quadratic	0.953369	0.908912	0.892351	8.471750	54.881255	1.89e-06	$PO=0.000116 \times AZI^2 + 0.052419 \times AZI + 23.871030$

TABLE 22. Best regression models for PO

Table 23 summarizes the actual and predicted polarizabilities of anticancer drugs based on the most forecasting index, and Figure 15 displays the corresponding graphical representation.

Drugs	Actual PO	Predicted PO	Residual	Drugs	Actual PO	Predicted PO	Residual
G_1	128.3	128.560230	-0.260230	G_8	108.3	107.848592	0.451408
G_2	55.5	60.127645	-4.627645	G_9	77.6	78.236154	-0.636154
G_3	58.3	54.140334	4.159666	G_{10}	56.1	51.955419	4.144581
G_4	46.3	48.060605	-1.760605	G_{11}	48.2	47.924398	0.275602
G_5	86.5	89.845405	-3.345405	G_{12}	92.9	91.663923	1.236077
G_6	97.8	95.340848	2.459152	G_{13}	87.5	87.101953	0.398047
G_7	44.8	46.794483	-1.994483	G_{14}	87.6	88.101953	0.398047

TABLE 23. Predicted vs Actual PO using H model.FIGURE 15. Actual and predicted PO using H model.

4.7. Comparative Evaluation of Regression Models for molar volume prediction. The $\mathbb{R}^2$ and adjusted $\mathbb{R}^2$ values for the linear regression model, logarithmic regression model, quadratic regression model, and cubic regression model are displayed in Table 24 and Figure 16. In these models, the dependent variable is the set of molar volume of fourteen drugs, and the independent variables are from the set of the ten degree-oriented indices.

In the linear model, the M_1 , M_2 , F , So , and AZI indices perform the best, as shown by Table 24 adjusted $\mathbb{R}^2$ values. The GA , ABC , H , χ and RI indices function best in the cubic model. Table 25 shows the Quantitative investigation of valuable regression models for every independent variable. The standard error, regression equation, p quantities, $\mathcal{F}$ -statistic, adjusted $\mathbb{R}^2$, and $\mathbb{R}$

Topological Invariant	Linear		Logarithmic		Quadratic		Cubic	
	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$
M_1	0.842635	0.829521	0.821310	0.806419	0.842639	0.814027	0.857427	0.814655
M_2	0.759674	0.739647	0.743438	0.722058	0.759681	0.715986	0.759731	0.687651
GA	0.888794	0.879527	0.863487	0.852110	0.888821	0.868607	0.919725	0.895643
ABC	0.906479	0.898685	0.889356	0.880135	0.907638	0.890845	0.942912	0.925786
H	0.934958	0.929538	0.911340	0.903952	0.934982	0.923161	0.966767	0.956797
F	0.789690	0.772164	0.773858	0.755012	0.789709	0.751474	0.790063	0.727082
χ	0.916489	0.909529	0.893706	0.884849	0.916572	0.901403	0.950688	0.935894
RI	0.937785	0.932601	0.919057	0.912312	0.938548	0.927375	0.970421	0.961548
So	0.848753	0.836149	0.828358	0.814054	0.848799	0.821308	0.864480	0.823824
AZI	0.791254	0.773859	0.764411	0.744778	0.793500	0.755955	0.795949	0.734734

TABLE 24. Comparison of $\mathbb{R}^2$ and adjusted $\mathbb{R}^2$ -values for different regression models.

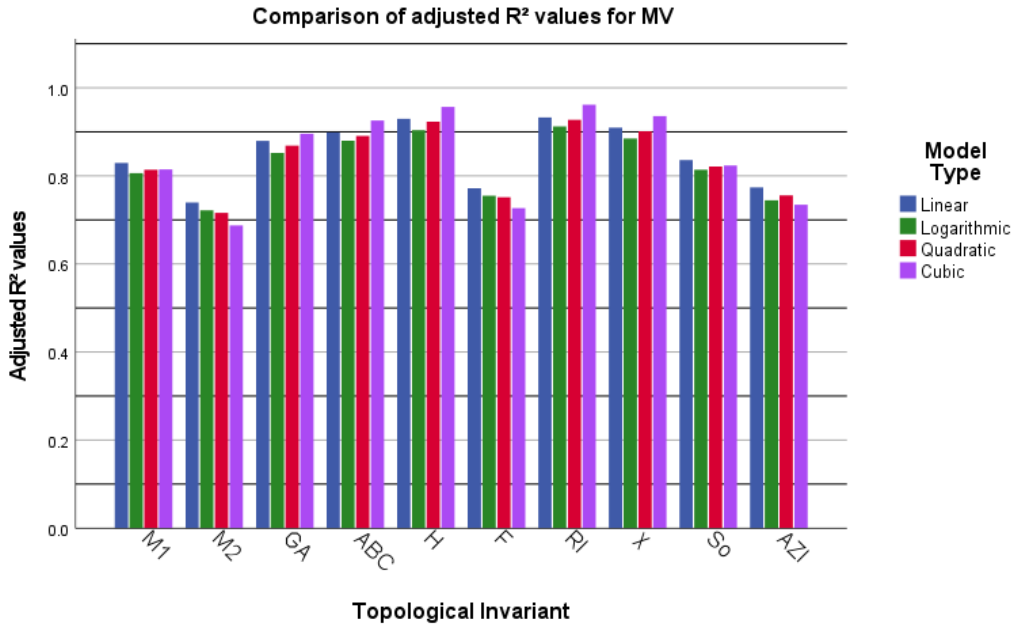


FIGURE 16. Comparison of adjusted $\mathbb{R}^2$ -values for MV.

are all included in this analysis. This Quantitative analysis demonstrates that the *RI* invariant is the strongest predictor index using a cubic model.

Predictor		Goodness of Fit				Sig.		
Indep. Vari-able	Model Type	R	R^2	adjusted. R^2	Std. Error	$\mathcal{F}$ -statistic	p -quantity	Regression Eq.
M_1	Linear	0.917952	0.842635	0.829521	82.846575	64.255870	4e-06	$MV=1.941823 \times M_1 + (-23.641504)$
M_2	Linear	0.871593	0.759674	0.739647	102.381328	37.932220	4.9e-05	$MV=1.456726 \times M_2 + 23.043887$
GA	Cubic	0.959023	0.919725	0.895643	64.818680	38.190819	8.72e-06	$MV=(-0.009081) \times GA^3 + 1.717265 \times GA^2 + (-91.047175) \times GA + 1803.242546$
ABC	Cubic	0.971037	0.942912	0.925786	54.661680	55.056225	1.60e-06	$MV=(-0.022352) \times ABC^3 + 3.150712 \times ABC^2 + (-124.548619) \times ABC + 1834.842691$
H	Cubic	0.983243	0.966767	0.956797	41.705855	96.968088	1.08e-07	$MV=(-0.112597) \times H^3 + 9.148502 \times H^2 + (-208.003238) \times H + 1775.107968$
F	Linear	0.888645	0.789690	0.772164	95.774746	45.058503	2.2e-05	$MV=0.0653898 \times F + 22.845751$
χ	Cubic	0.975032	0.950688	0.935894	50.802909	64.263131	7.73e-07	$MV=(-0.089549) \times \chi^3 + 7.969805 \times \chi^2 + (-199.377694) \times \chi + 1854.862149$
RI	Cubic	0.985100	0.970421	0.961548	39.345983	109.360547	6.05e-8	$MV=(-0.092743) \times RI^3 + 7.894897 \times RI^2 + (-186.670818) \times RI + 1677.136520$
So	Linear	0.921278	0.848753	0.836149	81.220155	67.340469	3e-6	$MV=2.65534 \times So + (-20.944103)$
AZI	Linear	0.889525	0.791254	0.773859	95.417839	45.486152	2.1e-5	$MV=1.176010 \times AZI + (-18.603993)$

TABLE 25. Best regression models for MV

Table 26 summarizes the actual and predicted molar volumes of anticancer drugs based on the most forecasting index, and Figure 17 displays the corresponding graphical representation.

Drugs	Actual MV	Predicted MV	Residual	Drugs	Actual MV	Predicted MV	Residual
G_1	880	890.925446	-10.225446	G_8	853.1	820.801867	32.298133
G_2	378.5	364.954883	13.545117	G_9	489.3	518.717452	-29.417452
G_3	393	334.355822	58.644178	G_{10}	353.1	331.531285	21.568715
G_4	301.8	335.054547	-33.254547	G_{11}	332.4	333.530754	-1.130754
G_5	610.6	651.508558	-40.908558	G_{12}	647.7	652.447719	-4.747719
G_6	773.5	705.513283	67.986717	G_{13}	590	612.297352	-22.297352
G_7	319.5	338.624482	-19.124482	G_{14}	586.9	619.942769	-33.042769

TABLE 26. Predicted vs Actual MV using RI model.

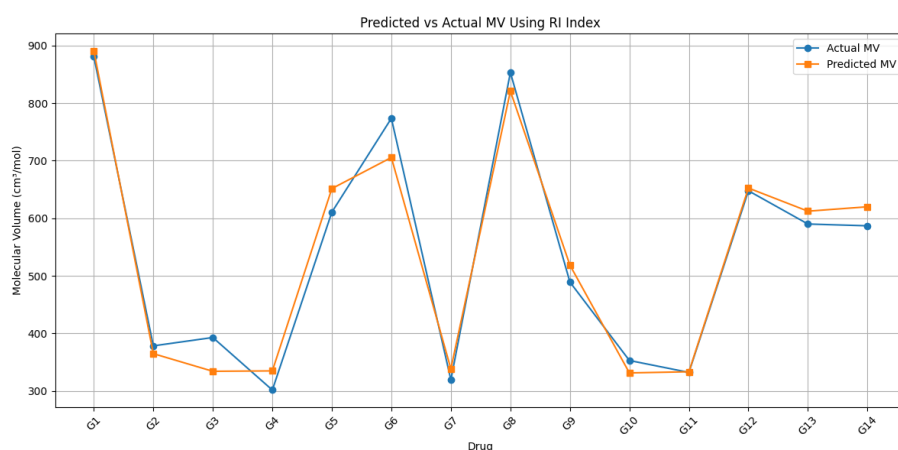


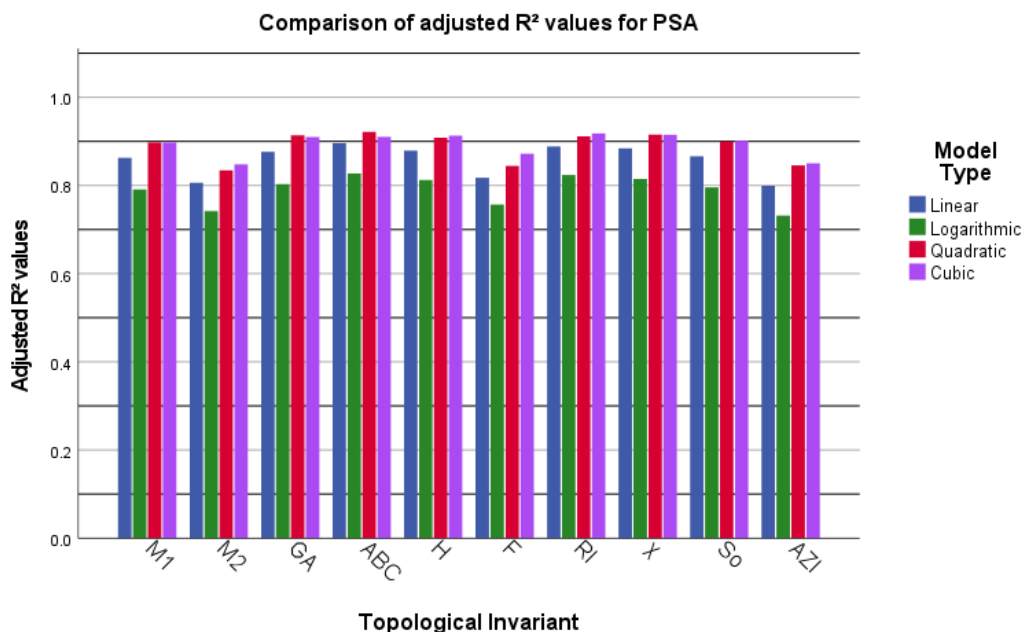
FIGURE 17. Actual and predicted MV using RI model.

4.8. Comparative Evaluation of Regression Models for Polar Surface Area prediction.

The R^2 and adjusted R^2 values for the linear regression model, logarithmic regression model, quadratic regression model, and cubic regression model are displayed in Table 27 and Figure 18. In these models, the dependent variable is the set of polar surface areas of fourteen drugs, and the independent variables are from the set of the ten degree oriented indices.

In the cubic model, the indices M_1 , M_2 , H , F , RI , So and AZI perform the best, as shown by Table 27 adjusted R^2 values. The GA , ABC and χ indices function best in the quadratic model. Table 28 shows the Quantitative analysis of the valuable regression models for every independent variable. The standard error, regression equation, p quantities, $\mathcal{F}$ -statistic, adjusted R^2 ,

Topological Invariant	Linear		Logarithmic		Quadratic		Cubic	
	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$	$\mathbb{R}^2$	adjusted $\mathbb{R}^2$
M_1	0.873517	0.862976	0.807330	0.791274	0.913686	0.897992	0.921684	0.898189
M_2	0.821385	0.806501	0.761846	0.742000	0.859871	0.834393	0.883137	0.848079
GA	0.885936	0.876431	0.818475	0.803348	0.927170	0.913928	0.930966	0.910255
ABC	0.904385	0.896417	0.840575	0.827290	0.933868	0.921844	0.938740	0.910355
H	0.888502	0.879210	0.827092	0.812683	0.922590	0.908516	0.933223	0.913190
F	0.831898	0.817890	0.775626	0.756928	0.868625	0.844739	0.901737	0.872258
χ	0.893388	0.884504	0.829317	0.815093	0.928430	0.915417	0.934896	0.915365
RI	0.897241	0.888677	0.837600	0.824066	0.925354	0.911782	0.937132	0.918272
So	0.876838	0.866574	0.811506	0.795799	0.915168	0.899744	0.924433	0.901763
AZI	0.814957	0.799537	0.752499	0.731874	0.869446	0.845708	0.884831	0.850280

TABLE 27. Comparison of $\mathbb{R}^2$ and adjusted $\mathbb{R}^2$ -values for 4 models.FIGURE 18. Comparison of adjusted $\mathbb{R}^2$ -values for PSA.

and $\mathbb{R}$ quantities are all included in this analysis. This Quantitative analysis demonstrates that the ABC index is the most predictive index using a cubic model.

Predictor		Goodness of Fit				Sig.		
Indep. Vari-able	Model Type	$\mathbb{R}$	$\mathbb{R}^2$	adjusted. $\mathbb{R}^2$	Std. Error	$\mathcal{F}$ -statistic	p -quantity	Regression Eq.
M_1	Cubic	0.960044	0.921684	0.898189	24.114531	39.229048	7.66e-06	PSA=0.000012 $\times M_1^3$ + (-0.009788) $\times M_1^2$ + 3.274728 $\times M_1$ + (-246.097320)
M_2	Cubic	0.939754	0.883137	0.848079	29.457112	25.190193	5.54e-05	PSA=0.000009 $\times M_2^3$ + (-0.009728) $\times M_2^2$ + 3.768477 $\times M_2$ + (-355.155611)
GA	Quadratic	0.962876	0.927130	0.913880	22.197215	69.976416	5.55e-07	PSA=0.047718 $\times GA^2$ + (-1.456502) $\times GA$ + 86.761321
ABC	Quadratic	0.966340	0.933813	0.921779	21.154752	77.598345	3.27e-07	PSA=0.066544 $\times ABC^2$ + (-0.463776) $\times ABC$ + 61.563487
H	Cubic	0.966035	0.933223	0.913190	22.267223	46.584009	3.51e-06	PSA=0.024529 $\times H^3$ + (-1.762843) $\times H^2$ + 48.574216 $\times H$ + (-325.037029)
F	Cubic	0.949598	0.901737	0.872258	27.011433	30.589202	2.34e-05	PSA=0.000001 $\times F^3$ + (-0.002516) $\times F^2$ + 2.174802 $\times F$ + (-480.638575)
χ	Quadratic	0.963516	0.928363	0.915339	22.008498	71.276345	5.05e-07	PSA=0.193696 $\times \chi^2$ + (-2.079233) $\times \chi$ + 76.336938
RI	Cubic	0.968056	0.937132	0.918272	21.605622	49.687925	2.06e-06	PSA=0.021235 $\times RI^3$ + (-1.644034) $\times RI^2$ + 48.222314 $\times RI$ + (-343.831479)
SO	Cubic	0.961474	0.924433	0.901763	23.687507	40.777459	6.42e-06	PSA=0.000032 $\times SO^3$ + (-0.020242) $\times SO^2$ + 4.925099 $\times SO$ + (-276.316918)
AZI	Cubic	0.940654	0.884831	0.850280	29.242904	25.609600	5.18e-05	PSA=0.000003 $\times AZI^3$ + (-0.004692) $\times AZI^2$ + 2.333546 $\times AZI$ + (-275.550647)

TABLE 28. Best regression models for PSA

The comparison of the anticancer drugs' actual and predicted Polar Surface Area based on the most forecasting index is summarized in Table 29, and the corresponding graphical representation is shown in Figure 19.

Drugs	Actual PSA	Predicted PSa	Residual	Drugs	Actual PSA	Predicted PSA	Residual
G_1	356	352.942601	3.057399	G_8	242	236.245205	5.754795
G_2	161	122.239647	38.760353	G_9	194	167.957823	26.042177
G_3	86.3	104.753144	-18.453144	G_{10}	102	105.479906	-3.479906
G_4	82.1	93.212565	-11.112565	G_{11}	100	94.153386	5.846614
G_5	221	198.560940	22.439060	G_{12}	183	197.229332	-14.229332
G_6	195	199.612520	-4.612520	G_{13}	154	188.153723	-34.153723
G_7	92.4	90.717626	1.682374	G_{14}	171	187.752817	-16.752817

TABLE 29. Predicted vs Actual PSA using *ABC* model.

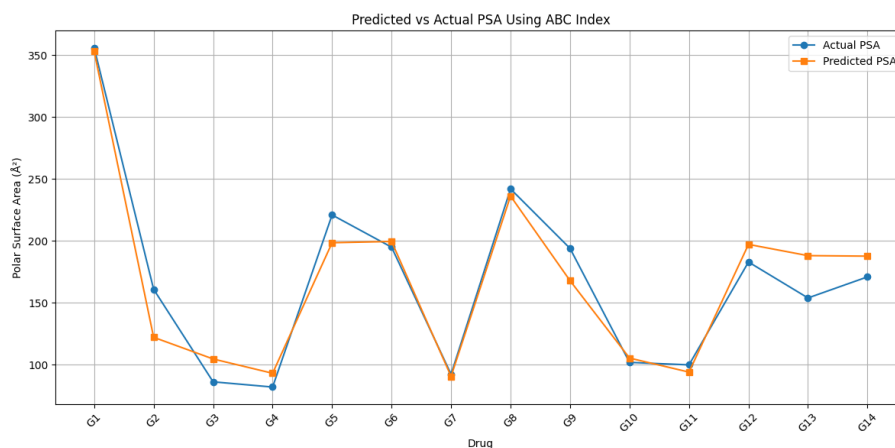


FIGURE 19. Actual and predicted PSA using *ABC* model.

5. CONCLUSION

Using QSPR analysis, this study methodically examined the predictive power of ten degree oriented graph theoretical indices for simulating the physicochemical characteristics of particular anticancer medications. The most suitable model index combinations were determined using statistical indicators like the correlation coefficient (R), coefficient of determination (R^2),

adjusted $\mathbb{R}^2$, $\mathcal{F}$ -statistics, standard error, and significance levels. A thorough comparative evaluation was carried out using linear, logarithmic, quadratic, and cubic regression models. This research used four regression models and degree oriented topological indices to thoroughly examine the relationship among the physicochemical characteristics and molecular structure of anticancer medication. The findings demonstrate that molecular branching and connectivity have a significant impact on molecular weight, with the Randić index yielding the most valuable predictor. Particularly under cubic regression models, heavy atom count showed remarkably strong correlations with degree oriented indices, suggesting that these indices accurately capture atomic composition. The Sombor index was found to be the most reliable predictor of molecular complexity when using quadratic regression, underscoring the significance of higher-order structural interactions. The augmented Zagreb index showed superior predictive capability despite incomplete experimental data, and cubic regression model proven better prediction accuracy of boiling point, a characteristic influenced by both molecular size and intermolecular interactions. Strong nonlinear correlations between molar refractivity and molecular topology were found; cubic models performed better than linear ones, and the harmonic index emerged as the most important predictor. The strong correlation between electronic deformability and molecular connectivity was confirmed by a similar pattern for polarizability, where the harmonic index once more offered the best predictive accuracy. Strong correlations between molar volume and degree oriented descriptors were found, suggesting that branching and connectivity cause molecular size and spatial occupation to rise. Degree oriented indices were similarly helpful in predicting polar surface area; nonlinear models performed best, highlighting the influence of molecule topology on surface-related and permeability-related features. Overall, degree oriented topological descriptors are strong, dependable, and effective tools for QSPR modeling of anticancer medicines, as demonstrated by the strong comparison among actual and predicted results across all characteristics.

5.1. Study Implications.

- Makes it possible to forecast important physicochemical features quickly and affordably.

- Facilitates early-stage anticancer chemical screening and computational medication design.
- Determines trustworthy topological indices for further QSPR research.
- Emphasizes how complicated pharmacological compounds require nonlinear modeling.

5.2. Limitations.

- A comparatively modest number of therapeutic compounds were examined.
- Some physicochemical characteristics have incomplete experimental data.
- Only degree-based topological indices are taken into account.
- The application of traditional regression approaches devoid of machine learning methodologies.

5.3. Future Research Directions.

- Incorporate a wider range of anticancer medications.
- Integrate additional molecular indices with degree oriented indices.
- Use hybrid modeling and machine learning techniques.
- Expand the framework to anticipate toxicity and biological activity.
- To increase the generalizability of the model, carry out external validation.

CONFLICT OF INTERESTS

The author(s) declare that there is no conflict of interests.

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